This Annual Report of the Institute of Atomic Energy describes the results of the research works carried out at the Institute at 1997. As in the preceding years the authors of the individual scientific reports published in this Annual Report are fully responsible for their content and layout. The Report contains the information on other activities of the Institute as well.

Editorial Committee:
Natalia Golnik
Janusz R. Mika
Krzysztof Wieteska

Editor:
Agnieszka Witak
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INTRODUCTION

Institute of Atomic Energy (Instytut Energii Atomowej, Polish abbreviation IEA) emerged in 1983 as one of three independent research institutes formed on the basis of the Institute of Nuclear Research founded in 1955.

Originally the main task of IAE was the research in the field of the nuclear reactor physics and development of techniques needed for nuclear power plants operation and maintenance. At the beginning of nineties the objectives of the Institute activity were generalised to development of new energy sources, new materials and environment protection.

The main research areas of IAE are:
- radiation dosimetry and protection,
- condensed matter physics,
- nuclear reactor physics,
- nuclear power plants,
- radioactive waste management,
- nuclear safety,
- irradiation of materials in the reactors,
- post-irradiation examination of materials,
- assessment of risk from industrial and nuclear installations.

The research and development activities in the field of radiation protection and dosimetry are performed by research group specialised in radiation dosimetry of mixed radiation fields.

Research in the field of condensed matter physics is based on the use of neutron and X-ray radiation scattering and Mössbauer techniques. The technologies of new crystalline and semi-crystalline materials were developed. The hot cell facilities allow to investigate the properties of irradiated materials.

The Seminar on Materials Investigation for Power Stations and Grids is organised every year to bring together scientists and engineers interested in inspection of the energy production and transmission facilities.

The method of probabilistic risk assessment for industrial installations was developed as a part for the prediction of the impact of industrial accidents on environment.

The Institute is involved in the development of the decision support system for nuclear emergencies in Europe (RODOS), which is a joint project of about thirty European institutions supported by the European Commission. The programme to create similar national decision support system for chemical accidents has been developed.

The EWA research reactor of 10 MW (th) power had been in continuous operation for 37 years and was shut down on 24 February, 1995. In 1997 the decommissioning of the reactor was in progress. The MARIA research reactor of 30 MW (th) has been upgraded and brought again into operation in December 1992. In 1997 the reactor was used for the production of radioisotope materials, activation analyses and neutron scattering studies.

The IAE is responsible for radioactive waste management in Poland and provides specialized services in collection, treatment and storage of radioactive waste for numerous customers.

The computer centre at IAE is equipped with the mini-super computer CONVEX C-3220 serving all institutions at Świerk. The local network linking many computer users at Świerk has access to Internet, with gateway to other network systems.

The international partners of IAE are: International Atomic Energy Agency, Russian National Scientific Centre „Kurchatov Institute” (Moscow), Gesellschaft für Reaktor Sicherheit (Karlsruhe, Germany), Energy Centre of Netherlands (Petten) and Joint Research Centre of the Commission of the European Communities in Ispra (Italy). In the area of neutron and condensed matter physics ties were kept with: DESY-HASYLAB (Hamburg), Laboratory for Neutron Studies (Studsvik, Sweden), CERN (Geneva, Switzerland), Laboratoire Leon Brillouin (Saclay, France), Institute for Nuclear Research and Nuclear Energy (Soča, Bulgaria), Institute of Metallurgy and Metal Physics (Moscow) and the Joint Institute for Nuclear Research (Dubna, Russia).
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<table>
<thead>
<tr>
<th>Lab Code</th>
<th>Laboratory Name</th>
<th>Person</th>
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</tr>
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<tbody>
<tr>
<td>L-1</td>
<td>Material Research Laboratory</td>
<td>Assoc. Prof. W. Szteke, M.Sc.</td>
<td>(22) 779-8663</td>
</tr>
<tr>
<td>L-3</td>
<td>CYFRONET Computing Centre</td>
<td>M. Sawa, M.Sc.</td>
<td>(22) 779-8841</td>
</tr>
<tr>
<td>L-4</td>
<td>Regional Laboratory of Neutronography</td>
<td>Prof. A. Czachor, Ph.D., D.Sc.</td>
<td>(22) 779-8805</td>
</tr>
</tbody>
</table>

The Scientific Council was elected on the 23 of May 1995 by the scientific, technical and administrative staff of the Institute. The Council has the right to confer PhD degree in physics.

Krzysztof Andrzejewski, Ph.D.  Institute of Atomic Energy
Mieczyslaw Borysiewicz, Ph.D.  Institute of Atomic Energy
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Zbigniew Woźnicki, Ph.D. Institute of Atomic Energy
Prof. Mieczysław Zielczyński, Ph.D., D.Sc. Institute of Atomic Energy

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Prof. Janusz R. Mika, PhD., D.Sc. Institute of Atomic Energy
Prof. Bronisław Słowiński, Ph.D., D.Sc. Institute of Atomic Energy

Chairman of the Scientific Council: Prof. Stefan Chwaszczewski, Ph.D., D.Sc.
Deputy chairmen:
Secretary Edmund Kmiotek, Ph.D., Deputy secretary Jan Wasiak, Ph.D.

have been elected by the members of the Council
Phone of the Secretary (22) 779-9481
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Bronislaw Slowirski, Ph.D., D.Sc
Zbigniew Strugalski, Ph.D., D.Sc
Jan Suwalski, Ph.D., D.Sc
Mieczyslaw Zielczynski, Ph.D., D.Sc

nuclear power and safety
solid state physics
solid state physics
mathematical methods in physics
solid state physics
nuclear and radiation physics
experimental physics, nuclear physics and particle physics
solid state physics
radiation dosimetry

ASSOCIATE PROFESSORS:

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Ewa Hajewska, Ph.D.
Edward Maliszewski, Ph.D., D.Sc
Kazimierz Mikke, Ph.D.
Maciej Nowak, Ph.D., D.Sc
Zofia Nowak, Ph.D., D.Sc
Andrzej Strupczewski, Ph.D.
Witold Szteke, M.Sc.
Witold Żyszkowski, Ph.D., D.Sc

analytical and radio-chemistry
metallurgy, corrosion of metals
solid state physics
solid state physics
organic chemistry and technology
organic chemistry and technology
nuclear safety
metallurgy, welding
nuclear energy and exchange of heat

SENIOR RESEARCHERS:

Krzysztof Andrzejewski, Ph.D.
Stanisław Bednarski, Ph.D.
Waldemar Bitous, Ph.D.
Konrad Blinowski, Ph.D.

reactor physics
solid state physics
materials science
solid state physics
<table>
<thead>
<tr>
<th>Name</th>
<th>Research Fields</th>
</tr>
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<tbody>
<tr>
<td>Mieczysław Borysiewicz, Ph.D.</td>
<td>applied mathematics and systems reliability analysis</td>
</tr>
<tr>
<td>Witold Bykowski, Ph.D.</td>
<td>reactor engineering</td>
</tr>
<tr>
<td>Wanda Czosnowska, Ph.D.</td>
<td>nuclear chemistry</td>
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<td>Ludwik Dąbrowski, Ph.D.</td>
<td>solid state physics</td>
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<td>Natalia Golnik, Ph.D., D.Sc.</td>
<td>health physics, dosimetry</td>
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<td>Ludwik Górski, Ph.D.</td>
<td>solid state physics</td>
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<td>Zbigniew Haratym, Ph.D.</td>
<td>gamma spectrometry</td>
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<td>Andrzej Hofman, Ph.D.</td>
<td>materials science</td>
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<td>Rajmund Janczak, Ph.D.</td>
<td>nuclear energy and exchange of heat</td>
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<tr>
<td>Jacek Janeczek, Ph.D.</td>
<td>radiation protection, medical physics</td>
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<tr>
<td>Henryk Jędrzejec, Ph.D.</td>
<td>nuclear physics</td>
</tr>
<tr>
<td>Krystyna Józefowicz, Ph.D.</td>
<td>radiation metrology</td>
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<tr>
<td>Edmund Kmiotek, Ph.D.</td>
<td>nuclear energy</td>
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<td>Teresa Kulikowska, Ph.D.</td>
<td>reactor physics</td>
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<td>Jan K.Maurin, Ph.D.</td>
<td>solid state physics</td>
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<tr>
<td>Andrzej T.Mikulski, Ph.D.</td>
<td>reactor physics and diagnostic systems</td>
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<td>Jan Oglaza, Ph.D.</td>
<td>radiochemistry</td>
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<td>Beata Paluchowska, Ph.D.</td>
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<td>Sławomir Potempski, Ph.D.</td>
<td>computer science and numerical analysis</td>
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<td>Krzysztof Pytel, Ph.D.</td>
<td>reactor physics</td>
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<td>Aldona Rajewska, Ph.D.</td>
<td>solid state physics</td>
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<td>Tomasz Skorek, Ph.D.</td>
<td>computer science</td>
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<td>Ernest Staroń, Ph.D.</td>
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<tr>
<td>Elżbieta Strugalska-Gola, Ph.D.</td>
<td>experimental physics, nuclear physics</td>
</tr>
<tr>
<td>Jan Szczurek, Ph.D.</td>
<td>nuclear safety analysis</td>
</tr>
<tr>
<td>Marcin Szuta, Ph.D., DSc.</td>
<td>nuclear engineering</td>
</tr>
<tr>
<td>Jan Wasiak, Ph.D.</td>
<td>materials science</td>
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<td>Krzysztof Wieteska, Ph.D.</td>
<td>solid state physics</td>
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</tbody>
</table>
Zbigniew J. Woźnicki, Ph.D. | numerical analysis
Janusz Zalewski, Ph.D. | computer science and numerical analysis
Piotr Zielczyński, Ph.D. | computer science, artificial intelligence

**RESEARCHERS:**

<table>
<thead>
<tr>
<th>Name</th>
<th>Field of Study</th>
</tr>
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<tbody>
<tr>
<td>Elżbieta Borek-Kruszewska, M.Sc.</td>
<td>nuclear energy and exchange of heat</td>
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<td>Wojciech Czajkowski, M.Sc.</td>
<td>nuclear energy and exchange of heat</td>
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<td>Piotr Czerski, M.Sc.</td>
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<tr>
<td>Edmund Fuksiewicz, M.Sc.</td>
<td>new technology and engineering</td>
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<td>Andrzej Furtek, M.Sc.</td>
<td>reliability analysis, nuclear physics</td>
</tr>
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<td>Joanna Jankowska-Kisielińska, M.Sc.</td>
<td>solid state physics</td>
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<td>Tadeusz Kochański, M.Sc.</td>
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<td>Marek Krasnowski, M.Sc.</td>
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<td>Janusz Licki, M.Sc.</td>
<td>new technology and engineering</td>
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<td>Krzysztof Maletka, M.Sc.</td>
<td>solid state physics</td>
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<td>Piotr Marks, M.Sc.</td>
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<td>Barbara Radzio, M.Sc.</td>
<td>new technology and engineering</td>
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<tr>
<td>Zdzisław Rusinowski, M.Sc.</td>
<td>radiation metrology</td>
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<tr>
<td>Kazimierz Salwa, M.Sc.</td>
<td>nuclear energy and exchange of heat</td>
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<tr>
<td>Leonard Strzałkowski, M.Sc.</td>
<td>nuclear energy and exchange of heat</td>
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<td>Marek Ślepowroński, M.Sc.</td>
<td>solid state physics</td>
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<td>Tadeusz Wagner, M.Sc.</td>
<td>materials sciences</td>
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<td>Mariusz Wieczorkowski, M.Sc.</td>
<td>metallurgy, welding</td>
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<tr>
<td>Henryk Wojciechowicz, M.Sc.</td>
<td>computer science and numerical analysis</td>
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<tr>
<td>Andrzej Wojciechowski, M.Sc.</td>
<td>computer science and numerical analysis</td>
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<tr>
<td>Zygmunt A. Wojciechowski, M.Sc.</td>
<td>material science</td>
</tr>
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## FINANCES AND PERSONNEL

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<td>Total revenues (MPLN)</td>
<td>8.0</td>
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<td>Total number of employees</td>
<td>644</td>
<td>638</td>
<td>573</td>
<td>530</td>
<td>482</td>
<td>445</td>
</tr>
</tbody>
</table>
TECHNICAL ACTIVITY
OPERATION AND SAFETY OF THE NUCLEAR FACILITIES AT THE REACTOR RESEARCH CENTRE
Grzegorz Krzysztofek, Ludwik Dąbkowski, Adam Hryczuk, Alojzy Moldysz
Research Reactor Centre, Institute of Atomic Energy

In the reported period the effort were focused on tasks and problems to be solved to maintain safe operation of the MARIA reactor and related nuclear facilities at the Reactor Research Centre at Świerk.

The multipurpose high neutron flux research reactor is water and beryllium moderated with graphite reflector, water cooled and of pool type with pressurised fuel channels containing concentric six- or five-tube assemblies of fuel elements. It has been designed with a high degree of flexibility. A vertical cross-section across the reactor pool is shown in Fig. 1. The fuel channels are situated in a matrix made of beryllium blocks and enclosed by lateral reflector made of graphite blocks in aluminium cans. Reactor MARIA is equipped with vertical channels for irradiation target materials, rabbit system and 6 horizontal neutron beam channels with the output neutron thermal flux is $3 \times 10^{13}$ n/m²/s.

Fig. 1. Vertical cross section of MARIA reactor
First criticality of MARIA reactor was reached in December 1974. The reactor was in operation until 1985 when it was shut down for modernisation.

The major tasks are as follows:

1. Reactor operation.
2. Dosimetric survey on the MARIA reactor.
3. Appropriate conditions for nuclear materials storing and control of materials and construction state in nuclear facilities.
4. Technical control and matching the quality requirements.
5. Training of nuclear facilities personnel.
6. Design and construction supervision on upgrading, repairs and maintenance of nuclear facilities.
7. Accomplishment of outfit, overhauls and maintenance of nuclear installations.
8. Checking out and assessment of thermal-hydraulic parameters in the nuclear facilities.
10. Activation analysis for the needs of MARIA reactor.
11. Adaptation of a new signalling, monitoring and control system of MARIA reactor.

In 1997 the reactor was started up 38 times and operated on power 16.1 to 22.6 MW during 36 cycles in compliance with the assumed time schedule. The individual cycles lasted from 43.9 to 120 h depending on the irradiation needs of target materials.

The reactor operational chart is shown in Fig. 2. The total operation time was 3856.3 h. During the reported period the configuration of the reactor core was changed 9 times. This was justified by the necessity to obtain:

- the neutron flux to be required in certain isotope channels,
- core reduction for maintaining the high neutron flux at lower reactor power,
- variation of channels lay-out for irradiation purposes.

Fig. 2. Schedule of the reactor MARIA operation in 1997
As an example in Fig. 3 is shown one of the consecutive core configurations. The irradiation of target materials in vertical channels and in reactor rabbit system have been accomplished on demand of the Isotope Research and Development Centre and the Institute of Chemistry and Nuclear Technology. It should be emphasised that very high specific activities for Ir-92 about 600 Ci/g and for P-32 about 12 Ci from 60 g of the target material have been attained.

In March the sterilisation of soil samples by means of using the gamma radiation emitted by the spent fuel elements was accomplished for the Lublin Microbiology Institute. The sample has been successfully sterilised by dose over 10 kGy in AR spent fuel pool.

In the rotary channel being installed in the socket k-9 the gallium arsenide monocrystal was irradiated.

---

**Fig. 3. One of core configurations**
One of the major topics from the point of view of reactor economical efficiency is fuel burn up to be achieved. At the beginning of 1977 seven fuel channels i-6, i-7, j-6, f-6, g-7, g-8 and h-7 have been selected for detailed monitoring of the fuel element state. The measurements encompassed regularly carried out read-outs once in a day in the 3NO measurement line of the fuel leakage detection system with established water flow in each of the above mentioned fuel channels.

It has been revealed that the burn-up of up to 120 MWd did not cause any changes of the examined MR-6 type fuel elements. All the elements maintained their design integrity. In parallel a research programme on examination of the MR-6 fuel elements which were delivered to the Institute in 1969 for the critical assembly AGATA, was launched. Three fuel elements have been successfully checked in the MARIA reactor and one can come to the following conclusions:

1. In the first five weeks of burning up of the aforementioned fuel elements the stationary dosimetric system has not revealed any boast of activity.
2. Signal values of monitoring of the seven selected measuring channels exhibited signal values clearly indicated that possible emission of noble gases and aerosols was substantially lower than the permitted release limits stated by the NAEA President.

The corrosion examination in-pile loop was installed in the reactor core. Test section is of the shape of Field tube and the loop is operating continuously.

All the reactor repair and maintenance works were carried under technical control and matching the quality assurance requirements.

It accomplished among others:

- survey, repair and examination of mechanisms of control rod channels,
- preparation of the quality documentation of materials and technology for manufacturing 30 fuel channels and 3 movable fuel elements,
- preparation of documentation for repair and control of removing the failures in four heat exchangers,
- testing and elaboration of survey reports of the technological systems and I&C apparatus.

At the end of 1997 due to the intensive training activities the authorised reactor operation personnel accounted 35 persons including 6 shift chiefs. It is enough to ensure the reactor operation time on a level of 3500 to 5000 hours a year.

An analysis and the preparation of the safety documentation on using the MR-5 five-tube fuel element was done. The conclusion from that report is the limitation of nominal power of one fuel element to 1.7 MW(th). Also, the operation safety report for MARIA reactor was completed, reviewed and accepted by the Nuclear Safety and Radiation Department of NAEA.

The measurements of neutron fluxes by means of activation methods were carried out. These measurements can be divided into two groups:

- in some selected spots in the reactor core for precise determination of irradiation parameters for target materials,
- at the neutron beams outlets.

In relation to the first group the distribution and values of neutron fluxes in aluminium block aimed for sulphur irradiation was measured. Also the neutron fluxes in other selected vertical channels were measured.

In relation to the second group the neutron fluxes at the outlet of H7 and H8 neutron beams were measured. The channel H8 is to be considered as a neutron source for the medical therapy encompassing destruction of cancer cells in the brain.

In spite of successful operation of MARIA reactor in 1997 one should realise that it has an aged control and safety system based on the construction from 1974. To improve it:

- the newwarning system of SAIA was installed, tested and implemented into operation,
- technical analysis on construction of a digital safety system based on „ABB PROCONTROL” modules for MARIA reactor was done,
- technical analysis of the implementation of Hartmann-Braun apparatus for MARIA reactor safety system was carried out.

In general, the MARIA reactor was safely and successfully operated in 1997.
THE ACTIVITIES OF THE DIVISION OF RADIATION PROTECTION SERVICE

Bogdan Filipiak, Zbigniew Haratym
Institute of Atomic Energy

The Division of Radiation Protection Service of the Institute of Atomic Energy is responsible for handling all problems concerning radiation protection in the Institute and in the vicinity of Świeck Nuclear Centre and of Central Radioactive Waste Repository, located at Rózän.

The main tasks are:
- radiation control on the Świeck site
- surveillance of nuclear material safeguards
- radioactive waste control
- emergency radiation protection
- improvement of radiation protection measurements
- personal dosimetry
- sewage water activity measurements
- environmental radiation monitoring.

The following laboratories and facilities are available in the Division:
- whole body counter
- counter of thyroid activity
- calibration laboratory
- gamma spectrometry laboratory
- environmental measurement laboratory
- radiochemical laboratory.

An outline of the Division's activities is presented below:
- Whole body monitoring was carried out for radiation workers from N.C. Świeck and for external customers. 362 measurements were made in 1997; 1 person was registered with internal contamination more than 1% of ALI (1.12% ALI for I-131). The results of measurements of the Cs-137 concentration in men, between 1986 and 1997, are presented in Fig. 1.
- Regular monitoring of Radioisotopic Center radiation workers for iodine contamination of the thyroid was carried out.
- Individual monitoring of radiation workers was carried out with film dosemeters. Individual dose equivalents registered were well below the Annual Dose Limit.
- The environmental monitoring within or outside Center's boundaries includes the measurements of direct or stray radiation due to the operation of reactors, accelerators etc. and the measurement of radioactivity in samples of air, river and underground water, precipitation, mud and vegetation taken on the Center's site and in its vicinity. In 1997 more than 1000 environmental samples were measured.

The results of measurements show that there is no registered influence on the environment and the population living in the Center's vicinity due to the operation of its facilities.

On December 31, 1997 Division of Radiation Protection Service employed 11 graduated staff members and 15 nongraduated.

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Fig. 1. The concentration of Cs-137 in men after the Charnobyl accident.
MANAGEMENT OF RADIOACTIVE WASTE

Wlodzimierz Tomczak, Andrzej Cholerzyński, Jerzy Świtalski
Institute of Atomic Energy

In Poland the Institute of Atomic Energy (IAE) takes responsibility for the waste management, waste disposal and for Research and Development. The work is supervised by Director of IAE.

The Radioactive Waste Management Department (ZDUOP) of the IAE at Świerk is in charge of the collection, treatment, conditioning and interim storage of radioactive wastes arising at the institute. ZDUOP also collects wastes from outside laboratories, hospitals and industrial isotope users for treatment at the IAE. It is further in charge of the transport of conditioned wastes to the radioactive waste repository (KSOP) in Różan and the operation of this repository.

There are 43 people working in the Radioactive Waste Management Department, five of them are university graduates. R & D are performed by people from various research groups of the IAE and from other scientific institutes.

Waste arisings
Radioactive waste comes from research reactors, scientific and educational institutions, industrial organisations and hospitals. At present there is one 30 MW reactor working at the Institute of Atomic Energy. Second reactor - EWA is in the decommissioning phase. More then two thousand laboratories are scattered over the country. Only low- and intermediate level waste is produced. The spent high activity gamma sources are transported back to the supplier abroad, but a number of them, mainly of Soviet origin, still remain at the users place.

About 70% of total amount of waste is produced at Świerk Centre. Remainder 30% come from isotope application, mainly for medical purposes (diagnostics, therapy).

In 1997, about 505 m$^3$ of low- and intermediate-level liquid waste, 120 m$^3$ of low-level solid waste and 28 m$^3$ of alpha contaminated waste were collected, transported and treated at IAE-Swierk.

The diagram of the radioactive waste management system is shown in Fig.1.

![Diagram of the radioactive waste management system in Poland](image-url)
Waste treatment and conditioning

ZDUOP is equipped with the following facilities necessary for treatment, conditioning and storage of all collected waste:

- chemical treatment station – 30 m³/d,
- hydraulic press 12 T,
- conditioning of spent ion-exchange resin unit – 10 m³/y,
- bituminization plant – 25 dm³/h evaporated water,
- cementation plant – 2,4 m³/d (12 of 200 l drums),
- low- and intermediate-level liquid waste storage farm consists of 6x50 m³, 2x4 m³, 3x1,6 m³ and 1x300 m³ tank,
- temporary storage facility at Świerk Centre,
- central repository in Rozan.

The low-level liquid wastes were treated with use of mixed synthetic inorganic sorbent composed out of barium carbonate and copper ferrocyanide. Decontamination factor achieved was 30. Precipitate obtained was further subjected to the bituminization.

Intermediate-level liquid wastes were concentrated by evaporation. The concentrate was conditioned by cementation.

The solid wastes were sorted. About 60% of total volume of the wastes were subjected to the bailing techniques with use of hydraulic press. Volume reduction factors obtained were ranging from 3 to 5 depending on the type of waste. Ion-exchange resins were conditioned by dewatering, drying and mixing with polyester resin. The solid and conditioned wastes were packed into the standard metal drums, zinc-plated or varnished on both sides.

In 1997 ZDUOP collected from different enterprises more than 33,000 thousand smoke detectors containing plutonium sources. Smoke detectors were dismantled and plutonium sources separately immobilized in 1 dm³ metal box with use of polyester resin. Metal boxes were subsequently placed in 50 dm³ zinc-plated metal drum and grouted. Other parts of the smoke detectors when plutonium contamination did not exceed the clearance level, had been released from the radioactive material restrictions.

ZDUOP has been also collected 29 spent radium sources (226Ra) which total activity was 65193 MBq. Radium sources were immobilized with the glass and placed into the brass container. Subsequently the brass container was located in the storage container and in a such from transported to the repository.

Storage container for spent radium sources is shown in Fig. 2.

---

**Fig. 2. Storage container for spent radium sources**
The diagram of the radioactive waste treatment and conditioning at the Institute of Atomic Energy is presented on Fig. 3.

Fig. 3. Radioactive waste treatment and conditioning at the Institute of Atomic Energy - Świerk
Waste storage and disposal

The National Central Radioactive Waste Repository (KSOP) is located in Różan, Ostrołęka District, 90 km from Warsaw and is in operation since 1961. It is superficial type repository.

This repository is considered as a final disposal site for low- and medium-level waste containing beta and gamma isotopes and as a temporary storage site for alpha bearing waste.

In 1997 about 102 m$^3$ solid and solidified waste was transported to KSOP for storage or final disposal. Total activity of these wastes, including more than 600 spent radiation sources, was 2.16 TBq equivalent to $\Sigma$ ALI = 4,442,244.

Total volume of the waste stored at Różan repository is about 3000 m$^3$ (without backfill, sealing and shielding materials) and its activity on 31.12.1997 was 35.6 TBq.

Isotope cake is shared as shown in Fig.4.

![Fig. 4. Radioisotopes share in the activity of the waste stored in Różan repository](image)

Technical developments and investment

In the frame of IAEA Technical Assistance, the new cementation plant was completed. Basic equipment was supplied by AEA Technology, U.K. Test of installation were carried out and the results of these tests showed the necessity of improvement of cement screw feeder as well as grout flow out. Starting the operation of this plant is planning in September '98.

A new evaporation plant is under construction. Basic apparatus is already located and connected in the host building. It is planning that forced circulation type of evaporator will be ready for commissioning in the midle of '99.
MATERIAL RESEARCH LABORATORY IEA

The Material Research Laboratory of the Institute of Atomic Energy is engaged in the research works covering all aspects of materials engineering and in the technological processes developed in the domain of powder metallurgy, welding, brazing and soldering. The investigations are carried out on both structural materials and their welded joints, including the examinations of irradiated materials. The Laboratory is equipped with modern devices for the scientific and applied research of materials. All work in MRL are carried out according to the Quality Assurance Program.

The MRL incorporates the Hot Laboratory, which was put into operation in February 1993 after the authorization by the National Inspectorate for Radiation and Nuclear Safety. The facility was designed to provide maximum flexibility for a broad research programmes involving the metallurgical, physical, and chemical testing of irradiated reactor structural materials.

The main part of the laboratory is the set of 12 hot cells with the lead shielding suitable for handling of radioactive materials up to 4 TBq related to $^{60}$Co. Every cell is equipped with up-to-date sophisticated devices for the examination of radioactive materials. The main equipment includes:

- Instron 8500 Dynamic Testing System with two 100 kN frames for testing of tensile strength, compressive strength, low cycle fatigue resistance, fracture toughness, bend characteristics and crack growth resistance at temperature range from 150°C to 350°C,
- Instrumented Wolpert Pendulum Impact Testing Machine PW 30/15 for dynamic tests of Charpy-V type specimens carried out at temperature range 150°C to 350°C for determination of significant force and deflection values, partial energy values, characteristical fracture-mechanical values,
- Wolpert Hardness Testing Machine DIATESTOR 7521 for testing of hardness using Brinell, Vickers and Rockwell procedures,
- X-ray Diffractometer type DRD-4 for structure analysis.

Above mentioned devices are fully automated, remotely operated and instrumented, equipped with the computer control systems for machine control during the course of experiments, data acquisition and analysis of results.

The remainder equipment of the hot cells complex provides an opportunity to perform:
- cutting out of the samples from the irradiated reactor components,
- samples preparation for metallographic and X-ray examinations,
- thinning of metallic samples for transmission electronic microscopy,
- optical microscopy and microhardness measurements,
- swelling control of materials and density determination,
- thermal treatments and annealing,
- stereo microscopic examination and stereo photography,
- chemical analysis.

Material Research Laboratory IEA received Certificate of Testing Laboratory Accreditation No L 25/1/95. This Certificate confirms that Material Research Laboratory at Institute of Atomic Energy is in conformance with the standard PN-EN 45001 and ISO/IEC Guide 25:1990.

In 1996 the Certificate of Testing Laboratory 2nd Degree Approval No L-II-001/27 was granted to the MRL by the Office of Technical Inspection. This indicates that Material Research Laboratory IEA fulfilled the criteria as set forth in PN-EN 4001:1993 and is in conformance with the Specification of the Office of Technical Inspection DT-L/95.
LABORATORY OF HIGH TEMPERATURE PROCESSES (LHTP)

The activity of the laboratory is concentrated on the problems of modern power generation and environment protection. It is designed for research works on the technology required for an advanced coal fuelled gas turbine power system, the coal slurry combustion technology, testing and developing of slagging coal combustors, testing of pulverized coal burner with electric arc plasmatrons, elaboration of liquid wastes disposal process by burning with simultaneous removal of environmental pollutants. The main activities of laboratory are dedicated to environment friendly technologies of electricity production from coal, reduction of sulfur and nitrogen oxides in fumes and developing technologies of waste disposal.

The basic components of LHTP facility are:
- main slagging combustor 4MW(th),
- slag tank,
- vitiated air heater,
- secondary combustor,
- coal feeding system,
- coal-water slurry system,
- MHD generator,
- electromagnet, scrubber, turbo-compressor, electric arc plasmatron,
- liquid oxygen storage,
- research installation for elaboration of liquid and solid waste disposal process by burning with simultaneous removal of environmental pollutants,
- research installation for investigations of pulverized coal burner with electric arc plasmatron.

The main goal of the laboratory in 1997 was to obtain a long-term and stable operation of the installation for quick pyrolysis of coal dust suspension. Many modifications were introduced to the plasmatron construction. Finally, the three experiments have been carried out, each of four hours duration. The laboratory was closed due to financial reasons at the end of June 1997.

CYFRONET COMPUTING CENTRE

Convex computer system C-3220 is the basic Computer of CYFRONET.

C-3220 is a 100 Mflops computer system with:
- Two 64-bits scalar-vector processors (40 μs cycle), 64 MB operating memory (800 MB virtual) and 64-bits data bus (200 MB/s).
- Three Sabre ST83220 disk stations, each has the 2.71 GB capacity and 4.67 MB/s transmission speed.
- Two MTD-204 magnetic tape stations with double speed (50ips/100ips), 1600 bpi and 6250 bpi density and 625 KB/s transmission speed.
- One DDS DAT tape drive specifically designed as 5.25-inch, characterized by high capacity and high performance - 1.3 GB (60 meter tape) or 2.0 GB (90 meter tape) of storage with a transfer rate of 183 kilobytes/second.
- Two high performance, VME Ethernet connections.
- One 600 lpm printer/plotter.

A list of software available at the CYFRONET Computer Centre:

1. Operational system: ConvexOS (UNIX type), an extension of 4.2 and 4.3 BSD, compatible with IEEE Posix P1003.11 standard, working under the Bourne- and C-shell.
2. Compiler: Assembler, CONVEX FORTRAN 77 (ANSI X3.9-1978), CONVEX C (ANSIX3.159 1989) - both with automatic vectorization and parallelization. The extensions are compatible with VAX/VMS, CRAY and SUN products.
3. Utilities: CXdeb, Convex Consultant, CXpa and the COVUE programs package with COVUEnet, COVUEbinary, COVUEshell, COVUElib, COVUEdit, COVUEbatch for VAX users.

Operation and services

C-3220 computer system is operating 5 days/week, 24-hours each day. The total production CPU time from 1997.01.01 to 1997.12.31 is 11206 hours. User CPU time is equal to 8984 hours what gives 80% of CPU
efficiency. Use of CPU time in 1997 year is shown in figure below.

![CPU Time Distribution](image)

Distribution of CPU time is given in the table below:

<table>
<thead>
<tr>
<th>Institution</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maria Curie-Sklodowska University - Lublin</td>
<td>36.9%</td>
</tr>
<tr>
<td>Institute of Atomic Energy - Świerk</td>
<td>14.0%</td>
</tr>
<tr>
<td>Institute of Nuclear Studies - Świerk</td>
<td>4.7%</td>
</tr>
<tr>
<td>Research Reactor Centre</td>
<td>22.9%</td>
</tr>
<tr>
<td>Other</td>
<td>1.5%</td>
</tr>
</tbody>
</table>

**REGIONAL LABORATORY OF NEUTRONOGRAPHY (RLN)**

**RESEARCH PURPOSE:**
Investigation of structures and internal dynamics of materials and devices, using horizontal neutron beams of the 20 MW nuclear reactor MARIA and neutron spectrometers installed there.

**SCIENTIFIC STAFF:**
- Prof. Andrzej Czachor - head of the RLN,
  tel. 48-22-779-8805, fax 48-22-779-3888,
  e-mail e08cza@cxl cyf.gov.pl.
- Konrad Blinowski, Ph.D.,
- Joanna Kisieleńska-Jankowska, M.Sc.,
- Assoc. Prof. Edward Maliszewski,
- Krzysztof Maletka, M.Sc.,
- Assoc. Prof. Kazimierz Mikke,
- Jacek Mikczarek, M.Sc.,
- Prof. Andrzej Murasik.

**TECHNICAL STAFF:**
Zdzislaw Jurkowski,
Jan Żołądek.

**PROJECT SELECTION BOARD**
Consists of the representatives of institutes and universities involved in doing research using neutron scattering. Chairman - Prof. Ludwik Dobrzyński from the Soltan Institute of Nuclear Studies, Świerk. The Board selects and qualifies the research projects to be performed on the neutron spectrometers. The proposals should be sent to Prof. Andrzej Czachor.

**AVAILABLE INSTRUMENTS AT HORIZONTAL CHANNELS (H 3-7) AND CONTACT PERSONS**

**H3** - double axis diffractometer to study crystalline or magnetic structures. It also enables one to do spectrometric measurements, i.e. the energy analysis of inelastically scattered neutrons. Contact:
- Krzysztof Maletka M.Sc., tel. 48-22-779-9324

**H4** - small angle spectrometer. Monoenergetic neutron beam is obtained by the Bragg reflection from ideal Ge single crystal. The halfwidth at half maximum of the neutron beam intensity distribution is 45°. The angular distribution of transmitted intensity may be measured in steps of 0.5°. This instrument is suitable to determine the size of magnetic domains, atomic clusters, or other micro-objects which cause neutron scattering. Contact:
- Jacek J. Mileczarek M.Sc., tel. 48-22-779-8801
H5 - polarized neutron spectrometer. Polarized neutron beam is produced by Bragg reflection, first from the (200) plane of the Cu monochromator and then - from magnetized Co-Fe single crystal.

Contact: Konrad Blinowski Ph.D., tel. 48-22-779-8805

H6 - triple-axis spectrometer. The instrument is destined to study the crystal and magnetic lattice dynamics by inelastic neutron scattering. If necessary it may be used as diffractometer with analyzer set for measurements in the so called elastic regime. Technical data: monochromator - PYG (0.4°), neutron flux at the sample position: 5.1x10^5 n/cm²/s for λ = 2.35 Å.

Contact: M. Szymański Ph.D., Warsaw University, tel. 48-22-628-3031 ext 197

H7 - triple-axis spectrometer, destination as above. Technical data: monochromator Zn (15°), neutron flux at the sample position: 5.5x10^5 n/cm²/s for λ = 1.523 Å.

Contact: Joanna Jankowska-Kisielińska M.Sc., tel. 48-22-779-8304

Each instrument is controlled by PC through the CAMAC electronic system. In order to standardize and facilitate measurements, the computer program for running the instruments complies with rather general operational requirements, including these for the polarized neutron spectrometry. The programs offer the window system with text mode or graphics mode, with zooming for data extraction, and visualization of measurements.

The diagram below shows the distribution of instruments in the MARIA reactor hall.
DATABASE SYSTEM FOR CHEMICAL INSTALLATIONS RISK ASSESSMENT

The calculation of the probability and consequences of an accidental release of a hazardous substance from manufacturing, transport and storage, may be effectively supported with appropriate computer data bank.

For these purposes the database system for chemical installations risk assessment is created and continuously updated. The system is composed of six main components:

- dangerous substances database,
- process equipment failure database,
- selecting hazard evaluation techniques for chemical installations,
- HAZOP-type procedure of analyses,
- review of computer programs for chemical substances atmospheric dispersion calculations,
- documentation,

each of which contains links to files with databases distributed with respect to the sort of data.

In each main component further detailed information is available. Thus:

- physical, chemical and toxicological properties for 1800 dangerous chemical substances,
- equipment failure rate data for 70 kinds of hardware (characterised as time-related and demand-related),
- detailed flowchart for selecting hazard evaluation techniques that may be used directly or to assist develop own procedure,
- detailed algorithm of HAZOP analysis that may be used directly or to be a guide for such procedure,
- characteristics of 33 computer programmes developed for modelling atmospheric dispersion of accidentally released gases (model type, release type, consider or not topographical data, terrain data etc.)
- zipped documentation (Word 6.0) to download.

The data included in the database system are continuously updated reviewed and verified accordingly to the users suggestions and needs. Database URL:
http://www2.cyf.gov.pl/chemia.html
RESEARCH
DETERMINATION OF AMBIENT DOSE EQUIVALENT IN MIXED RADIATION FIELDS BY RECOMBINATION CHAMBER

Natalia Golnik, Mieczysław Zielczyński
Institute of Atomic Energy

Ambient dose equivalent, H*(10), was defined by International Commission on Radiation Units and Measurements (ICRU) [1] in 1985 and became the basic operational quantity for strongly penetrating radiation. In 1992, the International Commission on Radiological Protection (ICRP) published its new recommendations (ICRP 60) [2] that seriously affected the principles of radiological protection. In 1997, the recommendations of the ICRP 60 were adopted by the Joint Task Group of ICRP and ICRU [3] bringing the definition of H*(10) into line with the recent European Directive [4]. New legislation following this Directive is expected to come into effect on 1 January 2000 in all European Community countries.

The international recommendations mentioned above created a need to develop such measuring methods that the response of radiation detectors would match the ambient dose equivalent.

The research project to develop recombination methods suitable for determination of H*(10) in mixed radiation fields started at IAE in 1992, almost contemporaneously with publication of the ICRP 60 Report. The main part of the project was completed in 1997 [5-8]. Some further studies on optimization of the developed methods and measuring systems are still foreseen.

In our method, H*(10) is calculated as a product of the absorbed dose (D) and the effective radiation quality factor (Q_{ICRP-60}), both determined by recombination chamber of REM-2 type [5] designed by M. Zielczyński in late 60’s.

The response of the chamber was proved to be extremely stable. Examples of saturation curves obtained with the $^{137}$Cs source are shown in Fig. 1 to illustrate the repeatability of the curves over long periods of time.

Two different methods were proposed for determination of the $Q_{ICRP-60}$ according to the ICRP-60 recommendations. The first one was based on measuring the recombination index of radiation quality ($Q_4$) and calculation of the $Q_{ICRP-60}$ using a specially proposed function [9]. The method was accurate within few percent for neutron radiation fields with low contribution of gamma radiation and within about 50% for the most complex radiation fields. Usually, such accuracy is sufficient for routine radiation protection, so the method could be recommended for fast estimation of the radiation quality factor.

The second, more accurate method [5,6] involves determination of the absorbed dose distribution, D(L), vs. LET (Linear Energy Transfer).

A new theoretical model has been developed for this purpose [5,10,11]. Using this model one can derive the D(L) distributions by fitting theoretical functions to the measured saturation curves of the recombination chamber. The fitting procedure was found to be reliable and only weakly influenced by experimental uncertainties.

The D(L) distributions are then used for calculation of radiation quality factor. Two slightly different calculation procedures were elaborated [8]. One of them results in values close to radiation weighting factors, (w_R), defined by ICRP in Ref. 2. The other gives the values of $Q_{ICRP-60}$ and is used for calculation of H*(10). Fig. 2. shows the results obtained for reference monoenergetic neutron beams at PTB Braunschweig.

![Fig. 1. Saturation curves of REM-2 recombination chamber determined with $^{137}$Cs for three series of measurements performed within a four year period: (*) September 1993; (•) March 1995; (▼) September 1997.](image1)

![Fig. 2. Comparison of the $w_R$ (○) and effective quality factor values (▼) experimentally determined by the REM-2 recombination chamber, with calculated values recommended by ICRP [3] (solid and dashed lines, respectively).](image2)
The response of the REM-2 chamber to \( H^*(10) \) was investigated in different radiation fields. All the experimental values were related to the reference (conventionally true) values of \( H^*(10) \). The results are summarized in Fig. 3 which presents the relative response of the REM-2 chamber to photons of different energies (diamonds), monoenergetic neutrons (triangles) and mixed neutron-gamma radiation fields of isotopic sources (squares).

Fig. 3 shows, for completeness, also the results obtained for high energy neutrons. Therapeutic neutron beam of maximum energy 660 MeV in Dubna is represented by the point at the neutron mean energy of 350 MeV. It should be stressed that accuracy of this result is relatively poor, mainly due to large uncertainty in calculating the reference \( H^*(10) \) values. The point at 100 MeV corresponds to CERN-CEC calibration field of high-energy stray radiation that simulates the cosmic radiation field on board of an aircraft during high-altitude flights.

It can be seen from Fig. 3 that the resulting relative \( H^*(10) \) value (related to a reference value) is between -20% and +40% for monoenergetic neutrons. In practical conditions of radiation protection, however, one usually deals with mixed radiation of broad neutron energy spectrum and some photon contamination. The results of measurements performed in radiation fields of isotopic neutron sources and in fields of neutron sources placed in filters (with photon component ranging from 10% to 72%) showed that in such conditions the \( H^*(10) \) response of the REM-2 chamber is within few percent from the reference value. The \( H^*(10) \) response of the REM-2 chamber to photons is only about 10% to 30% lower comparing with the response to \(^{241}\text{Am}-\text{Be}\) neutrons used for calibration and is nearly independent of photon energy.

The dose rate which is easily accessible for the chamber in routine operation ranges from 1 \( \mu \text{Gy} \cdot \text{h}^{-1} \) to 0.25 \( \text{Gy} \cdot \text{h}^{-1} \), which corresponds to the \( H^*(10) \) values from 1 \( \mu \text{Sv} \cdot \text{h}^{-1} \) up to approximately 1 \( \text{Sv} \cdot \text{h}^{-1} \). There is practically no limitation on LET and energy range of detected radiation. Recombination chambers can be considered as an alternative to TEPC-instruments or neutron remmeters. There is a large variety of such instruments and comparison with different types may lead to somewhat different conclusions. Nevertheless, it is rather clear that the ambient dose equivalent response of the recombination chamber is generally less dependent on neutron energy than that of most known TEPC-systems and of commercial neutron dose meters. We expect that for most of realistic radiation fields with broad energy spectrum our instrument should give similar response as the best TEPC systems.

REFERENCES:
Tests of the IAE Dose Equivalent Meter in Radiation Field of High Energy Calibration Facility at SPS-CERN

Zdzisław Rusinowski, Natalia Golnik
Institute of Atomic Energy

The IAE ambient dose equivalent meter [1] based on REM-2 recombination chamber, was designed for use in mixed radiation fields. Up to now, the IAE device was tested in fields of isotope radiation sources only but the features of the detector predestine the device for use in the vicinity of accelerators. In 1997 the performance tests of the device were carried out in reference high-energy fields that are provided outside shielding configurations of the H6 beam of the Super Proton Synchrotron (SPS) at CERN. In this unsteady, pulsed radiation beam, the device was working with its own monitoring circuit not used during the earlier tests. The beam intensity was also monitored with a Precision Ionization Chamber (PIC) placed in the beam line. The signal of PIC was later used as the primary signal for comparison of our results with the reference values.

An example of the results obtained during the measurements is shown in Figure 1. In its upper part the dose rate measured by the IAE device (solid line) is compared with the beam intensity measured by the PIC (dotted line). Sharp drops to zero seen in the PIC count curve indicate loses of single pulses of the beam (no protons on the target). The fact that not all the loses of the beam pulses are reflected in the dose rate curve is due to the dead time of the device during the voltage switching and stabilization. Generally, this does not influence the mean value of the dose rate.

The lower part of the Figure 1 shows the measured values of the recombination index of radiation quality, RIQ, approximating the radiation quality factor. It can be seen that the mean value of RIQ = 3.35 ± 0.07 was obtained with standard deviation of about 2% only. Somewhat higher variations of the RIQ value (but still below 10%) were observed only during the period of strong instability of the beam and may reflect the real variations of the quality factor. Practically, such deviations of the RIQ value are of very small importance.

The mean value of the ambient dose equivalent rate obtained by the IAE device was equal to \( H^*(10) = (3.82 ± 0.15) \times 10^{-10} \) Sv per PIC-count. This value can be compared with the reference value of \( (3.75 ± 0.41) \times 10^{-10} \) Sv per PIC-count.

The tests described above proved the sound performance of the device. Moreover, the chambers do not need any kind of service and their sensitivity changed by less than 1.5% during last 12 years. With such features the IAE device can be especially suitable for continuous monitoring of complex mixed radiation fields.

Acknowledgements. The work was supported by the Polish State Committee for Scientific Research under KBN grant No. 4 P05D 033 11.

REFERENCES:

Fig. 4. Upper part - the dose rate measured by the IAE device (solid line, left axis) and the beam intensity as monitored by PIC (dotted line, right axis). Lower part - recombination index of radiation quality approximating the ICRP-21 radiation quality factor.
A thin-walled recombination chamber has been developed [1] for direct determination of radiation protection operational quantities H'(0.07) and H'(3) recommended for dosimetry of weakly penetrating radiation.

Ionization chambers operated at saturation are recommended and widely used for dosimetry in fields of low energy photons and electrons but they cannot provide any information about radiation quality so that their application in fields of low energy alpha particles or heavy ions is much limited. This problem can be solved by use of a specially designed thin-walled recombination chamber. Such a chamber will be also a useful tool for some special measurements needed sometimes both in routine radiation protection and in research, e.g. for the determination of contamination of higher energy photon beams with low energy photons or for the determination of radiation field close to the body or phantom surface where the conditions of electron equilibrium are not fulfilled.

The thin-walled recombination chamber denoted as KR-16 was designed as a planar, tissue-equivalent ionization chamber, with the gas cavity under a tissue-equivalent absorber of 0.012 mm thick backed by a thick layer of tissue-equivalent plastic having similar backscattering characteristics as tissue. Cross-section of the recombination chamber is shown in Figure 1. Almost all the details of the chamber are made of a tissue-equivalent material. A thin (0.012 mm) Mylar foil stretched on a solid isolating ring serve as the polarizing electrode and entrance window. The collecting electrode and the guard ring of the chamber form a common flat surface ensuring the uniform electrical field strength and well defined active volume in the chamber. A specific property of the KR-16 chamber design is that the voltage insulators are „invisible” from any point of the active volume. Such configuration ensures very good time stability of the electrical field strength in the active volume of the chamber and enables reading of the ionization current in short time after changing the supplying voltage from saturation to the recombination one and from positive to negative polarity. The chamber is filled with butadien and operated with a gas flow system at gas flow rate of about 3 cm$^3$/min.

The tests of the chamber were performed in the fields of $^{137}\text{Cs}$ gamma and $^{239}\text{Pu}$ alpha radiations. It was proved that the chamber was working correctly and could ensure repeatability of the results within statistical uncertainty of measurements. The dark current of the chamber was below 3 fA. The recombination index of radiation quality measured for $^{239}\text{Pu}$ alpha particles was equal to $Q_{r}=15^2$.

Unfortunately, there is a serious limitation for possible routine application of the KR-16 chamber filled with C$_4$H$_6$ due to ageing processes in the chamber. It was observed that some heavy hydrocarbon fraction appeared on inner part of the chamber after three months of intensive work and irradiation with the dose of about 10 Gy. The Mylar electrode became degraded and had to be replaced by a new one. The replacement is not difficult in laboratory conditions but inconvenient for routine radiation protection.

Acknowledgements. The work was supported by the Polish State Committee for Scientific Research under KBN grant No. 4 P05D 033 11.

REFERENCES:
[1]. M. Zielczyński, N. Golnik: Thin-walled recombination chamber for determination of directional dose equivalent H'(0.07). Raport IEA B-70/97.
IMPROVED DETERMINATION OF NEUTRON AMBIENT DOSE EQUIVALENT H*(10), IN IAE STANDARD NEUTRON FIELDS

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Standard fields of neutron sources $^{241}$Am-Be and $^{252}$Cf, recommended by ISO [1], have been examined in the Institute of Atomic Energy in 1986-87 [2]. Total neutron emission rate of the sources was measured in National Physical Laboratory, Teddington, Great Britain. Basic physical and dosimetrical parameters of neutron fields of sources, exposed in IAE calibration hall, were determined [2]. $^{239}$Pu-Be neutron source served for routine use. Its emission is growing in a not well predicted way.

After ten years it became necessary to confirm the earlier measurements, to revise the results, according to new recommendations, and to renew the traceability of IAE sources to NPL.

Verification of the neutron sources emission through the transfer instrument calibration has been chosen, with Studsvik 2202D remmeter as a transfer instrument. New calibration of Studsvik has been done at NPL with standard sources $^{241}$Am-Be and $^{252}$Cf, giving the values of fluence response of remmeter. The Studsvik counting rates in IAE calibration hall, in the distance of 1 m from the sources, were taken as a basis for the determination of neutron emission rate of the sources.

Neutron ambient dose equivalent rates of isotope sources, exposed free in air in calibration hall, have been measured versus the distance from the source, using Studsvik.

![Fig. 1. Neutron dose equivalent rate of $^{241}$Am-Be vs. distance, measured in 1996 and 1986.](image)

New values of fluence-dose equivalent conversion factors [3], together with the response mentioned above, have been used for the evaluation of results of earlier and new measurements, recalculation into ambient dose equivalent $H^*(10)_n$, for the date of 31 December 1997. Some results are shown in Figures 1 and 2, the full data are given in internal report [4].

![Fig. 2. Neutron dose equivalent rate of $^{252}$Cf vs. distance, measured in 1996 and 1987.](image)

Measurements performed in 1996 resulted in values of emission of the sources higher by 1 % for $^{241}$Am-Be and nearly 4 % for $^{252}$Cf, comparing with the results from 1986 and 1987.

Neutron emission of $^{239}$Pu-Be source has been measured during 12 years, in comparison with the neutron emission of standard $^{241}$Am-Be neutron source. Results are shown in Figure 3. The source has to be periodically checked.

![Fig. 3. The growth of the neutron emission of IAE $^{239}$Pu-Be source.](image)

REFERENCES:
STRUCTURAL AND MAGNETIC PROPERTIES OF Fe-Cr-Al ALLOYS WITH DO3-TYPE STRUCTURE

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The results reported here were published in [1]. Fe3Si and Fe3Al alloys are very interesting intermetallic compounds for number of reasons. They crystallize in DO3 - type structure (Fig.1), in which iron occupies two inequivalent positions. One of these is surrounded in the nearest-neighbour shell by eight iron atoms in bcc iron and possesses a high magnetic moment of the order of 2.2-2.5 μB.

Fig. 1. DO3-type structure

This site is usually abbreviated by B, whereas the letters A and C stand for other sublattices in which iron is surrounded by four iron and four Si or Al atoms. The magnetic moment found at these sites is much lower and equals about 1.1 μB in Fe3Si and 1.4 μB in Fe3Al. The fourth position D is occupied uniquely when perfect order is achieved, by silicon or aluminium atoms. The presence of the two inequivalent positions in the lattice make the alloys almost ideally suited for studies of the magnetic moment dependence on the local environment. In addition, the structure itself changes to B2 and A2 under disordering so the physical origins of the order-disorder process can be studied as well. The two isomorphous alloys, according to the band structure calculations, should show very similar properties but this is not the case. The most striking differences can also be seen in their mechanical properties: Fe3Si is brittle, whereas Fe3Al is ductile. It is also interesting to note that the DO3 ordering is rather easily achieved in the Fe3Si alloy, whereas it is extremely difficult to order Fe3Al alloy fully. A rather small difference in the lattice constants (5.655 Å for Fe3Si compared to 5.793 Å for Fe3Al) results nonetheless in a great decrease of the effective exchange interaction from about 22 meV in Fe3Si to about 9 meV in Fe3Al, yet the magnetic moments per formula unit (4.86 and 5.08 μB at room temperature, respectively) as well as the Curie temperatures (830 and 760 K) do not differ significantly.

Actually the property which raised the most of interest in these alloys is the preferential occupation of sites by the transition metal impurities substituted for iron. In the number of papers it has been shown that in the Fe3Si alloy, the elements to the left of iron in the periodic table of elements occupy preferentially B-sites, whereas those to the right of iron locate at (A,C)-sites. Observed changes of the local hyperfine fields have been explained in the framework of the local-environment model implying that - at least as far as the hyperfine fields are concerned - configuration of the nearest-neighbour shell is the only important factor in these alloys. The spin wave studies [2] indicated, however, that the exchange forces are of much longer range, calling in fact for the band structure approach. Such an approach was used to explain the mechanism of preferential site occupation in Ref. [3]. Although this explanation for Fe3Si-based alloys should apply seemingly well to the Fe3Al-based alloys, it has been noticed that the preferential occupation of sites in the latter alloy is not so clear if Mn is substituted for iron [4].

In the recent studies of Fe3Si alloy with Cr substitution [5], [6], it was found, to the authors' surprise, that chromium does not locate preferentially at the B-sites but rather spreads evenly between A-, B- and C-sites. It was also found that chromium may assume magnetic moments comparable to the iron ones at both sites. How-
ever, in contrast to the behaviour of Mn impurity, the chromium moments are oriented antiparallel to the direction of the iron moments. Therefore it became interesting to study the behaviour of chromium in Fe₃Al alloy.

Magnetization studies using the magnetic balance were performed at the Institute of Physics in Bialystok. Also X-ray powder diffraction diagrams were obtained in Bialystok on the X-ray diffractometer with Fe Ka radiation (λ=1.93597 Å). Powder neutron diffraction experiments were conducted on the D20 diffractometer at the Institute Laue-Langevin in Grenoble, while polarized neutron research was carried out on POLAR 2 diffractometer at the Studsvik Neutron Research Laboratory.

The powder sample compositions have been checked by means of X-ray microanalysis. The composition of the bulk samples dedicated to polarized neutron studies have been estimated from the difference of masses measured before and after arc-melting.

The analysis of the neutron intensities cannot discriminate between aluminium and chromium because the neutron scattering lengths of these two elements are not much different (3.45 and 3.64 fm, respectively). Because it is apparent that in our samples rather strong A-D disorder is present, the analysis of neutron data themselves can show unambiguously the occupation of sites by iron only. Happily, one can combine neutron and Mössbauer data [7]. Inspection of both leaves no doubt that chromium enters predominantly B-sites, and it is reasonable to expect that the only other position which can be occupied by chromium will be the D-site which has the same nearest environment as the B-sites.

X-ray, neutron, magnetization and Mössbauer effect studies carried out on Fe₃₋ₓCrₓAl alloys with x<0.6 showed that chromium atoms occupy preferentially B-sites and enter also D-positions [1]. Their magnetic moments are small, if any, and they diminish the value of the neighbouring iron moments by roughly 0.1 μₜ per chromium atom. This value agrees well with the one found in Ref. [8]. In spite of high counting statistics in neutron diffraction patterns, the determination of magnetic moments for various crystallographic sites did not allow either detection of the nonzero magnetic moment of chromium or a difference between the iron moments at the B- and D-sites.

Therefore, the final data analysis has been carried out under an assumption of zero magnetic moments of chromium atoms, and identical iron moments of iron at the B- and D-sites. The undisturbed magnetic moments of iron at (A,C)- and B- (or D)-sites were estimated to be 1.54 (22) and 2.58 (22) μₜ, respectively, at T=10 K, 1.51 (27) and 2.32 (14) μₜ, respectively, at T=300 K. These values agree well with the ones obtained in Ref. [9] for Fe₃Al. It is also shown that the iron moments decrease if an extra aluminium atom is found in the nearest surrounding, and this decrease is 0.37 (10) and 0.26 (6) μₜ at T=10 K and 300 K, respectively. A markedly different behaviour of chromium in Fe₃Si and in Fe₃Al concerns the occupation of atomic sites by chromium, the value of its magnetic moment, as well as a change of lattice constant with the chromium content. On the grounds of known differences in exchange interactions in both parent alloys [2], [10], it is suggested that different behaviour of chromium is due to a subtle interplay of magnetic and nonmagnetic interactions.

REFERENCES:
THE GREEN'S FUNCTION BASED INSIGHT INTO ATOMIC DYNAMICS OF DISORDERED ISOTROPIC SOLIDS, USING NEUTRON AND LIGHT INELASTIC SCATTERING AND INFRARED ABSORPTION

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Results of the Average-Local-Information-Transfer-Approximation (ALITA) study of atomic dynamics in disordered solids have been summarized [1]. As the results of the neutron (NIS) and light (first order Raman, FOR) inelastic scattering, and infrared absorption (IRA) experiments can be represented in terms of the same time and space dependent Green's functions for atomic displacements, interesting features of and some relations between the measured spectra do appear. It was shown and verified that the phonon density of states for glasses is given as a superposition of the Raman and IRA spectra. Peaks in the IRA spectra should be, for multatomic systems, attributed to some frequency gaps in their phonon spectra. Neutron profiles in the Q-constant NIS experiment for a monoatomic solid have been shown to be a deformed spectrum of local (Einstein) frequencies of the solid.

This spectrum of local frequencies is a very informative characteristic of disorder - for example it consists of the single δ-function line for a monoatomic regular crystal, while for the amorphous edition of the same substance the spectrum can have a considerable width and rich structure. A formula has been derived, linking the phonon density of states and the spectrum of local frequencies. Using it, and taking the experimental FOR spectrum for amorphous Si as a good representation of its phonon density of states, the form of the local frequency spectrum for amorphous Si has been established, see Fig. 1.

REFERENCES:

Fig. 1. Spectrum of local frequencies E(ω) for amorphous Si.
EXACT CALCULATION OF THERMODYNAMIC FUNCTIONS IN THERMODYNAMIC LIMIT FOR A MODEL ANTIFERROMAGNET WITH IDENTICAL COUPLING BETWEEN ALL SPINS

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Specific heat and magnetic susceptibility for the Kittel, Shore and Kac (KSK) model magnet consisting of N Ising or vector spins $S=1/2$, interacting identically with each other and with magnetic field, have been calculated in the thermodynamic limit $N \to \infty$, assuming the antiferromagnetic interspin coupling $I/N$, $I<0$. To achieve it the Kac mathematical procedures have been properly generalized and completed. It has been found that, due to a fast decline of the high-energy density of states vs the energy, the specific heat (per one spin) goes to zero in this limit. In general the specific heat in thermodynamic limit is shown to be proportional to the field squared. The magnetic susceptibility shows in this limit the same paramagnetic type of temperature dependence both for Ising and vector spins, see e.g. Fig.1 for vector spins.

There is no phase transition in this case. Characteristic dependence of the susceptibility on $N$ being even or odd can also be seen in this plot, for finite $N$.

The results obtained are exact and thus can be used to verify approximate theories one has often to introduce to investigate more realistic magnetic systems.

REFERENCE:

Fig. 1. Sequence of the magnetic susceptibility vs $T$ (both in dimensionless units) plots for growing $N$, assuming vector spins $S=1/2$ coupled identically and antiferromagnetically, showing the way the susceptibility converges to the thermodynamic limit value, given by the "$N \to \infty$" heavy line.
In order to understand the role of thermal phonons in anomalous physical properties of the fcc Ni-Fe invar alloys, we have undertaken experimental lattice dynamics studies of the Ni$_{1-x}$Fe$_x$ system in the Fe concentration range where the fcc lattice is formed. From the literature on invar problems [1] it follows that the systematic lattice dynamics studies of the Ni$_{1-x}$Fe$_x$ system can give indispensable and important information related to the invar anomalies. Measurements of phonon dispersion relations $\omega(q)$ by inelastic neutron scattering in Ni$_{1-x}$Fe$_x$ lead to the determination of their frequency changes $\Delta\omega(q)$ and self-energy $\Sigma(q,\omega(q))$, versus the Fe concentration, in comparison with the dispersion curves of the Ni matrix crystal. This method proved to be useful in the studies of lattice dynamics of disordered crystals. Results of such investigations of the lattice dynamics for Ni-rich alloys (Ni, Ni$_{0.88}$Fe$_{0.12}$, Ni$_{0.76}$Fe$_{0.24}$) were already published [2]. The studies of lattice dynamics of Ni$_{0.65}$Fe$_{0.35}$ [3] and Ni$_{0.50}$Fe$_{0.50}$ [4] we also presented.

In the paper, reported here, prepared for publication and for Report IAE B-1/98 [5] we present the results of the investigations of the invar Fe$_{0.65}$Ni$_{0.35}$ lattice dynamics. The application of the experimental method mentioned above, elaborated for disordered crystal of solid solutions, to Fe$_{0.65}$Ni$_{0.35}$ made it possible to disclose the softening of the longitudinal branches.

The softening of the longitudinal branches disclosed by $\Delta\omega(q)$ and $\Sigma$ functions has not been observed up to now. This lack complicated explaining theoretical models of invar effects. The $\Sigma$ functions plotted in Fig 1 display a dynamical picture of the Fe$_{0.65}$Ni$_{0.35}$ Invar. The rich oscillating structure of these functions ($\Delta\omega,\Sigma$), which strongly depends on wave vectors and on polarization, would make it possible to analyse theoretically an influence of different interactions on the lattice dynamics of Fe$_{0.65}$Ni$_{0.35}$ and on its anomalous physical properties.

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[2]. E. Maliszewski S. Bednarski: The Lattice Dynamics of Ni$_{0.88}$Fe$_{0.12}$, Ni$_{0.76}$Fe$_{0.24}$ and Ni Single Crystals, phys. stat.sol. (b)200, pp. 435-444, (1997).

Fig. 1. The self-energy functions divided by the average atomic mass vs. the reduced wave vectors for Fe$_{0.65}$Ni$_{0.35}$, determined from the phonon frequencies for Fe$_{0.65}$Ni$_{0.35}$ and Ni.
ANISOTROPY OF THE GENERALISED SUSCEPTIBILITY IN Mn(38%Ni) ALLOY IN THE MAGNETIC PHASE TRANSITION REGION

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The previous studies [1,2] of the magnetic phase transition in the fcc γ-Mn-Fe and γ-Mn-Ni alloys revealed a large directional anisotropy of the transverse spin-correlation lengths. This effect is similar to the one found in USb [3]. It is interesting that both effects were observed in cubic systems.

The aim of the experiment was to determine the anisotropy and dynamics of the transverse and longitudinal components of the generalized susceptibility near the Néel temperature for the Mn (38%Ni) alloy.

The Mn (38%Ni) alloy undergoes the continuous P-AF1 phase transition at 400 K in the fcc lattice. The critical exponent for the sublattice magnetisation is close to 0.4. The transverse fluctuations were found to increase significantly at the transition point although their correlation lengths were finite at the Néel temperature.

The neutron scattering measurements were performed by 3-axis neutron spectrometer at Orphée reactor in LLB CEN Saclay. The measurements with zero energy transfer were performed in the vicinity of (100) and (110) rlp in (001) and (1,-1,0) planes. The intensity distribution determined in the (001) plane around (100) rlp confirmed the large, independent of temperature, anisotropy of the transverse component of the static generalized susceptibility. The intensity distribution measured in the same plane in the vicinity of (110) rlp revealed no significant departures from the isotropic features, i.e. circular constant intensity contours. The measurements performed in the (1,-1,0) plane around both (001) and (110) rlp have shown that the correlation length in the [001] direction is larger than the correlation length in the [110] direction.

These results indicate that the anisotropy axis is parallel to the direction of wave vector of the spin density wave which, according to current theories, describes the magnetic structure of the alloy.

For the first time the critical inelastic neutron scattering was investigated in the Mn(38%Ni) alloy. The observed effect was discussed in terms of the anisotropic static generalized susceptibility and anisotropic dynamic component:

$$\chi^{\text{ex}}(q, \omega) \propto \frac{M}{1 + \left(\xi_{s} q_s^2 + \xi_{l} q_l^2\right)} \frac{\Gamma(q)}{\Gamma_0(q) + \omega^2}$$

where

$$\Gamma(q) = \Gamma_0 \left(1 + \left(\xi_{s} q_s^2 + \xi_{l} q_l^2\right)^2\right).$$

The dependence of the spectral width $\Gamma(q)$ on $q$ appears to be less anisotropic than assumed. The temperature dependence of $\Gamma_0$ is characteristic for the continuous phase transitions, as shown in Fig. 1.

![Fig. 1. Temperature dependence of the spectral width $\Gamma(q = 0)$.](image)

This work was partly supported by the "Human Capital and Mobility - Access to Large Scale Facilities PECO Extention" Program (Contract N° ERB CIPD CT 940080).

REFERENCES:
INFLUENCE OF MAGNETIC ORDERING ON PHASE EQUILIBRIA IN SPINODALLY DECOMPOSED Fe-Cr-Co-V ALLOY

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Alloys based on the Fe-Cr-Co system are known to be very suitable for ductile permanent magnet production. Magnetic ordering in these alloys causes the appearance of a specific shape of the miscibility gap of a solid solution of the ferromagnetic phase $\alpha_1$ and the paramagnetic phase $\alpha_2$. Precise determination of its shape and elaboration of a thermodynamical model describing these effects are vital for developing the techniques for the production of various hardmagnetic materials based on the Fe-Cr-Co system.

The studies of the Fe-Cr-Co alloys with Mo and V additions were presented in [1,2]. In the present work we use the thermodynamical model described in [3] for Fe-Cr-Co-V alloys.

The thermodynamical model includes the chemical and magnetic contributions to the free energy of the alloy. The chemical contribution is based on a model of subregular solid solutions. The magnetic one, is calculated using the data on $T_C$, magnetization and magnetic contribution to alloy heat capacity ($C_m$). The basis of the model of this last contribution in a solid solution is given by the formula:

$$C_m = \begin{cases} A_1 \left( \frac{T}{T_C} \right) & \text{if } T < T_C \\ A_1 \left( \frac{T}{T_C} \right) \exp\left(\frac{(T-T_C)}{mT_C}\right) & \text{if } T > T_C \end{cases}$$

where:

$$A_1 = A / (m-1/n),$$

$$A = A_F \sum_{i=1}^{N} d_i c_i,$$

$$T_C = T_{CP} + \sum_{i=1}^{N} \left( a_i c_i + b_i c_i^2 \right).$$

The parameter $n$ describes the long range magnetic ordering and $m$ is the short-range magnetic ordering at $T > T_C$. $A$ is the integral of the entropy change near $T_C$. The parameters $m, n, a, b, d$ should be estimated from the experimental data, $c_i$ - are the concentrations of the alloy components, $N = 4$ is the number of components. Contributions to the free energy were calculated by integrating the heat capacity.

In our experimental work [4] we obtained the data on $T_C$ and on the boundaries of the miscibility gap $T_d$ in some Fe (16-25%) Cr-15%Co-3%V alloys (fig.1). They were used for the detailed choice of the parameters: $a_v = 900$ K and $b_v = 1000$ K. The data on the miscibility gap boundaries yield the parameters’ values: $n = 2.7$, $d_v = -0.1$. All other parameters were taken from [3].

![Fig. 1. Binodals calculated for different values of the model parameters $n$ and $m$.](image)

The value of $n (=2.7)$ differs from that for pure Fe ($n=5$) and from one found for Fe-Cr-Co-Mo alloys ($n=3$). According to the model described in [5] this change might result from the decrease of the degree of correlation between atomic magnetic moments in a magnetic alloy. Cr and V additions are known to destroy the ferromagnetic ordering of Fe atoms. They also lower the saturation magnetization of Fe-Cr-Co-based alloys, since magnetic moment of Cr atoms is known to be antiparallel to that of Fe atoms [5].

REFERENCES:
PLASTIC DEFORMATION EFFECT ON THE CRYSTALLINE AND MAGNETIC STRUCTURE OF THE Mn SHAPE MEMORY ALLOYS

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Some γ-Mn alloys exhibit outstanding properties such as shape memory effect (SME), high damping capacity (HDC) or elinvar anomaly. These alloys undergo a diffusionless magnetostructural phase transformation, leading to the long range antiferromagnetic ordering and the reduction of symmetry from the initial fcc to tetragonal fct [1]. The specific twin microstructure, formed in the process of transformation, results in the twin boundary displacement under the action of the external stresses. The single crystals of Mn₇₅Cu₂₅ and Mn₇₅Fe₁₀Cu₃₀ alloys have been investigated. The samples were cut from single crystals in such a way that their edges were coincident with the [100] direction of the parent high temperature fcc structure. The uniaxial deformation of the samples (ε = 4%) was carried out by compression along the long axes of the samples denoted as [001]. The step by step deformation along all three axes of single crystal was also performed with ε = 5% along [100], [010] and [001].

The deformation of the samples along the [001] axis causes a pronounced redistribution of the scattered intensity in X-ray profiles (Fig. 1). For the Mn-Fe sample the above redistribution is typical for the single domain structure. The deformation of the Mn₇₅Cu₂₅ alloy causes the transformation of the initial fct structure to the structure which is a mixture of the two tetragonal phases with different “c” parameters: (c₁ = 3.676 Å, c₂ = 3.625 Å). This is related to the spinodal decomposition of this alloy and induced fcc-fct transformation [2,3], when the tetragonal shear of the regions enriched in Mn is propagating to the Mn depleted regions.

The plastic deformation of the Mn₇₅Cu₂₅ alloy leads to a smoother magnetization decrease with temperature (Fig. 2). The character of the dependence deviates from the Brillouin curve and the transition from long to short order occurs more smoothly. The transition to the two phase (fct₁ + fct₂) structure might mean that initial single phase magnetic structure with the average magnetization value M transforms to the two-phase magnetic structure with (M₁ + M₂).

Fig. 1. X-ray profiles of the (200) type peaks after successive deformation along 3 axes for the Mn (25%Cu) sample taken for reflections from the plane parallel (a) and perpendicular (b) to the axis of the last deformation.

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Fig. 2. Temperature dependence of the square root of the intensity at (110) for Mn (25%Cu) alloy.

REFERENCES:
NEUTRON SCATTERING IN 2,6 LUTIDINE CONFINE IN POROUS GLASS

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The properties of fluid imprisoned in porous medium attracted much attention in the last few years. A variety of novel effects might be expected in some polar liquids confined in porous media. Study of the 2,6 - lutidine confined in a porous glass Vycor (Na₂O - 7 mol %, B₂O₃ - 23 mol %, SiO₂ - 70 mol %) showed unusual behaviour of heat capacity at t = 21° C [1,2]. The character of the unusual heat capacity behaviour looks like a smeared first order phase transition. The phenomenological theory of phase transitions does not explain this phenomenon. It turns out that this phenomenon takes place in the ordered layer of 2,6 - lutidine formed on the glass surface and connects probably with the orientational phase transition in this layer. In our experiment the small angle neutron scattering method (TOF SANS) was used to the study of the polar liquid 2,6 - lutidine confined in small volume of the porous glass on the spectrometer of the IBR - 2 pulsed neutron source [3] at FLNP, JINR in Dubna (Russia).

The measurements were performed for temperature from 20° C to 28° C and for the scattering vector q = 0.01 - 0.2 Å⁻¹. The sample was placed in the aluminium cell, size 1.4 x 2.5 x 0.1 cm. The characteristic size of the Vycor - matrix pores was about 100 Å. The results of our measurements for temperatures 20° C and 21.6° C are given in, Fig.1. Phase transition was observed between the temperatures 20° - 22° C. Our earlier investigations [2] showed that porous media strongly modify thermodynamic properties of a substance both quantitatively and qualitatively. The values of the heat capacity and latent heat of the phase transitions of samples confined in porous medium are smaller than in bulk. The temperature of the phase transitions is changed. For the first time we observed a qualitative modification in the heat capacity behaviour of the polar liquids and liquid crystals confined in porous glass matrixes manifested as “crevasse” in a curve. The character of the heat capacity behaviour near “crevasse” looks like a smeared first order phase transition with liberation of heat.

The well-known bulk phase transitions are accompanied by absorption of heat (smeared δ-function in the heat capacity) if this is first order phase transition or have a fluctuation anomaly (or discontinuity) of the heat capacity in the case of the second order phase transition. Thus the character of the heat capacity behaviour near the bulk phase transition is reverse to the observed one. The effect of porous medium on confined fluid is takes place through fluid molecules - hard surface interplay on one hand and the effects of confined pore space and pore geometry on the other hand. This gives rise to situations which are more complex than in the bulk and one can expect new phase transition that was not yet predicted even by sophisticated theories.

Fig. 1. The intensity of neutron scattering vs scattering vector q for the vycor+lutidine in temperatures 20° C and 21.6° C.

REFERENCES:
STRUCTURE AND PHASE TRANSITIONS IN SOME Me$_2$UX$_6$ IONIC CONDUCTORS

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The uranium halides Me$_2$UX$_6$ (Me = Na, Li, K, Rb, Cs; X = Cl, Br, I) form a series of interesting compounds with a closely related structure, and exhibiting several interesting properties such as sequences of structural phase transitions and fast ionic conductivity at elevated temperatures. In the course of neutron diffraction investigations of structural properties of these systems, we continued works with the following compounds: Li$_2$UBr$_6$, Na$_2$UCl$_6$, Li$_2$UCl$_6$, and Rb$_2$UBr$_6$. The measurements were carried out on the NPD and SLAD diffractometer installed at the Studsvik Neutron Research Laboratory. Obtained results can be summarised as follows:

1. **Li$_2$UBr$_6$**

The compound crystallises in two forms. The first one is characterised by long range ordering of cations' sublattices (LRO - form) whereas in the second one the short range orders of cations' sublattices were observed (SRO - form). The crystal structure of both forms of Li$_2$UBr$_6$ has been studied as a function of the temperature by neutron powder diffraction. The room and high temperature structures have been determined. At 300 K the LRO-form crystallises in a trigonal unit cell (space group P-31m) with lattice constants: $a = b = 6.8893(4)$, $c = 12.6462(9)$ Å. Above the phase transition occurring at 505 K the space group is found to be monoclinic C2/m. The SRO form at 300 K is trigonal. Above 505 K the structure is monoclinic C/2m but with unordered sublattice of uranium ions. The sublattices of uranium become ordered in the manner observed in the LRO forms above 670 K. (Fig. 1).

2. **Na$_2$UCl$_6$ and Li$_2$UCl$_6$**

The behaviour of the Na$_2$UCl$_6$ and Li$_2$UCl$_6$ was studied as a function of temperature by neutron powder diffraction. The Na$_2$UCl$_6$ up to 711 K, crystallises in a trigonal unit cell, with space group P-3m1. The lattice cell constants at 711 K are: $a = b = 11.951(7)$, $c = 6.568(5)$ Å. It is shown that at room temperature the Li$_2$UCl$_6$ crystallises in hexagonal unit cell, with space group P6$_3$/mmc. The unit cell constants are: $a = b = 11.174(1)$, $c = 18.104(3)$ Å. In the room temperature structure, the sublattices of uranium and lithium ions are disordered. The high temperature structures of Li$_2$UCl$_6$ have been determined. It was shown that above 640 K the Li$_2$UCl$_6$ crystallizes in a trigonal unit cell. At 711 K the lattice cell constants are: $a = b = 11.483(4)$, $c = 12.639(5)$ Å. At this temperature the compound crystallizes with space group P-3c1. It has been found that in contrast to room temperature phase, the sublattice of uranium ions is ordered in a manner similar to Na$_2$UCl$_6$.

3. **Rb$_2$UBr$_6$**

The behaviour of Rb$_2$UBr$_6$ ionic conductor has been studied as a function of temperature by neutron powder diffraction. The low, room and high temperature structures have been determined. In the temperature range 4.2 - 80 K, the compound crystallises in a monoclinic unit cell with P2$_1$/c space group. Between 80 and 843 K the compound crystallises in a tetragonal unit cell with space group P4/mmc. At 300 K the lattice cell constants are: $a = b = 6.8893(4)$, $c = 12.6462(9)$ Å. In the temperature range 843 - 967 K a trigonal phase with P-3m1 space group was observed. Above phase transition at 967 K the compound crystallises in a cubic unit cell with Fm3m space group (Fig. 2). Basing on the literature data known so far on structures and phase transitions, we conclude that observed in the Rb$_2$UBr$_6$ sequences of phase transitions appears to be typical for the Me$_2$UX$_6$ compounds with the ionic radius of Me$^+ > 1$ Å.
Fig. 1. The structures of Li₂UBr₆: (a) LRO-form at 300 K, (b) LRO-form at 550 K and (c) SRO-form at 550 K. The large circles represent bromide ions. The dashed small circles represent lithium ions. The small open circles represent U-ions (b) or octahedral sites randomly occupied by two uranium ions (c).

Fig. 2. (a) Transition from the pseudo-tetragonal to monoclinic unit cell appropriate to P2₁/c space group. (b) Relation between the pseudo-cubic and tetragonal unit cell. (c) Relation between trigonal and cubic unit cell. For the sake of clarity only U ions are shown.

REFERENCES:
THE PIN-HOLE MICRO-LAUE PATTERNS OF IMPLANTED LAYERS

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The important advantage of the synchrotron source is high initial collimation of the beam in the range of arc seconds. This feature significantly increases the possibilities of a well known Laue method especially when the size of the beam is very small.

In the present investigation such kind of a micro-Laue method was applied for studying the implanted layers in silicon and AlB multicom-pound epitaxial layers. This was an important completion of our other studies by means of Bragg case section and multicrystal methods. The micro-Laue patterns were exposed using a white beam limited by a pin-hole to a diameter in the range 5-30 μm. The geometry of the experiment was similar to Bragg case section experiments [1,2] and the conclusions were drawn comparing the results of both methods.

The Bragg case section patterns of investigated layered structures formed by epitaxy and/or implantation contained a series of stripes corresponding to different layers. Exposing the patterns with large film-to-crystal distance increased the effects caused by lattice deformation. Corresponding to that the pin-hole pattern contained a fragments coming from different regions and the deformation components produced also some azimuthal rotation between these parts especially significant in the case of skew asymmetrical reflections.

As a representative result we present here the one which is characteristic for the implantation with light and heavy ions.

In the case of the light ion implantation where the defects are concentrated in the relatively thin layer the characteristic feature is a poor visibility of deformation effects. The lattice deformation effects were revealed in strongly overexposed patterns by activation of forbidden reflections due to lattice tetragonalization. The representative pattern is shown in Fig. 1. The longer line in the picture corresponds to the plane of diffraction. We may also notice additional distinct streak caused by the most deformed layer.

It was found that the long tail corresponding to the diffraction plane is produced by all interference effects caused either by crystal curvature or some lattice parameter gradients in the bulk crystal.

The second streak was visible only in the case of reflection corresponding to low indexed forbidden one.

The direction of this second contrast corresponds to the rotation of the diffraction vector along the intersection of the reflecting plane with the surface. That was confirmed by the theoretical simulation of the azimuths of these two kinds of contrast shown in Fig. 2.

Fig. 1. The pin-hole Bragg case spot of the silicon implanted with 1.6 MeV protons to the dose $2 \times 10^{17}$ cm$^{-2}$ in 602 reflection selecting 0.65 Å.

Fig. 2. The calculated directions of the two streaks visible in Fig. 1 for a fragment of the Laue pattern. The angle between two lines for 602 spot is the same as in Fig. 1.

In the case of heavy ion implantation no distinct shot-through layer is produced and the implanted layer forms a distinct spot translated with respect to the other parts of the image due to lattice deformation. It may be seen in Fig. 3. The three spots corresponding subsequently to the implanted layer, not implanted part of the epitaxy and to the substrate are located along one direction again corresponding to the rotation of the diffraction vector about the intersection of the reflecting plane with the surface.
Strongly overexposed spots revealed also some effects of diffuse scattering due to the lattice defects or thermal vibrations of the lattice. The present geometry enabled the determination of the layer responsible for diffuse scattering.

The work was supported from Polish-German cooperation POL-GER-N-100-95/BO (204/P-3).

REFERENCES:

SYNCHROTRON X-RAY INVESTIGATIONS OF $\text{Al}_x\text{Ga}_{1-x}\text{As}$ EPITAXIAL LAYERS IMPLANTED WITH Se IONS

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The implantation induced effects in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and other multi-element semiconducting compounds are interesting both in scientific and practical aspect. The formation of the implantation defects in this type of materials was described in some papers [1-4], but there is a practical need of amorphising dose evaluation for different practical applications.

In the present work, 1.5 MeV Se implanted $\text{Al}_x\text{Ga}_{1-x}\text{As}$ layers were studied with a number of methods, especially the Bragg-case section topography [5,6].

The high dose implantation with 1.5 MeV Se ions was performed at Rossendorf Research Centre in two series of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ epitaxial layers grown with MOCVD method. The first series of layers with $x=0.2$ were deposited on substrates cut from LEC grown undoped semi insulating crystal with the dislocation density greater than $10^7$/cm. The second series of layers with $x=0.45$ was deposited on substrates cut out from Bridgman grown crystal heavily doped with 0.3% indium and dislocation density not exceeding $10^7$/cm. The thickness of the epitaxial layers was close to 3 µm, and in the first stadium of the process the 0.2 µm undoped GaAs buffer layer was deposited.

A very narrow synchrotron white beam limited by horizontal 5µm slit was used, analogously as in [5,6]. Using film to crystal distances greater than 30 cm it was possible to reveal the effect of lattice deformation caused by relatively large lattice parameter differences between the implanted layer, $\text{Al}_x\text{Ga}_{1-x}\text{As}$ epitaxial layer and GaAs substrate.

Apart from section topography, the white beam experiments included also taking projection topographs and "pin hole" (micro Laue) patterns in the similar geometry.

The synchrotron monochromatic beam experiments included recording rocking curves in symmetrical 400 reflection of 1 Å radiation. The curves reveal the actual lattice parameter difference between the different layers, and seems be a necessary completion of the white beam experiments. The second series of samples, was examined also with conventional double-crystal spectrometer in CuKα radiation.

As may be noticed in Fig. 1 in the case of the sample from the first series implanted with the dose $8\times10^{13}$/cm$^2$ the patterns produced by narrow beam contained three well separated stripes.
Fig. 1. The pattern obtained using 5μm wide synchrotron white beam and 30 cm film to crystal distance in 533 reflection of 1.05 Å for Al\(_x\)Ga\(_{1-x}\)As sample with \(x=0.24\) implanted with 1.5 MeV Se ions at room temperature at the dose \(8 \times 10^{13}/\text{cm}^2\).

The splitting of stripes was caused by tetragonal deformation in the epitaxial and implanted epitaxial layer. As may be easily evaluated, the deformation in the implanted layer producing the uppermost stripe is more than four times greater than in the not penetrated part of the epitaxial layer producing the middle stripe. The lowest stripe comes from the bulk. The section pattern corresponded well with the rocking curves in 400 symmetrical reflection which exhibited three peaks. The highest of these peaks was situated on the low angle side and corresponded to the implanted region, the lowest middle to the not penetrated part of Al\(_x\)Ga\(_{1-x}\)As epitaxy and the most right to the GaAs substrate.

Despite high dislocation density the rocking curve of the first sample exhibited some traces of interference maxima. These fringes are much better visible in the case of second series of epitaxial layers. The obtained rocking curves point greater depth of lattice parameter changes than may be concluded from the TRIM-95 calculation providing of ion ranges 0.7 - 0.8 μm. Also the height of the implanted layer peak points that the lattice parameter seems be almost constant in the greater part of implanted layer.

The first attempts of theoretical rocking curve simulation were performed in the case of the second series of samples where the experimental curves were not affected by a high density of dislocations. It was not possible to obtain the correspondence between experimental and theoretical curves approximating the lattice parameter depth distribution profiles equal to vacancy distribution obtained with Monte-Carlo method similarly as in [5,6].

Fig. 2. a - The experimental rocking curve in slightly asymmetric 511 CuKα reflection taken in almost parallel arrangement with Ge monochromator for highly perfect Al\(_x\)Ga\(_{1-x}\)As epitaxial layer implanted with 1.5 Se ions to the dose \(6 \times 10^{13}\). b - The theoretical rocking curve exhibiting a good correspondence in the heights of the main maxima with the curve shown in a.

As may be seen in Fig. 2 a certain agreement was obtained assuming the diffusion of the defects - i.e. transforming the profile by numerical integration of the diffusion equation and then also flattening its maximal part close to the surface. The first operation increased the depth range of lattice parameter changes almost twice. The character of the necessary profile modifications shown in Fig. 3 is in a good agreement with the results of Xiong et al. [7] of theoretical rocking curves fitting in 2 MeV oxygen implanted GaAs.

Fig. 3. The comparison of vacancy distribution obtained for 1.5 MeV Se\(^+\) implantation into Al\(_x\)Ga\(_{1-x}\)As from TRIM 96 program (dashed line)
with a modified profile assumed in the calculation of the curve shown in Fig. 2 b (continuous line).

The work was supported by the Polish-German State Co-operation POL-GER-N-100-95/BO (204/P-3).

REFERENCES:

SYNCHROTRON X-RAY INVESTIGATION OF POROUS SILICON AND SILICON EPITAXY GROWN ON POROUS SILICON

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The interest in porous silicon is connected both with its physical properties and with perspective application in SOI (silicon on insulator) technology where the important point is the deposition of silicon epitaxial layers on the of porous layer. The most characteristic results reported by previous papers [1-4] is a significant increase of lattice parameter in the porous layer.

In the present paper porous layers of different porosity and epitaxial layers deposited on porous silicon were studied with a number of X-ray diffraction methods including the use of synchrotron Bragg-case section topography similarly as in [5,6]. They were prepared from highly boron doped crystals with the resistivity 0.02Ωcm. The porous layers were produced by electrochemical etching in HF solution, while the boundary part of the sample was masked by a seal. The samples differed in thickness of porous layers in the range 2-5 μm and in ratio of porosity in the range 30-50%. The slightly boron doped epitaxial layers were deposited by means of CVD method at 900°C with a growth rate 80 nm/min. The resistivity of the layer was close to 1Ωcm.

The Bragg-case section topographs were exposed using synchrotron white beam limited by horizontal 5 μm slit. The topographs were taken both at small 5-10 cm and at relatively large 23-50 cm film-to-crystal distances. In the first case the effect of different depth location of the subsequent layer and fine details of the interference fringes were studied. Comparing the exposure at small and large film to crystal distances it was possible to separate the effect of lattice deformation.

It should be noticed that presence of porous or epitaxial layer caused elastic bending of samples with thickness close to 400 μm. It is well known that bending causes formation of distinct long-range interference fringes in Bragg-case section pattern in silicon [6,7], absent in the case of flat samples.

The synchrotron multi-crystal investigations included recording rocking curves and taking topographs in symmetrical 333 reflection of 1 Å radiation. Less sensitive conventional double-crystal spectrometer studies with the Cu Kα radiation enabled comparison of rocking curves in different reflections. These experiments were performed in parallel set-ups with silicon monochromator. The rocking curves were recorded in 333, 531, 440, 400 and 422 reflections and in the case of asymmetrical reflections both in the geometry with lower and higher angle of incidence. This combination allowed to evaluate both the lattice parameter difference and the lattice deformation. In addition the observation of (110) and (111) cleavage faces was performed with the Zeiss Digital Scanning Electron Microscope 950. The cleavage faces perpendicular or slightly inclined to the surfaces were studied in high resolution secondary electron images. That allowed
direct measurement of the thickness of the subsequent layers and observation of the porous layer morphology.

Similarly as in [1-4] the rocking curves in porous silicon exhibited two peaks separated up to hundreds of angular seconds. The layer peak was usually wider and less regular than the substrate peak but in some stronger reflections e.g. 422 this difference was not very distinct.

In the Bragg-case section patterns the porous silicon produced additional stripe, separated mainly due to lattice deformation. The separation of the stripes increased proportionally to the distance film-crystal as may be seen in Fig. 1. In many reflections we observed the Pendellösung fringes, similar as in the case of bent single crystals, shown in Fig. 1 c.

The mechanism of fringe formation discussed by Chukhovski et al. [7] assumes the reflection of wave fields redirected by the lattice curvature from the back side of the entrance surface. It may be then expected that a rather irregular boundary of the porous layer retain similar reflecting possibilities as a well prepared crystal surface. In the case of epitaxy deposited on the porous silicon the Bragg-case section pattern contained again only two stripes. It was found that additional stripe is caused by reflection from the epitaxial layer and the separation is caused mainly by the depth location. The lack of the maximum due to the porous layer was also a characteristic feature of recorded rocking curves. The maximum due to the epitaxial layer was often affected by some systems of interference maxima. The explanation of that is high deformation of the delicate porous silicon layer, under the epitaxial deposit layer. The evidence of that was found in the strongest, overexposed reflections exhibiting large tails corresponding to much larger reflection range.

Fig. 1. The representative Bragg-case section patterns of 4.6 μm porous silicon layer with 50% porosity on (100) oriented silicon wafer. Similarly as in the Figs.2,3 the left parts of the topographs correspond to the area without porous layer. The contribution from the porous layer appears as a separate stripe in the upper part:

a - in 620 reflection of 0.6 Å and 7.5 cm film-to-crystal distance,
b - in the same reflection as in 1 a. and 33 cm film-to-crystal range.
c - in 115 1 reflection of 0.6 Å showing system of interference fringes characteristic for bent crystals.

The difference in lattice deformation between porous and epitaxial layers may be in particular proved by the rocking curves shown in Fig. 2. The lattice spacing difference between the porous layer and the substrate for the planes parallel to the surface evaluated from curve shown in Fig. 2a is 2.6 times greater than analogous difference for (440) planes inclined at 45° evaluated from the pair of curves shown in Fig. 2b and Fig. 2c. The analogous ratio for epitaxial layer should be close to 1.5. That proves that the lattice spacing in porous silicon decrease faster with the inclination of planes, and the planes steeper to the surface have smaller spacing in porous layer than in the substrate.

Together with subsidiary maxima in the rocking curves we observed interference fringes in the plane wave topographs of the epitaxial layers grown on the porous silicon as is shown in Fig. 3. The density of these fringes was dependent on the point of the rocking curve and they seemed to be connected mainly with the variation of porous silicon layer thickness. In some cases the fringes formed very irregular "fractal-like" patterns.
Fig. 2. Set of conventional double-crystal rocking curves in Cu Kα radiation of 4.6 μm porous silicon layer with a porosity 50% used enabling studying of lattice deformation:
a - in symmetrical 400 reflection,
b - in highly asymmetric 440 reflection with glancing angle $\Theta - \varphi = 8^\circ$,
c - in highly asymmetric 440 reflection with glancing angle $\Theta + \varphi = 99^\circ$, where $\varphi$ is the inclination of reflecting planes.

Fig. 3. Synchrotron double-crystal topograph in 333 reflection of 1.0 Å of edge fragment 2.3 μm of epitaxial layer on 4 μm porous silicon layer.

The work was supported by the Polish-German State Cooperation POL-GER-N-100-95/BO (204/P-3).

REFERENCES:

TEMPERATURE DEPENDENCE MEASUREMENT OF MANGANIN RESISTANCE

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2 Institute of Physics, Warsaw University of Technology

Manganin which is the Cu based alloy with an admixture of 2.5-3% of Ni and 11-13.5% of Mn, is commonly used as a convenient pressure gauge within the large range of values above about 100 MPa owing to the linear dependence of its electric resistance on pressure (see, for example, [1]). Nevertheless, the manganin resistance reveals acceptable weak temperature dependence within too narrow temperature interval only what may cause some systematic errors, difficult to be allowed for. So, attempts have been made to widen this interval using ion implantation techniques and some promising results were obtained so far at rather low doses of Ar and Xe ions, equivalent to the implanted ion concentration of about $10^{18}$ cm$^{-3}$ within the layers of thickness of 0.25 and 0.34 μm, respectively [2]. But the observed effect of a slight shift of the temperature dependence of manganin resistance after implantation (shown in the figure) should be studied with particular precautions taken to eliminate the influence of possible background factors and, first of all a non-uniformity of temperature regime during the measurements. Therefore, a simple computer controlled assembly satisfying the requirement of temperature stabilisation in the volume of manganin sample location has been developed and preliminarily tested. In the figure, in which our previous results are also depicted, the temperature dependence of nonimplanted manganin resistance is displayed showing a good consistence of all data. Further investigation is in progress.
Temperature dependence of the relative resistance of implanted and nonimplanted manganin slices [2]. Added are the results obtained using our temperature stabilisation assembly.

REFERENCES:
MAGNETIC STRUCTURE OF THE STRONTIUM - IRON - VANADIUM PEROVSKITE MONOCRISTAL

Janusz Ozimkowski, Jan Suwalski,
Institute of Atomic Energy

Experimental data are obtained for the antiferromagnetic < 256 K < ferrimagnetic single crystals Sr$_2$FeVO$_6$ by the Mössbauer technique. The strontium - iron - vanadium perovskite exhibits interesting properties, viz. the quantization axis of the spins of the iron ions changes direction by 90° in the range 265 - 380 K. The changes of the hyperfine interactions parameter: internal effective magnetic field, quadrupole splitting and isomer shift at the transition temperatures are studies in detail. The magnetic field $H$. $\downarrow$ drops abruptly by 0.6 Tesla on changes of spin quantization axis. Quadrupole splitting changes sign and magnitude from -0.208 mm/s for 78 K to +0.108 mm/s for 500K respectively and isomer shift IS changes linearly with temperature.

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Table 1. Mössbauer spectrum parameters changes with temperature.

A MOSSBAUER SPECTROSCOPY STUDY OF THE SPIN REORIENTATION TRANSITION IN Sr$_2$FeVO$_{6.5}$ PEROVSKITE

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Perovskites of the general formula ABO$_3$ have been the subject of intense investigation for many years. Recently, the subject of great interest have become double perovskites whose general formula is A' A'B'B'O$_6$, where the primes denote the possible involvement of different ions. The crystalline structure of these compounds has been rather well recognised [1], but much less is known about their magnetic properties which are the subject of this work. In general, magnetic properties of the compounds of this type are determined by the B cations. In double perovskites they can be arranged in three types of sublattices namely: random, rock salt and layered.

Detailed studies of magnetic properties of the Sr$_2$FeVO$_{6.4}$ (0≤δ≤0.4) double perovskite are reported in ref. [2, 3]. This compound of a distorted perovskite structure with orthodrom-bic symmetry is ferrimagnetic with the Neel temperature of about 753K and a hard magnetic material with magnetic heterostructure [2]. Considerable oxygen deficiency appears in particular in the good homogeneity samples of Sr$_2$FeVO$_5$ called shortly SFVO of monoclinic symmetry which have been fired at high
temperatures. In these materials iron and vanadium ions are only trivalent. This compound for $\delta<1$ is antiferromagnetic with the Néel temperature of 910 K [6] and below this point is shows weak ferrimagnetism and the reorientation transition temperature of about 264 K at external field 0.42 T [5,6]. This paper raports direct observation of the AFM$\rightarrow$WFM transition in SFVO by Mössbauer effect study.

The preparation of Sr$_2$FeVO$_6\delta$ ($\delta<1$) single crystals and magnetic data are described in refs. [4-6]. Prior to the Mössbauer spectra recording, the samples were ground to fine powder. The Mössbauer equipment of conventional transmission type with a $^{57}$Co(Rh) - 50mCi source and krypton filled proportional counter was used. Calibration spectra were recorded for a natural α-iron foil (25µm) at room temperature. The optimum absorber thickness was established to be 68 mg/cm$^2$ of the coarsely powdered small monocrystals. The temperatures from the range 78K to 500K were secured with the use of the liquid nitrogen cryostat and the furnace. The sample heat treatment in vacuum at 500K was proved to have no influence on the Mössbauer spectra of SFVO.

Mössbauer spectra of SFVO have been taken in temperatures from 78K to 500K. The spectra taken at $T<265K$ and $T>380K$ show the normal Zeeman sextet split while for $265K < T < 380K$, the range covering the Morin transition [5,6], the spectra reveal the superposition of two hyperfine - split sextets whose amplitude changes with temperature are shown in Fig. 1. The temperature dependence of the effective magnetic field at the nucleus ($H_{\text{eff}}$) and the quadrupole splitting $Q.S.$, are shown in Fig. 2 and Fig. 3.

Distinct separation of sextets in the region of transition 265K$< T < 380$ K as well as the rapid changes in the value and sign of the quadrupole splitting indicate the coexistence of magnetically ordered phases with spin oriented at the $0^\circ$ or $90^\circ$ to the b axis. Below the spin transition temperature $T_{\text{M}}=265K$ the spins point along the b axis which means $\theta = 0^\circ$. Above 380 K the spins are perpendicular to the b axis and $\theta = 90^\circ$.

A rapid change of $H_{\text{eff}}$ near the Morin transition temperature is clearly visible. The effective magnetic field in SFVO is suddenly reduced by 0.6 T on heating of this material through the transition temperature. The quadrupole splitting near the spin transition region decreases with temperature. Such a course has often been observed in compounds containing Fe$^{3+}$ [7]. It is reasonable to assume that all internal distances change in proportion to the changes in the length of the a-, b- and c-axes, the phenomena is known as homogeneous contraction [8,9]. As a consequence, the thermal expansion is highly anisotropic. Therefore, the ion positions along the a-axis change more rapidly with temperature than along the b- and c-axes [10]. A sudden change of the lattice parameters of the crystal at the Morin point indicates that the reorientational transition in SFVO does not occur by smooth change of the spin positions but the spin rotation is jumpwise. The reorientational spin transition observed for SFVO by ME effect indicates the presence of a disordered distribution of equivalent iron and vanadium ions in the crystal lattice which is responsible for the diffused character of the transition. The first order transition in SFVO observed by AFMR experiment [5] and magnetic measurement [6] at $T_{\text{M}}$ explained in terms of Dzialohinsky-Moriya interaction should be accompanied by a change in slope of the temperature dependence of I.S. However, the difference in the slopes in the regions 240-260K and 295-380 K viz. $-7x10^{-7}$ mms$^{-1}$K$^{-1}$ and $-8.4x10^{-7}$ mms$^{-1}$k$^{-1}$, respectively can hardly be called significant. The expansion of the lattice and monoclinic distortion resulting from the deficiency of oxygen reduces the covalent contribution of the anions to the 3d levels of iron and vanadium. Introduction of anion vacancies to the perovskite structure is manifested as a quadrupole splitting of Fe$^{3+}$ and V$^{3+}$ ions.

![Fig. 1. Normalised amplitude of M.E. sextets $I_1$ and $I_2$.](image-url)
ON THE ENERGY STRUCTURE OF $C_{60}$Fe COMPLEX

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Iron was introduced into fullerites by diffusion and decomposition of ferrocene at elevated temperatures. In order to identify iron ions we applied the Mössbauer spectroscopy at various temperatures. The results suggest that the ionisation of Fe depends on the temperature.

To the most striking effect belong the non-monotonous dependence of the quadrupole splitting on the temperature. The properties are discussed on the grounds of a simple model derived from the energy structure calculated in the extended Hückel approximation.
An original method of evaluation of the cluster population in carbon martensite has been developed [1]. Using this method it was shown that the Kurdiumov's model of a carbon redistribution within the different octahedral site sublattices can quantitatively account for both observed normal and abnormal tetragonality in carbon martensite. It was also shown that an existence of the internal strains in martensite constitues a necessary and sufficient condition for the energetic preference of tetrahedral site over the cubic one. The presence of the residual tetragonal distortion in the quasi-cubic phase of \( \kappa \)-martensite is associated with the presence of the mixed clusters formed of the atoms belonging to \( \Omega_c \) sublattice as well as to remaining ones.

The long - range ordering parameter \( \eta \) is associated with the mean carbon concentration on sublattice \( C(O_{a}) \), \( C(O_{b}) \) and \( C(O_{c}) \) by the following relations :

\[
C(O_{a}) = C(O_{b}) = C(1-\eta)/3
\]

(1)

\[
C(O_{c}) = C(1+2\eta)/3
\]

On the other hand, the internal energy, may be expressed as:

\[
U = N \sum V_n C_n
\]

(2)

where: \( V_n \) - binding energy per atom,

\( C_n \) - probability that a given atom belongs to cluster \( n \)

\( N \) - total number of iron atoms.

Taking into account eq. (1) and the law of conservation of the total number of particles in the sublattices, we obtain:

\[
\Sigma_{(a)} C_{a} + \Sigma_{(b)} (a_{\gamma}/n_{\gamma}) C_{\gamma} = C(1+2\eta)/3
\]

(3)

\[
\Sigma_{(b)} C_{b} + \Sigma_{(c)} b_{\gamma}/n_{\gamma} C_{\gamma} = C(1+2\eta)/3
\]

where the subscript \( a \) labels the clusters composed of the atoms located in \( O_{a} \) or \( O_{b} \) sites. The \( \gamma \) subscript labels the mixing of the atoms in \( n \)-particle clusters with \( a_{\gamma} \) atoms in \( O_{c} \) and \( b_{\gamma} \) atoms in \( O_{a} \) or \( O_{b} \) sublattices.

The entropy \( S \) can be expressed as:

\[
S = S_{L} + S_{sh}
\]

(4)

where \( S_{L} \) is the entropy connected with long-range ordering, \( S_{sh} \) the entropy connected with short-range ordering. Taking into account eq. (1), the entropy \( S_{L} \) can be expressed as:

\[
S_{L} = kN(1+2\eta)/3 \ln C(1+2\eta)/3 + (1-C)/3 \ln C(1-C)/3 + 2(1-C)/3 \ln C(1-C)/3
\]

(5)

The entropy \( S_{sh} \), may be obtain in the form:

\[
S_{sh} = -kN \Sigma (a\alpha) R_{\alpha} \ln (1-C_{a}/R_{\alpha}) + \Sigma (b\beta) R_{\beta} \ln (1-C_{b}/R_{\beta}) + \Sigma (c\gamma) C_{\gamma} \ln (1-C_{c}/R_{\gamma})
\]

(6)

where \( R_{\alpha} \beta \gamma \) are numbers of possibilities of rotations transforming a given cluster into another one. Concentrations \( C_{a} \), \( C_{b} \) and \( C_{c} \) must satisfy the equation (3). For equilibrium state, from the condition of minimum free energy, we have a system of equations from which all order parameters can be derived. Omitting technical details of calculations we obtain:

\[
C_{a}/(R_{a} - C_{a}) = N_{1} \exp(-V_{a}/kT)
\]

\[
C_{b}/(R_{b} - C_{b}) = N_{2} \exp(-V_{b}/kT)
\]

(7)

\[
C_{c}/(R_{c} - C_{c}) = (N_{1})^{\alpha\gamma}/(N_{2})^{\beta\gamma} \exp(-V_{c}/kT)
\]

where normalization constants \( N_{1} \) and \( N_{2} \) can be found numerically using jointly eq.(7) and eq.(3).

REFERENCES:

CLUSTERS IN CARBON MARTENSITE. PART II.
THE MARTENSITE IN NON-EQUILIBRIUM STATE

Ludwik Dąbrowski
Institute of Atomic Energy

Table 1.

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By using a computer simulation of the dynamical behavior of carbon martensite approaching the thermodynamical equilibrium, it was found that the ultimate state of this system is strongly beyond the thermal equilibrium [1]. Even after long-term aging, the free energy is far beyond the minimum value allowed for this system. The reason for such a behavior and the possible aging processes proceeding in this system are discussed on the molecular level. All the ordering parameters are affected by aging process. However, the evolution proceeds in the distinctly different time intervals for different parameters. At first, the long-range ordering parameter which determines the tetragonality of martensite evolves and reaches the stable value. In the next stage, a formation and then disintegration of the two-particle clusters occurs. Disintegration of two-particle clusters coincides with the stage when three-particle cluster formation occurs at a high rate. Three-particle clusters also disintegrate when some time elapses. The same pattern repeats as regards four-, five-, six-, seven-, and eight-particle clusters. To simplify the calculations, the nine-particle clusters are assumed to be the largest possible and are identified with an existence of superstructure. The formation of 100% of nine-particle clusters with no contribution of free atoms in an alloy stops all aging processes. The evolution of these processes is illustrated graphically in the time range from 16 seconds to 1500 years, as estimated on the basis of experimental data.

Table 1. Type of clusters and their building energy per atom (column 8). Column 1 - the order of clusters, column 2 - their symbol, according to [1], column 3 - basic initial cluster, columns 4 - 7 - lattice positions of atoms r, -r, m, bound in a given cluster. Lattice positions are determined with respect to the first carbon atom located at (000) position in O sublattice.

REFERENCES:
MÖSSBAUER STUDIES OF THE MAGNETIC OSCILLATOR COUPLING IN Li-Ti-Zn INDUCED BY EXTERNAL MAGNETIC FIELD

Sylwester Ligenza, Jerzy Ozimkowski
Institute of Atomic Energy

A self-assembled magnetic cellular structure arises in Li-Ti-Zn ferrite during annealing at about 800 K, as a result of thermal diffusion of ions and of the tendency of the system to reach a minimum of free energy. The linear dimension of cells is about 14 nm. The magnetic cells are separated by walls having the average dimension of 1 nm [1-3]. These magnetic cells have increased concentration of paramagnetic ions relative to walls, which contain mainly the diamagnetic ions. Taking into account these data and the information from neutron measurements, the average value of magnetic moment of cells was calculated as $M_c = 6350 \mu_B$.

The phenomenon of appearing of self-assembled magnetic cellular structure in Li-Ti-Zn ferrite, was discovered by neutron scattering and Mössbauer effect measurements [1-3]. The appearing of the self-assembled magnetic cellular structure is observed for the first time in the crystal structure of magnetic materials.

During the analysis of the neutron depolarisation measurements [4-5] the existence of perpendicular magnetisation induction $<B>_\perp$ was observed at room temperature and interpreted as due to the appearing of correlated dipole interactions between magnetic moments of cells. The external magnetic field induced the correlated magnetic oscillator coupling between cells. It was established that maximum of $<B>_\perp$ appeared at external magnetic field $H_{ex} = 44$ Oe.

It was found that perpendicular component of magnetic induction $<B>_x$ induced by external field is described by the formula:

$$<B>_x = ((<B>_z^2 + <B>_\parallel^2)^{1/2} / [1 + k(H_{ex} - 44)^4])$$

(1)

where $<B>_z = 424$ G, and $k$ is the fitted parameter obtained as 0.0625 [4]. The determined values of $<B>_\parallel$ and $<B>_\perp$ versus external magnetic field $H_{ex}$ are given in [4]. The correlated magnetic oscillator coupling between magnetic cells in crystal structure of solid state was observed for the first time and is similar to the oscillator coupling observed in biology [6,7].

The Mössbauer effect investigations on this ferrite system was carried out in order to study the influence of external magnetic field $H_{ex}$ on the intensities of Mössbauer Zeeman lines. It is known that relative intensities of Zeeman lines depend on the direction of magnetisation of sample relative to the direction of gamma rays:

$I(1,6) = 9/4 (1 + \cos^2 \Theta)$

$I(2,5) = 3 \sin^2 \Theta$

$I(3,4) = 3/4 (1 + \cos^2 \Theta)$

(2)

where $\Theta$ is the angle of magnetisation relative to the gamma rays. In the case of $H_{ex} = 0$ the direction of the magnetisation of sample would be random so the average square of $\cos \Theta$ is equal $<\cos^2 \Theta> = 1/3$ and relative intensities are

3:2:1 for $I(1,6)$: $I(2,5)$: $I(3,4)$

(3)

respectively.

Measurements were made for the external field $H_{ex}$ to perpendicular the gamma rays (parallel to the plain of absorber). In this geometry the demagnetisation coefficient of sample was negligible. It was expected that the appearing of the perpendicular component of magnetic induction $<B>_\perp$ with the maximum at 44 Oe would influence the intensities of Mössbauer lines. In the present measurements the intensities of Zeeman lines $I(1,6)$ and $I(2,5)$ were measured as a function of $H_{ex}$ at room temperature. The Mössbauer measurements at 78 K and 293 K for Li-Ti-Zn ferrite cellular system are given in Fig. 1.

Fig. 1. Comparison of Mössbauer effect measurements at 78 and 293 K for $H_{ex} = 0$. 
It can be seen that the Zeeman lines at 78 K are well separated and their relative intensities I(1,6): I(2,5): I(3,4) are 3:2:1 respectively, like expected from the theory. At 293 K the Zeeman lines are much perturbed by superparamagnetic relaxation of magnetic cellular structure. The lines are broadened and their intensities decrease.

Fig. 2 presents the relative intensities of I(1,6) and I(2,5) at 293 K (given as points) measured versus external magnetic field from $H_\text{ex} = 0$ to $H_\text{ex} = 100$ Oe.

Fig. 2. Experimental relative intensities of Mössbauer Zeeman peaks versus external magnetic field.

The experimental points were scaled relative to the intensities of I(3,4) taken as 1. As it is seen from Fig. 2 the intensities I(1,6) and I(2,5) at small $H_\text{ex}$ are not as 3 and 2 respectively.

In Fig. 3 the theoretical intensities of I(1,6) and I(2,5) are compared with experimental ones as a function of $H_\text{ex}$. The relative intensities were calculated taking into account the parallel $<B>_\parallel$ and perpendicular $<B>_\perp$ components of magnetic induction [4]. The resulting magnetisation was computed as a vector sum of above magnetic induction components. The angle $\Theta$ between resulting magnetisation of sample and gamma direction was calculated as a function of external magnetic field and substituted into equations (2). As a result, the dependence of relative intensities I(1,6) and I(2,5) versus $H_\text{ex}$ were obtained and presented in Fig. 3 as a solid lines.

The experimental points in Fig. 3 were adapted to the theoretical ones at high values of external field.

Fig. 3. A comparison of experimental and theoretical relative intensities of Mössbauer Zeeman peaks versus external magnetic field.

As it is seen in Fig. 3, the appearing of perpendicular component of magnetic induction $<B>_\perp$ (caused by external field in magnetic cellular structure) with maximum at $H_\text{ex} \approx 44$ Oe is confirmed by Mössbauer intensity measurements. The disagreement between experiments and theory at low $H_\text{ex}$ is connected with superparamagnetic relaxation of magnetic moments in magnetic cellular structure. The relative intensities at $H_\text{ex} = 0$ are not 3:2 for I(1,6): I(2,5), respectively, contrary to the measurement made at 78 K. This disagreement between Zeeman relative intensities for Li-Ti-Zn sample at room temperature may be connected with the value of $<\cos^2\Theta>$ different from 1/3. It may be due to the existence of cellular magnetic structure.

REFERENCES:
STRUCTURE OF METHYL 4-C-(2,5-DIMETHOXY-4-METHYLPHENYL)-
2,3,6-TRIDEOXY-α-L-ERYTHRO-HEX-2-ENOPYRANOSIDE

Osman Achmatowicz 1, Barbara Szechner 2, Jan K. Maurin

1 Institute of Atomic Energy
2 Pharmaceutical Research Institute, Warsaw

The crystal and molecular structure of the title compound shown in Fig. 1 was synthetized as one of the products during our studies on addition of organolithium reagents to some carbohydrate enones.

Fig. 1. The Ortep view [1] of the molecular structure with atomic numbering and 30% probability ellipsoids for non-H atoms.

This reaction was interesting as the important part of the new route of the total synthesis of anthracycline antibiotics e.g. daunomycin or adriamycin.

REFERENCES:

MOLECULAR RIBBONS COMPOSED OF CALCIUM ATOMS BRIDGED BY CARBOXYLATE OXYGENS IN THE X-RAY STRUCTURE OF CALCIUM COMPLEX WITH 3-AMINOPYRAZINE-2-CARBOXYLIC ACID

Janusz Leciejewicz 1, Halina Ptasiewicz-Bąk 1, Beata Paluchowska 2

1 Institute of Nuclear Chemistry and Technology
2 Institute of Atomic Energy

Coordination compounds of 3d metals, uranyl, calcium, strontium and barium with pyrazine-2-carboxylic acid (PZCA) show the same coordination scheme: the central ion is chelated by a heteroring nitrogen atom and an oxygen atom belonging to the nearest to it monodentate carboxylic group. In all the above complexes two pyrazinic acid molecules are bonded to the metal atom forming monomeric molecules with the characteristic for each central ion coordination completed by water molecules. Monomeric molecules have also been found in the structure of magnesium complex with 3-aminopyrazine-2-carboxylic acid (APZC), however, the study of the crystal structure of the calcium complex of the acid revealed entirely molecular pattern.

The crystals of monoaquabis(μ-3-aminopyrazinato) calcium(II) are monoclinic, space group Cc, a=22.785(5), b=6.367(1), c=9.906(2) Å, β=110.58(3)°, Z=4.
Fig. 1. The first coordination sphere of Ca atom in monoaquabis (μ-3-amino - 2-pyrazinato) calcium(II).

In contrast to all up to now studied complexes of divalent ions with pyrazinic acid and magnesium complex of APZC, which in crystals appear as monomeric molecules, the structure of calcium aminopyrazinate is polymeric. It is composed of molecular ribbons propagating in the c direction of the unit cell. A fragment of the ribbon with full coordination sphere of Ca cation is displayed in Fig. 1. The packing diagram viewed along the b axis is displayed in Fig. 2. Each calcium atom is coordinated by two aminopyrazinate molecules situated on the same level via their heteroring nitrogen atoms and nearest to them carboxylic oxygens. The Ca-N and Ca-O bond distances are typical for calcium complexes and amount to 2.594 Å and 2.385 Å, respectively (average values). An oxygen atom belonging to a water molecule is attached to each calcium ion at a distance of 2.344 Å. The maximum deviation from the mean plane defined by the calcium ion, the water oxygen and the coordinated carboxylate oxygens and nitrogen atoms is 0.48(1) Å. Two more oxygens are coordinated by the calcium ion: one of them is above this plane with Ca-O distance of 2.360 Å, the other one below with Ca-O bond length of 2.363 Å. They belong to the carboxylic groups located on the adjacent planes above and below and thus act in bridging manner producing a molecular ribbon. These Ca-O contacts are almost collinear, since the O12-Ca-O21 angle is 169.6 °. Thus the coordination polyhedron around the calcium ion is a distorted pentagonal bipyramid. This coordination represents entirely different geometry from that observed in calcium pyrazinate\(^3\); its monomeric molecule consist of two pyrazinic acid moieties attached to calcium ion via the heteroring nitrogen and the oxygen atoms of the nearest to it monodentate carboxylic group. Four water oxygens complete the coordination of dodecahedron. The polymeric structure of the title compound might be brought about by the presence of steric disturbance introduced by the aminogroup, which activates the carboxylic group to act as a bidentate. The second heteroring nitrogen atom does not participate in direct bonding the central ion indicating that the aminogroup does not influence its activity for coordination.

The geometry of pyrazine rings as well as the carboxylic and amino groups is close to that found in APZC itself\(^4\). The mean plane of pyrazine ring makes a dihedral angle of 53.7(8) °. With the mean plane of pyrazine ring, (see Fig. 1) the dihedral angles between planes of the carboxylic moiety and the pyrazine ring in the aminopyrazinate molecules and pyrazine ring are 13.9(8) ° and 14.6(8)°, respectively. The ribbons are held by a system of hydrogen bonds in which the water molecule coordinated by the calcium ion plays a significant role. Hydrogen bonds of 2.71(1) and 2.74(1) Å link the water oxygen with carboxylate oxygens in the adjacent ribbons. Weak interactions joining heteroring nitrogens with aminogroup nitrogens of neighboring molecules can be also recognized by their lengths of more than 3 Å.

Fig. 2. Packing diagram of Ca(APZA)\(_2\)H\(_2\)O structure viewed along b axis.

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DIMERIC MOLECULES OF CO(II) AND Zn(II) COMPLEXES WITH FURAN-2-CARBOXYLATE LIGANDS STABILIZED BY THE SYSTEM OF INTERCONNECTED C-H-O WATER HYDROGEN BONDS

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2- and 3-furancarboxylic acids (denoted hereafter as 2-FCA and 3-FCA) as well as many of their compounds are of interest due to their natural derivation and biological activity[1]. Also some 3d metal complexes of 2-FCA and 3-FCA exert antimicrobial activity against a number of gram+, gram- bacteria and fungi[2]. The X-ray diffraction of calcium[3], strontium[4], and barium[5] complexes of 2-FCA have confirmed that during the process of coordination, also the furan ring oxygen takes part also in chelating the central ion. In the case of 3-furancarboxylate complexes of Ca[6], Sr[6] and Ba[5], where direct O-F-metal contacts are sterically impossible, the oxygen from the furan ring reveals their electron donor properties acting as acceptors in C-H-O hydrogen bonds system. Complexes of divalent cations with 2-FCA and 3-FCA show also that the first coordination sphere of metal ion is usually build up not only from 2-or 3-furancarboxylate anions but from the water molecules as well. Apart from the carboxylate groups of respective anions, these molecules act in some compounds as bridging ligands giving rise to a variety of coordination schemes. In the uranyl furoate[7], hydroxo bridged dimers linked through carboxylate ligands form extensive molecular chains. In the complexes with magnesium[8], the Mg²⁺ cations are linked via water molecules. On the other hand, in the nickel 2-furoate[9] the nickel atom is coordinated by five oxygens from water molecules and one oxygen donated by a (FCA)⁻ anion acting in the monodentate mode. The second (FCA)⁻ ligand (the same geometry within the e.s.d. of all bonds and angles as the first one) is bonded to the [Ni(H₂O)₆(FCA)]⁺ cation via hydrogen bonds only. Thus, it is worth to emphasize the great importance of the water molecules and variety of hydrogen bond types for their role in steering molecular association in the furancarboxylate complexes. The careful analyze of the crystal structures of compounds which engage π-electrons in its bonding system (aromatic and unsaturated compounds), collected in the Cambridge Structural Database[10], leads to the conclusion that two cases of O-H-π interactions clearly extends beyond van der Waals separations. One of them is of T-shape type, reported lately among the terminal terminal alkynes[11]. The second one is similar to the O(C)-H-π interactions in aromatic compounds where O-H vectors are nearly orthogonal to the centre of aromatic ring, gaining the contacts with the centre of π-electron system. A survey of CSD reveals a number of hints where O-H-π hydrogen bonds seem to influence packing arrangement of the molecules in which five-membered, unsaturated ring is a structural element (cyclopentadien, furan, thiophene, pyrrole). Among the crystal structure of the compounds comprising furen ring there are at least 17 cases in which one can pointed out an orthogonal approach of the O-H vector towards the centre of the π bond, indicating T-shape type of interaction. Significantly less examples of this type of contacts are among the compounds with pyrrole or thiophene ring. Cyclopentadienyl rings exhibits rather these type of O-H-π interactions which is attributed to the aromatic moieties (the O-H vector directed to the midpoint of the ring). The results of database search can be explained by the effecting the π-electron density distribution within the ring due to the presence of heteroatom of certain electron structure[1]. It thus shows direct dependence of the existence and geometry of O-H-π hydrogen bonds on kind of heteroatom build in the ring. As the furan ring is significantly less aromatic than benzene and exhibits more localized system of π-electrons, in the case of compounds comprising furan, thiophene and pyrrole ring, the most favorable geometry of these bonds is one in which O-H bond is nearly normal to the C=C double bond edge of ring. As most biological systems encounter an aqueous environment during their normal functions, the interaction of water molecules with aromatic moieties is of great importance[12]. It was therefore of interest to examine other structures of metal furoates where
water molecules are build in to the coordination sphere or acts as a solvation shell of the complex. The results of the experiments carried out for cobalt and zinc compounds are reported in this study.

The crystals of both title compounds are isomorphous (Fig.1). They consist of dinuclear molecules with distorted octahedral environment. The Col - Co2 and Zn1 - Zn2 intramolecular distances are 3.483(2) Å and 3.505(2) Å, respectively. The coordination around the Co1 and Co2 as well as around Zn1 and Zn2 involves four oxygen atoms donated by FCA ligands and two oxygen atoms from water molecules. However, the Co1(Zn1) and Co2 (Zn2) environments differ in the way in which the bonding of one FCA anion is accomplished. While in the case of Co1 (Zn1) the ligands denoted as FCA1 are monodentatedly bonded to the respective cation, in the case of Co2 (Zn2) these FCA3 anions are bonded in bidentate way. Moreover, the FCA2 ligand bridges the metal ions in the O-O,O mode, while the remaining two ligands, FCA2 and FCA4 bridge the respective cations in the O:O mode. The geometry of all FCA ligands is not affected by the process of coordination, since all of them remain planar within their e.s.d and the bond distances and angles within the furan ring fit reasonably well to those reported for the furan-2-carboxylic acid. The Co-O bond distances range from 2.034(3) to 2.206(3) Å and Zn-O from 2.003(3) to 2.221(3) Å, typical for the coordination compounds of the respective metals. The angles O-Co1(Zn1)-O and O-Co2(Zn2)-O indicate that the coordination deviates from perfectly octahedral. Obviously, the coordination around Co2(Zn2) is more distorted than around Co1(Zn1) due to the steric conditions imposed by the observed bridging mode of the FCA3 ligand.

Both structures are stabilized by a system of interconnected hydrogen bonds. All water molecules are involved in intra- and intermolecular interactions acting as proton donors either to carboxyl oxygens of the adjacent ligands or to the symmetry related molecules of solvation water. Three of them (O3, O5, O6) act three times as donors taking part in one normal and one bifurcated (H30, H50, H6) hydrogen bonds. Moreover O5 molecule participates in the Owater - H⋯π hydrogen bond system, where C41 and C51 furan ring carbon atoms serve as acceptor of H51 atom. The geometry of this interaction is nearly the same as in the other structures collected in CSD[10]. (Owater-H vector nearly orthogonal to the C=C bond). The distances from the H5 atom to the center of the C41 - C51 π bond are 2.28 and 2.27 Å for the cobalt and zinc compounds respectively. In the case of FCA2 and FCA3 ligands, the furan ring oxygens (O32 and O33) act as acceptors for the H atoms. The packing of dimeric molecules in the crystal suggests also the existence of weak C-H⋯O contacts in which the C-H⋯Owater and C-H⋯Ocarboxyl are involved with interaction distances in the range from 3.08 to 3.49 Å. The existence of so complicated hydrogen bonds network is probably due to a cooperative effect with an O-H⋯O and C-H⋯O interactions of various types. In each structure heteroatoms from the furan rings play a significant role in creating this network.

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THE CONFORMATION RELATED REACTION EFFICIENCY OF GLUTARIMIDES WITH PHENYLLITHIUM. X-RAY AND THEORETICAL STUDY

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In the course of our synthetic evaluation of the reactivity of organolithium compounds towards substituted glutarimides, it has been found [1, 2] that phenyllithium reacts with polimethyl-substituted glutarimides to form products whose structures depend on the number of the methyl groups attached to the imide ring. When glutarimide (1) itself was used as a substrate, a ketoamide (2) was found to be the only product. With traces of acids it dehydrated quantitatively forming an enamide (3).

Fig. 1. Reactivity of various glutarimides with phenyllithium.

Treatment of 4,4-dimethylglutarimide (4) with phenyllithium caused the formation of two compounds (5) and (6) in approximately 1:1 ratio, being in relatively fast tautomeric equilibrium. Addition of acids, even in trace amounts, accelerated the equilibration, causing also the dehydratation into a final enamide (7). The structures of both tautomeric compounds (5) and (6) were established on the basis on their spectroscopic examination (1H NMR) upon their separation in pure forms [2].

When 3,3,5,5-tetramethylglutarimide (8) was reacted with phenyllithium, a single compound (9) was formed in 95% isolated yield [2]. The yield of the product (9) is much better than in the case of compounds (3), (5) and (6), proving a higher susceptibility of the imide carbonyls in (8) for a nucleophilic attack. The cyclic form of (9) was proposed by comparison of its 1H NMR spectrum with the spectra of tautomers (5) and (6).

The fact of increasing stability of the cyclic structures of the products derived from imides (1), (4), and (8) can be rationalised in terms of gem-dialkyl groups stabilisation known as the Thorpe-Ingold effect (Eliel, 1962).

X-ray structure determinations of 3,3,5,5-tetramethylglutarimide (8) and 2-hydroxy-2-phenyl-3,3,5,5-tetramethyl-6-piperidone (9) were performed in order to assure the ring structure of (9) as well as to evaluate the reasons for the relatively high reactivity of imide (8) with the organolithium reagent.

Different glutarimides represent a class of attractive starting materials in the synthesis of 2- and/or 6-substituted piperidines by means of the reaction of imide carbonyl groups with Grignard or organolithium compounds. However, when the use of N-protecting group is omitted, the first reaction to occur is the salt formation, in which the negative charge at the N atom diminishes the electrophilic character of the carbonyls. That
accounts for low to intermediate yields of these reactions [3]. Contrary to these results we found that compound (8) reacts with phenyllithium giving product (9) in virtually quantitative yield. That difference may be attributed to the presence of neighboring *gem*-disubstituted carbon atoms in (8). Indeed, there are some literature indications of unexpected increase of reactivity of the carbonyl group at C-2 in 3,3-dialkylsuccinimides [4].

Structure of (8) is monoclinic P2₁/c, \(a=7.715(2), \ b=11.136(2), \ c=11.707(2) \ \text{Å}, \ \beta=105.63(3)^\circ\). The molecular geometry is shown on Fig. 2.

![Fig. 2. Molecular geometry of structure (8).](image)

The structure of 2-hydroxy-2-phenyl-3,3,5,5-tetramethyl-6-piperidone (9) is triclinic P-1 \(a=6.1685(6), \ b=11.1475(10), \ c=11.526(2) \ \text{Å}, \ \alpha=117.100(10), \ \beta=103.390(10), \ \gamma=91.288(7)^\circ\). Fig. 3 shows its molecular geometry.

![Fig. 3. Molecular geometry of (9).](image)

Since the different methyl-substituted glutarimides give products with the substantially different efficiencies, we looked more closely into their geometries searching for the reason for this effect. The first look at the bond lengths of structures of glutarimide (1) [5], 4,4-dimethylglutarimide (4) [6] and the present structure of 3,3,5,5-tetramethylglutarimide (8) gives no answer. The bond lengths as well as the bond angles differ only slightly. However, a more careful analysis reveals some discrepancies. Although the fragment N, C2, C3, C5, C6 (in the notation used in this paper) is planar in structures of glutarimide and its 4,4-disubstituted derivative (rms deviations 0.008 and 0.015 Å), it is significantly less planar in the present structure (rms deviation 0.069 Å). The differences in carbonyl O atoms positions with respect to those planes could also be seen. In non-substituted glutarimide they are almost in the plane whereas in disubstituted derivative they deviates more and in tetrabstituted are distinctly out of plane. Those findings made us study this problem further, especially because of the observed disorder in structure of 3,3,5,5-tetramethylglutarimide which might suppress a little bit the results. We used the crystallographic results as the starting points for the geometry optimization in terms of *ab initio* quantum chemical calculations.

The molecular structures of glutarimide (1), 4,4-dimethylglutarimide (4) and 3,3,5,5-tetramethyl-glutarimide (8) were optimized using three different methods: RHF SCF method with the standard basis 6-31G**, MP2 method with the basis 6-31G** which involves two electron correlations and also the DFT formalism with the B3PW91 functional. All methods gave the similar results confirming the X-ray structural results and showing that 3,3,5,5-tetramethylglutarimide is the least planar molecule of three glutarimides studied. The calculations prove also that in the tetrabstituted derivative both carbonyl oxygen are displaced from the plane defined by N, C2, C3, C5, C6 atoms. The MP2 method gives the best restoration of the conformation for all three X-ray structures.

The comparison of both crystallographic results and the quantum chemical calculations for glutarimides lead to the conclusion that in 3,3,5,5-tetramethylglutarimide the carbonyl groups are rotated slightly around respective N-C bonds making their positions less favorable to participate in conjunction with the two 2p electrons of the nitrogen atom. This explains the larger negative charges located on the O and N atoms with increased positive charges on both carbonyl carbons. Such separation of partial charges in the carbonyl group should result in higher reactivity of this compound towards substitution.
REFERENCES:

STRUCTURE OF (S)-(1-PHENYL)ETHYLAMMONIUM (R,S)-4-CYANO-2-ETHYL-2-(4-NITROPHENYL)-HEXAMOATE DOUBLE SALT

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The title structure is monoclinic P21 with a=7.200(3), b=13.998(3), c=20.724(4) Å, β=97.17(3)°. The salt of the racemic cyanoacid with the chiral amine was synthesized with the intention to obtain crystals of pure enantiomeric form of the acide. This is one of the well known methods used for separation enantiomers [1]. This method failed, however, this time. The unit cell of the double salt is composed of 4 molecules of protonated base, 4 anions of acid (two of each enantiomer) and 2 molecules of water. Although the intensity statistics pointed to the noncentrosymmetric space group, the unit cell content resemble the centrosymmetric case with one base and one acid molecule in the asymmetric part of the unit cell with the coordinate system shifted by the vector [0.25, 0, 0.25] and P21/n symmetry. The similarity of both structures depend not only on the number of molecules in the unit cell but also on enantiomeric content of the crystal. As far as all amine molecules are (S) enantiomers, the unit cell contain racemate of the acid [two (R) and two (S) enantiomer molecules]. Moreover the geometry of protonated amino group -NH3+ resembles the methyl group, and this makes similar (S) and (R)-enantiomers of amine. The difference between P21 and P21/n cases is the content of water - the asymmetric part containing only one water molecule. Fig. 1 shows the view of the part of the crystal lattice displaying all types of hydrogen bonds (shown as the dashed lines). For the clarity of the drawing, all molecules are denoted with capital letters (A through E). The "primes" correspond to the symmetry related molecules. The amine "A" forms a slightly longer bifurcated hydrogen bonds with both molecules of the acid, comparing to those formed by molecule "B". The third hydrogen atom of the amino group of molecule "A" is involved in hydrogen bond with the water molecule, whereas molecule "B" is H-bonded to nitrile group of "D" molecule.

The amino fragment of "A" molecule and the carboxyl group of "D" molecule are partly disordered (for the clarity only one orientation of either disordered group is shown on the drawings). The geometries of the two amino molecules differ slightly. As far as both sp³ carbon atoms are almost ideally co-planar with the phenyl rings, the whole amino substituents are differently rotated in respect to the ring. The dihedral angle between the ring plane and the plane defined by C11, C17 and H17 (C21, C27 and H27, for the second molecule) are 12.3(4) and 25.3(3)°, respectively.
The geometries of both enantiomeric acid anions are very similar (apart from the absolute configuration on the C37 and C57 atoms). The planar phenyl rings make dihedral angles with the nitro group of 16.0(7)° and 19.8(6)°, for molecules “C” and “D”, respectively. The carboxylate group is nearly perpendicular to the ring (the dihedral angles 81.2(3)° and 84(2)° for molecules “C” and “D”, respectively). The disorder of the amino group of the molecule “A” (0.89 occupation factor for the main orientation) was realized by the small shift of N-atom, what resulted in amino H-atoms and H17 atom displacement. Also one oxygen atom of the carboxylate group of molecule “D” occupies two different positions (the main position has the occupation factor of 0.81).

REFERENCES:
EVALUATION OF CURRENT SAFETY STATUS OF RBMK REACTORS

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The RBMK graphite-moderated, boiling water cooled power reactors have been developed and operated in the former Soviet Union since early 1970s. Due to the possibility of on-line refuelling, they have excellent performance indicators. However, they often used to operate close to their safety limits. After the Chernobyl accident in April 1986, safety concern about the remaining NPPs with RBMKs is expressed worldwide.

The operable RBMKs belong to three various generations that differ from one another by plant safety features. The first generation primarily had the emergency core cooling system (ECCS) of limited capacity and did not include any containment system. The second generation, comprising most of the units, is provided with a 'wet' type accident localization system and the ECCS capacity is extended to cope with a guillotine break of the reactor cooling system (RCS) pipeline with maximum diameter. The third generation includes the contemporary, post-Chernobyl safety requirements and is represented by one unit, Smolensk Unit 3. There is also a unit under construction at Kursk site where the unique core physical features will improve its safety significantly.

Since the accident, a lot of work aimed at improving the plant safety has been made in all units with RBMKs: at Leningrad, Kursk, Smolensk (Russia), Chernobyl (Ukraine) and Ignalina (Lithuania) NPPs. The intention was primarily to exclude the possibility of a reactivity initiated accident that might be caused by positive void reactivity feedback. Fast-acting scram systems have been introduced, the operational reactivity margin increased, and fuel elements with higher enrichment loaded in all the operating units. These and further modifications in RBMK design introduced recently, including detailed tables with the status of individual safety improvements in all units, have been investigated and summarized in [1].

The recent status of most units is far more adequate to satisfy Western safety standards but significantly varies from one plant to another and strongly depends on reconstruction funding, domestic as well as international. The results of probabilistic safety assessments performed until now show that the core damage frequency has fallen down 3 times to \((1 - 2) \times 10^{-5}\) per reactor-year as a result of the reconstruction.

Still, a number of safety deficiencies in the units of this type remains. They are provided with no full-pressure containment and the existing accident localization systems do not include all the components of the reactor cooling system, especially the drum separators. The key question is to increase the capacity of the reactor cavity emergency venting system and to improve the thermal-hydraulic characteristics of drum separators. A great deal of work has been made at Leningrad NPP where the reconstructed drum separators can also serve for long-term core cooling system. Another important deficiency is related to the reactor control and protection system that cannot provide physical separation of operational and safety functions, unlike Western-designed reactors where part of the control rods is designed to perform safety functions only. There is still the trend to limit the reactor power level in case of emergency rather than shut down the reactor. Strong dependence on the operators' knowledge and actions remains while the safety culture is generally low. The distribution of responsibility between the plant, the general designer and the regulatory authorities is not clear in many cases.

Despite the opinions of Western experts to decommission the RBMK reactors, the recent statements expressed in Russia say that the plants can be upgraded continuously to meet their design lifetime and even plant life extension might be considered until new types of reactors with passive safety features are put into operation.

REFERENCES:
IN-VESSEL THERMAL-HYDRAULIC PHENOMENA DURING COOLDOWN OF WWER-440 REACTORS

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A study of the procedure of cooling down the primary circuit in a WWER-440/213 reactor with special consideration of the phenomena in the reactor pressure vessel (RPV) upper head volume was performed.

The calculation model was based on the 3-loop model [1]. The calculations were performed by RELAP5/MOD3.0 code [2].

The initial conditions for the calculations were nominal for the beginning of a fuel cycle. The transient starts when all of the 6 MCPs are tripped. After 3 s the signal for scram and 10 s later for turbine trip is initiated. The primary pressure and pressurizer level at first drop rapidly, then start to rise and close to 300 s stabilize when steam is removed from all SGs. Natural circulation is established in the system. The feedwater delivery to the SGs is provided by two auxiliary feedwater pumps which are controlled by SG fine scale level.

Later on, the primary circuit is cooled down by manual opening of the BRU-K steam dump valve in 2 hours (7200 s). The BRU-K discharge flow rate decreases slowly all the time. The coolant in RPV head where practically no circulation exists is also cooled down, mainly by compartment ventilation. These two stages are not included in the figure, neither are sensitivity studies performed.

Two cases with different cooldown rates were studied. When the cooldown is slower, it would be very difficult for the operator to control the steam dump keeping the cooldown rate. The case requires the operator to follow the heat generation continuously in order to maintain the rate of primary cooldown. The final RPV head temperature depends only on the process time while the cooling rate is similar for both cases.

In the case with compartment venting off, the coolant temperature in RPV head was kept practically constant for all the time investigated. During the early phase of transient, the secondary pressure was higher and reached the setpoint of the steam dump valve.

The transient was also analyzed with the pressurizer heaters switched off. As the pressure was not maintained, the makeup system operation was considered in view to keep the pressure higher. The injection led to rapid pressure increase so that the pressurizer relief valve setpoint was reached. Then the makeup system was remaining on for about 10% of the total time interval. The calculations show that operation of the pressurizer heaters is of key importance for maintaining the primary pressure.

As the starting point for further analyses, the calculated results of the above stage of transient were taken.

An auxiliary spray system injecting water from the auxiliary makeup pump was applied. The injection rate was maintained at the minimum controlled value in order not to cause too rapid depressurization. Several calculations with various assumptions on system availability were performed showing the results as follows:

- Depressurization with the pressurizer heaters switched off meets the limit of the emergency signals in a rather short time.
- The pressurizer heaters operation makes the depressurization slower but the above problem remains.
- The makeup system has no observable influence on depressurization.

In order to avoid the problem, the steam dump should be open widely enough to provide passing by the system limitations.

Two transients were investigated, one aimed at avoiding boiling under RPV head, the other at maximum steam bubble creation. The first one led to the following conclusions:

a) When the calculation reaches the saturation parameters under the reactor head, staying at that point leads to temperature and pressure increase and to achieving the temperature limitation.

b) Secondary cooldown with pressurizer heaters on increases the pressure relatively rapidly.

c) Cooldown with heaters off makes the steam fraction under RPV head rise significantly.

The first procedure seems to be the only prospective for successful cooldown but very time-consuming so it should not be applied for cooling down the reactor vessel.

Another scenario (Fig.1) was started with primary depressurization by the auxiliary spray system. In order to avoid the pressure limitation, the sprays were switched off then and the steam dump opened. The pressurizer level decreased to the protection signal.

At another stage of spraying, the saturation parameters under the RPV head were reached. The steam bubble grows then pushing down hot water from RPV head so that the hot leg temperature increase is observed shortly after then. In reality this phenomenon may be not so rapid because of continuous water mixing. The depressurization was continued to create
maximum steam bubble. The starting point for further calculations and sensitivity studies is the one when 100% steam under RPV head is reached.

Various approaches were considered for condensating the bubble. Repressurization results in increasing back the hot leg temperature at less convenient conditions. With simultaneous cooldown, the liquid level in the pressurizer drops to the emergency setpoint. There are limitations for every step considered starting from the latter point so fulfillment of all system requirements seems impossible.

In order to find a successful path, starting from the point when 100% steam fraction is achieved, no operator action is undertaken for 30 min. Then secondary cooldown begins with parallel primary makeup to avoid emptying the pressurizer. For cooling the primary system down it is necessary to use the so called "super emergency" feedwater system. It is also needed to follow the diminishing cooldown rate by opening the steam dump valve. The pressurizer heaters were not applied during any step of the above procedure as it could be expected. The process finished successfully with its total duration of 13.5 h from the initial point.

Fig. 1. p(T)-diagram of the cooldown scenario

If the emergency steam removal line connecting the RPV head with the pressurizer relief bubbler tank is opened, all the steam is removed in about 20 min. At the end of venting, the transient becomes extremely rapid and all the remaining steam is removed in less than 1 min. The problem may be related to the code instability when avoiding underpressure. The volume is filled by the coolant and the pressurizer level decrease can be observed. The makeup pump is not able to cope with the level drop at rapid refilling but it may help to keep the level above the limit.

The results with all 6 MCPs restarted show quite different character of the transient, namely process is rather slow instead of rapid coolant mixing and subsequent condensation. Although the calculations were extended to 2 hours, the steam was not fully condensed. Moreover, the whole circuit was heated up and finally the parameters in both the primary and the secondary system became equal. The reason of the observed behaviour may be limitation of the models or code applied. A three-dimensional modelling would be more suitable to predict the physical phenomena correctly.

General conclusions concerning this type of transients can be summarized as follows:

As the heat generated in the primary circuit is higher than can be dissipated in the surrounding compartments, secondary cooldown is necessary for any long-term process in order not to heat up the primary system. In such a case, however, significant drop of the pressurizer level must be taken into account. In general, all the processes without cooldown should be avoided unless they are the only way to provide successful course of transient.

Special care should be taken on maintaining the pressurizer liquid level within the required limits, using makeup system if necessary. However, applying the makeup system at high steam fraction under RPV head may lead to very rapid increase of primary pressure and to certain instabilities. The reactor vessel behaves then like an additional, second pressurizer for the primary circuit. This is not a WWER-specific phenomenon and was also observed in numerous experiments for Western PWR conditions [4], but it is enforced in WWER-type plants by lack of a vertical steam generator.

During the emergency spray operation there is no need to use other actions because the whole process is relatively short.

At the last stage of cooldown, in order to reach the desired temperature in the primary circuit, the secondary side should be supplied with cold feedwater from the condenser.

REFERENCES:
TEST LOOP FOR STUDIES OF CORROSION PRODUCT TRANSPORT

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An in-pile test facility for studies of corrosion product transport in water-cooled reactors has been constructed in the MARIA reactor. Part of the SBM Reactor Test Facility [1], namely the system designed originally for cooling the unloaded channel, has been used for this purpose.

The facility consists of a Field tube type in-pile channel and a branched out-of-pile loop. The channel is placed in the reactor core and filled with cooling water with no fuel. An outer gap is also provided to increase the efficiency of cooling the channel material. The loop, located in a single reactor compartment, comprises two branches, one with a heat exchanger to provide cooling of the reactor water, and a circulation pump after the junction of both branches. In the branch parallel to the heat exchanger an out-of-pile test section has been installed where material samples are placed. There is also a possibility of water sampling through one of the letdown valves. The loop is connected to atmosphere by a makeup tank. A schematic diagram of the facility is depicted in Fig. 1. In order to facilitate the correct monitoring of corrosion product behaviour, all the facility surface has been made of a uniform chromium-nickel austenitic steel material.

The facility is instrumented with pressure, temperature, and flow rate measuring devices. Pressure difference at the out-of-pile section is also measured. There is a possibility to add more measuring points on various pipelines in the loop when necessary. Due to this, it can be used to investigate the steady-state and transient corrosion phenomena in multi-loop systems with individual branches either operating or cut off.

Fig. 1. Schematic diagram of the loop

Water and steel samples are investigated in the research laboratories of MARIA reactor. The activity of corrosion products of interest in the coolant as well as those deposited on the surface is determined by quantitative spectroscopy analysis with a germanium detector. Main chemical parameters are also measured in the samples.

The facility was started up on December 8th, 1997. Measurements are under way without disturbing the normal reactor operating cycle.

REFERENCES:

ANALYSIS OF INVENTORIES, NEUTRALISATION AND DISPOSAL OF THE RADWASTE AND SPENT FUEL FROM NUCLEAR POWER REACTORS IN POLAND

Stefan Chwaszczerwski, Mieczysław Kwiatkowski, Andrzej Jastrzębski, Ryszard Krochmalski, Stefania Stankiewicz, Włodzimierz Tomczak, Andrzej Cholerzyński, Jerzy W. Światalski, Alojzy Molędz

1 Institute of Atomic Energy, 2 Polish Power Grid Company, 3 Institute of Power Engineering

This analysis was done in the assumption, that nuclear power plant would be undertaken in Poland and it covers the period 2010 - 2100. Here the first stage of the analysis done in 1997 is presented. The items covered are given below:
1. Scenarios of the development of nuclear power in Poland until 2050 based on the available solutions for new generation nuclear power plants.
2. Quantity of spent fuel and radwaste from nuclear power plants including the radwastes produced during the decommissioning of nuclear power units.
3. Review of the existing and being under preparation technologies of proceedings and disposal with:
   - radwaste arisen from spent fuel reprocessing;
   - spent fuel;
   - low and intermediate radwaste.

There have been considered two scenarios of macro economical development of Poland till 2020:
- upper scenario - the GDP annual rate increase 4.34% and population 42 mln and
- lower scenario - the GDP annual rate increase 3.1% and population 40.4 mln.

The forecasted demand for electric energy in 2020 for the lower scenario is 191 TWh/a and for the upper scenario 229 TWh/a which corresponds to the magnitude of installed power 37.5 GW(e) and 45.4 GW(e) respectively. The Integrated Resource Planning System foresees the partial covering of the electric power demand in 2020 by a nuclear power plant of 50 TWh/a electricity production for lower scenario and 56 TWh/a in upper scenario.

The preliminary analysis of forecasted demand for electric energy in 2050 is 490 TWh/a for upper scenario and 390 TWh/a for lower scenario. The nuclear power share will be evaluated in next stage of this work.

As concern to the spent fuel management, the detailed analysis of long storage and direct disposal technology was done. The review covered the technologies developed in Sweden, Finland, Canada, Spain and Germany was done. The technologies of fuel reprocessing and disposal of radwaste from reprocessing processes will be done in the next stage of this work.

The management policy concerning the low and intermediate radwastes were analysed. The nature and quantities of radwastes from a nuclear power plant depend on the type of reactor, its construction, procedures of operation, constrains, conditions and operational runs as well as on the quality (leak tighness) of fuel elements, were analysed. Typical handling procedures for different radwastes arising from BWR, PWR, CANDU and GCR reactors were described.

REFERENCES:

COST OF THE ELECTRICITY GENERATION IN NUCLEAR POWER PLANT

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Institute of Atomic Energy

This work was performed for presentation on the XI Conference "Problems of Energy Fuels in the National Economy" organised by the Mineral and Energy Economy Research Centre of Polish Academy of Science as an invited paper[1]. Based on the level of primary energy consumption density in Europe ~ 400 toe per square kilometre in year (the mean value of the world is 65 toe per square kilometre in year) it was shown, that only nuclear energy can stabilise the environmental pollution due to power generation in the present level.

The analysis of costs of energy production in nuclear power plants was performed using the Discounted Cash Flow method proposed by the IEA, UNIPEDE, IAEA and NEA organisations [2]. According to this method, the mean cost of the unit energy production $k$ is given by the relation:

$$k = \frac{\sum_{t=0}^{T} (I_t + O_t + F_t) \cdot (1+r)^t \cdot E_t}{\sum_{t=0}^{T} E_t (1+r)^t}$$

where:
- $I_t$ - investment cost in year $t$, including costs of nuclear plant decommissioning;
- $O_t$ - operation and maintenance cost in year $t$, including costs of radwaste management;
- $F_t$ - fuel cost in year $t$ including costs of spent fuel management;
- $r$ - discount ratio;
- $E_t$ - energy produced in year $t$;
- $T$ - the period of design, construction, exploitation and decommissioning of NPP.

Based on the available information [3], [4] of the investment costs, costs of the NPP decommissioning, costs of operation and maintenance, cost of radwaste management, fuel cost and spent fuel management in OECD...
countries, the costs of electricity production were calculated and analysed for two discount ratio: 5% per year and 10% per year. It was shown, that due to long period of radwaste and spent fuel management processes, and long predicted time of exploitation of new generation of NPP, the cost of electricity production very slowly depends on the discount ratio. In some countries, with strong policy of radwaste and spent fuel management, the cost of electricity generation is smaller with discount ratio 10% than with 5%. E.g. in Germany cost of 1 kWh production in NPP is 0,0511 US$ for r=5% and 0,0503 US$ for r=10%. In Fig. 1 the distributions of the investment cost, O&M costs and fuel cost for analysed countries were shown. There were shown for discount ratio 10%.

Fig. 1. The components of costs of electricity generation in NPP in OECD countries. (discount ratio 10%).

The results of analysis of the present situation in the uranium market were presented. It was shown that present price of natural uranium is relatively small and lies between 38 and 43 US$/kgU. The uranium price will depend on the demand of nuclear fuel. But influence of uranium price on the cost of electricity generation is relatively small[5].

REFERENCES:

MECHANISM OF NUCLEI DISINTEGRATION BY HADRONS WITH ENERGIES OVER PION PRODUCTION THRESHOLD

Elżbieta Strugalska-Gola, Zbigniew Strugalski, Andrzej Wojciechowski
Institute of Atomic Energy

The mechanism of nuclei the disintegration process in collisions with hadrons at energies over the pion production threshold is revealed experimentally [1-7]. The disintegration appears as a complicated nuclear process developing in time and space in intranuclear matter, consisting at least of three stages which last together about 10^24 - 10^16 s after the impact.

At the first stage, which, lasts about 10^24 to 10^22 s, depending on the target-nucleus diameter and the impact parameter, the fast incident hadron (e.g. a pion or a nucleon) passes through intranuclear matter and the target-nucleus is locally damaged. The cylindrical damage appears as centered around the hadron course with the radius approximately as large as the nucleon diameter. All the nucleons from this cylindrical volume are emitted; they are observed as the fast nucleons with kinetic energies from about 20 up to about 500 MeV (as the gray track particles if registered in photoemulsions).

At the second stage, lasting about 10^22 to 10^16 s, the damaged and therefore unstable residual target-nucleus evaporates light fragments - mainly nucleons, deuterons, tritons, α-particles.

At the final stage, the residual target- nucleus decays into two or more nuclear fragments.

It was shown that the energy changes induced in massive targets by high energy hadronic projectiles can be well estimated on the basis of experimental data [5]. In the fast collision stage, definite energy portion of the incident hadron energy is used only for the nucleus local damage, its values were estimated in [3]. All the nuclear processes - the nucleon configuration transformations in the damaged nucleus, in the second and the third stages, are realized on account of the
internal energy of the damaged residual target nucleus.

The number of the emitted fast nucleons is
\[ n_N = \pi R_N^2 \lambda < \rho > \approx \pi D_s^2 \lambda < \rho > , \]  
where \( D_s \) in fm is the diameter of the nucleon, \( D_s=3R_N \) - strong interaction range, \( \lambda \) in fm is the length of the path of the hadron in the nucleus, \( <\rho> \) in nucleons/fm\(^3\) is the mean density of nucleons along \( \lambda \).

The relation between the number \( n_j \) of emitted fast protons (in emulsions) and the mean number \( n_f \) of the evaporated nuclear fragments was obtained experimentally [8] as:
\[ <n_j>=1.21 n_p +1.49, \]  
for proton collisions with Ag and Br nuclei in emulsions at 6.2 and 22.5 GeV. Similar result has been obtained for the proton-nuclei collisions in emulsions at 67, 200 and 400 GeV, and for pion nuclei collisions in emulsions at 200 GeV [9].

Our experiments were performed mainly by means of the 26 litre Xenon bubble chamber of the JINR, Dubna and the 180 litre bubble chamber of the ITEPh, Moscow.

The relation (2) may be simply derived from the working hypothesis [10] that the evaporation of the nuclear fragments from the residual target-nucleus is from surfaces of the local damages inside it; the formula derived in such a way is [10]:
\[ <n_f> = 1.25(n_p + \frac{A-Z}{Z}) , \]  
where \( n_p \) - the number of emitted fast protons in our experiments; \( n_p=\bar{n}_p \) if in emulsions. For Ag and Br nuclei in emulsions, it gives \( <n_p>=1.25n_p+1.61 \), what is almost the same as obtained in experiments [10].

Summing up, we can conclude that taking into account the properties of the hadron passage through intranuclear matter [11,12], one can state:

The nuclei disintegration by hadrons with energies over pion production threshold is realized in two stages:
1. the first - fast one, in which, during about \( 10^{-24}+10^{-25} \) s, the target nucleus is damaged locally, due to incident hadron kinetic energy.
2. the second - slow one, in which, during about \( 10^{-22}+10^{-19} \) s, the damaged residual target nucleus transits into stable light fragments and some stable parts, due to its internal nuclear energy.

For the target-nucleus damage definite portion of the incident hadron energy is used only [3].

If the incident hadron energy used for the damage of the target \( \Delta E_{nd} \) is smaller than the internal nuclear energy \( \Delta E_{nf} \) emitted from the residual target nucleus transiting into stable fragments,
\[ \Delta E_{nf}>\Delta E_{nd} , \]  
then an overcompensated hadron-nucleus nuclear collision occurs.

REFERENCES:
EXCITATION OF ATOMIC NUCLEI BY FAST HADRONIC PROJECTILES

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Institute of Atomic Energy

To any bound configuration of nucleons in a nucleus, corresponds an appropriate state of internal nuclear energy. The configuration is stable when its energy level is the lowest possible. In changing this configuration, the nucleus may be raised to higher internal energy states - some quasistable states.

Two ways for the configuration changes are evidently natural, therefore:
1) when additional energy from outside is supplied to an atomic nucleus;
2) when a nucleus massive enough is damaged, and the residual nucleus is raised to a new internal energy state and, therefore, to an quasistable or an excited state.

In other words, the changes may be realized in hadrons and nuclei collisions with nuclei. In the collisions, nuclear reactions may occur - nucleons may be added to, removed from, or rearranged within colliding nuclei; the colliding nuclei are always damaged in hadron-nucleus and nucleus-nucleus collisions. The damage is usually local.

In this work, the hadron-nucleus collisions are of special interest - as such which are leading to target-nuclei excitation in its simplest form.

The projectile-hadron energy lost in the fast stage of hadron-nucleus collision is limited [1-4]. The target-nucleus is damaged only due to the projectile energy expenses. The fast nucleons (with kinetic energies from about 20 up to about 500 MeV) and intermediate objects by which the particles may be produced [5], escape the residual parent nucleus in this stage and carry away a corresponding portion of the energy lost. Only some damage of the target-nucleus is caused in the fast stage of the collision [4]. The damaged residual target-nucleus is exited and instable, therefore, it must transit into stable fragments. The internal nuclear energy of this residual nucleus $E_a$ is smaller than the internal energy of the target-nucleus $E_a$, $E_a < E_a$, but this energy $E_a$ may be larger than the summary internal energy $\sum E_{t\beta}$ of $k$ final states appeared after the residual nucleus transition into these $k$ nuclear fragments. The portion of the internal excitation energy:

$$ E_{exc} \approx E_{ir} - \sum_k E^t_{t\beta} = \Delta \tag{2} $$

will be exuded when the residual target nucleus transit into nuclear fragments; this portion $\Delta$ may be treated as some useful nuclear energy per nuclear reaction.

When $\Delta$ is larger than the energy $\Delta_d$ lost for the target damage, the intranuclear reaction is the energy overcompensating one. The energetic yield in the reactions is depending on the target-nucleus mass number, the incident hadron identity, and the collision impact parameter. At energies of incident nucleons higher than 8 MeV and incident pions higher than about 4 GeV, it is independent of the projectile energy as well, for the heaviest target nuclei [2,4].

A summing of facts observed in hadron-nucleon collision events, and taking into account the nature and properties of the hadron interaction mechanism in intranuclear matter, it may be stated that:

A nucleus excitation by fast hadrons is realized through the nucleus local damage only. It causes the damaged, and therefore instable nucleus, to transit into a number of more stable fragments.

REFERENCES

TOTAL DISINTEGRATION OF HEAVY NUCLEI BY FAST HADRONS AND NUCLEI

Elżbieta Strugalska-Gola
Institute of Atomic Energy

The subject matter in this report is a presentation of results from hadron-nucleus and nucleus-nucleus collision experimental studies. Recognition of the mechanisms and characteristics of the nuclei total disintegration processes are important as forming a physical basis for nuclei transmutations by fast hadrons and nuclei. An understanding of the intranuclear processes will have wide applicability in an activity based on new generation of nuclear power plants, in ecology and medicine.

The studies were based on our experimental material and on data collected by several other authors in experimental investigations performed during many years with use of photographic emulsions and heavy liquid bubble chambers [1-5].

Our aim was to discover a manifestation of the laws which govern inside target nuclei, within the extremely small volumes \(10^{-15}\) m, acting in two phases during time intervals of the order of \(10^{-24}\) to \(10^{-22}\) s, and then of \(10^{-12}\) to \(10^{-16}\) s. The mechanism of nuclei disintegration process was revealed experimentally in our works [3-6].

It has been shown [7] that the total disintegration of nuclei by fast hadrons and nuclei sometimes occurs.

The total disintegration of a fast nucleus, colliding with some other similar nucleus resting in the lab. system is proposed to be defined as such in which the incident nucleus is completely dispersed into its parent nucleons, and the struck nucleus is also shattered. Independently of any of the reference systems, the total disintegration (or the total destruction) of a nucleus in collisions with a hadron or a nucleus is proposed to be defined as such in which the nucleus in a hadron-nucleus collision or nuclei in a nucleus-nucleus collisions are totally disrupted into the parent nucleons.

In conclusion, it may be stated that heavy nuclei may be totally disintegrated in central or almost central impact with other nuclei of similar mass number only; light nuclei, formed of a few nucleons, may be totally disintegrated in central impact with a single hadron (e.g.: pion, nucleon). This conclusion is based on observations of appropriate collision events [1], and it is the consequence of the properties of fundamental phenomenon - the hadron passage through layers of intranuclear matter [8,9].

Light nuclei may be totally disintegrated by fast hadrons and nuclei; for heavier nuclei it may happen only in central or almost central collisions with nuclei of similar mass numbers.

As the consequence of such a scenario, one observes in experiments at colliders two collimated beams of nucleons from the colliding nuclei in their mass center systems.

In the head-on collision the multiplicity of both of the observed opposite beams of nucleons is equal to corresponding mass numbers of the colliding nuclei.

REFERENCES:
FISSION GAS RELEASE FROM FUEL RODS OF QINSHAN NUCLEAR POWER PLANT

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The defect trap model (DTM) of fission gas behaviour in UO$_2$ fuel which has been applied to the assessment of the number of gas leaking fuel elements in the VVER-440 nuclear power plant [1] can also be applied to the Qinshan Nuclear Power Plant [2].

The idea to apply the DTM model to the VVER-440 reactors is based on the $^{85}$Kr volumetric activity measurement carried out by a radiation monitoring system and on three actual technological parameters: $T$ - the coolant temperature at inlet, $P$ - the thermal power and $W$ - the coolant flow rate. The three technological parameters allow to evaluate the fission rate and fuel temperature distribution which is needed to evaluate the fission gas release FGR to fuel-clad gap. The $^{85}$Kr volumetric activity measurement enables to assess the number of gas-leaking fuel rods and coolant contamination by other fission gas products.

The fission gas release to fuel-cladding gap is to be evaluated first, so the above mentioned code can be adopted to evaluate the fission gas release from the experimental rod tested in the High Temperature and High Pressure Light Test Loop (HTHPTL) of the Heavy Water Research Reactor (HWRR) at the Institute of Atomic Energy of China.

The algorithm described in the paper [1] has been adopted to write a program for the assessment of the number of gas-leaking fuel rods and of the volumetric activity of fission gas products in the coolant of the Qinshan NPP.

There were, however, several differences between this and the application to the VVER reactor. The first one was the adoption of $^{133}$Xe as the isotope of interest as opposed to $^{85}$Kr used previously. The second difference was the adoption of another equation for calculation of the thermal conductivity of the fuel.

The thermal conductivity of the fuel was calculated using the formula presented in [3].

The third difference was the introduction of a relation between specific surface area and burn-up, as it was thought that the range of power and burn-up experienced by the fuel could result in grain boundary interlinkage and hence in increase of the fission product release.

It was assumed that the increase of surface to volume ratio versus burn-up can be described by the following equation:

$$ S = S_0 + S_1(1 - \exp(-(b - b_o / \tau)) ) $$  \hspace{1cm} (1)

where $S = 37.4$ cm$^{-1}$, $S_1 = 300$ cm$^{-1}$, $b_o = 13$ Mwd/kg U, $\tau = 10$ Mwd/kg U, $b$ - actual burn-up. It is further assumed that if $b < b_o$ then $S$ is equal $S_o$ and if $b \geq b_o$ then $S$ varies according to the equation above.

Clearly the values of the constants depend on the history of irradiation. For the high power, the increase of surface to volume ratio occurs at earlier burn-up.

The equation (1) is based on the experience from the gas flow rig IFA-504 irradiated in the Halden Boiling Water Reactor and reported in paper [4].

The updated model of the fission gas release was evaluated by comparing the calculations of the code with experimental data obtained in the framework of the OECD Halden Reactor Project. A fairly good agreement was obtained [5].

Tab. 1 presents the predictions assuming one defected fuel rod for the burnup of 25 Mwd/kg U: $R_2$ are the theoretical release rates in atoms/s, $F_2$ are the fractional fission gas release rates from the fuel rod and $A_2$ are the predicted coolant activities for several radioactive gases. For the nominal parameters of the Qinshan NPP used, the most highly rated fuel rod has a linear power of around 290 W/cm and a calculated maximal fuel center temperature of 1459°C. Thus, dividing the measured coolant activity, $A_0$, by the values for $A_2$ in the Tab. 1 gives the number of defective fuel rods present.

It is worth nothing that for a single defect, the model gives a coolant activity for $^{133}$Xe of about 2.0 GBq/m$^3$ for fresh un-interlinked fuel and about 12.9 GBq/m$^3$ for a fully interlinked rod (for burn-up 25 Mwd/kg U). This range of activities should be compared with German experimental data [Ref. 6] of 10–20 GBq/m$^3$, Swiss data [Ref. 7] of 10 GBq/m$^3$ and French data [Ref. 8] of 0.6–2 GBq/m$^3$. 
The algorithms of FGR from the fuel rod of Qinshan type described above were adopted to the assessment of FGR to the fuel-cladding gap of an experimental rod tested in the High Temperature and High Pressure Loop (HTHPL) of the HWRR [9].

Table 1. Predictions of fission gas release for one defected fuel rod at 25 MWd/kgU burn-up.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>RZ [atoms/s]</th>
<th>FZ</th>
<th>A₁ [Gbq/m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>³⁵Xe</td>
<td>3.3E12</td>
<td>4.0E-2</td>
<td>12.9</td>
</tr>
<tr>
<td>¹³⁵Xe</td>
<td>3.9E11</td>
<td>4.0E-3</td>
<td>1.1</td>
</tr>
<tr>
<td>⁵⁸Kr</td>
<td>4.9E10</td>
<td>2.2E-3</td>
<td>1.9E-1</td>
</tr>
<tr>
<td>⁸⁸Kr</td>
<td>8.5E10</td>
<td>1.6E-3</td>
<td>3.3E-1</td>
</tr>
<tr>
<td>⁸⁷Kr</td>
<td>3.7E10</td>
<td>1.0E-3</td>
<td>1.5E-1</td>
</tr>
<tr>
<td>¹³⁸Xe</td>
<td>5.0E10</td>
<td>5.8E-4</td>
<td>2.0E-1</td>
</tr>
<tr>
<td>¹³³Xe</td>
<td>1.5E10</td>
<td>5.8E-4</td>
<td>6.0E-2</td>
</tr>
<tr>
<td>¹³⁷Xe</td>
<td>3.9E10</td>
<td>4.4E-4</td>
<td>1.5E-1</td>
</tr>
<tr>
<td>⁸⁵Kr</td>
<td>2.9E10</td>
<td>4.2E-4</td>
<td>1.1E-1</td>
</tr>
</tbody>
</table>

A post irradiation examination of the fuel element rods tested in the HTHPL loop [9] has shown that the fractional fission gas release increases comparatively very much with a very small change of the maximal linear power.

If the temperature of the fuel exceeds the threshold temperature-temperature of recrystallization, a great amount of fission gas trapped in the fuel is released. Accordingly we can divide the fuel rod volume into the area where the defect trap model is applied (below 1670 °C) and the area above the threshold temperature where process of recrystallization occurs.

The calculation data show that a change in the power by about 8 % (from 407 to 435 W/cm) causes an increase of the fission gas release for ¹³³Xe by 100 %. This explains the experimentally observed increase of the fractional release by more than 100 % (from 10 % to 23 % fractional FGR) for a power increase of only about 8 % (from 407 to 435 W/cm).

The more flat is the distribution of temperature versus fuel length the higher is the expected increase in the fractional gas release with the increase of linear power as the area of a fuel rod expands very fast with temperature above the threshold temperature.

REFERENCES:
ELECTROMAGNETIC CASCADES IN DENSE AMORPHOUS MATERIALS

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A search for scaling description of basic characteristics of electromagnetic cascades produced by high enough energy particles (mainly by photons and electrons) in amorphous media is presently one of the most important problems both from the cognitive and practical point of view. As it has been shown earlier (see [1] and the references quoted therein) the longitudinal shower profile (LSP) and its fluctuation allows such a presentation with respect of energy E of shower initiating particles within appreciably large interval of E. But the problem still remains whether and to what extent such an approach is admissible if another substantial cascade parameter - a cut-off energy $E_c$ of cascade electrons and positrons - is taken into account. Moreover, it is equally of great practical importance to get an universal description of the LSP and other characteristics of cascades developing in different amorphous media. For lack of relevant experimental information the above mentioned problems are to be investigated mostly using the technique of computer modelling of the phenomenon under discussion after appropriate checking the results with experimental data whenever they are available. In the present communication we report some results concerning the longitudinal cascades development in amorphous materials being of particular interest from the practical point of view.

It is well known that lead glass Cherenkov counters are widely used for high energy gamma ray detection. Their operation is based on collecting of the Cherenkov light emitted by charged particles of the electromagnetic shower generated by high-energy photons in a dense material. We have carried out a Monte Carlo simulation of the longitudinal development of electromagnetic cascades using the code system EGS4 [6] running on HP 735 workstation. Special attention is paid to the longitudinal development of photon initiated electromagnetic shower in SF5 lead glass at the cut-off energy $E_c + m_e = 1$ MeV, as well as in liquid xenon for energy range from 500 to 3375 MeV at the cut-off energy $E_c + m_e = 1.5 \pm 0.5$ MeV. The reason is that the same values of these parameters were used in experiment [1]. The composition of the SF5 is given in Tab. 1.

<table>
<thead>
<tr>
<th>Compound</th>
<th>% weight</th>
<th>molecular weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO$_2$</td>
<td>0.385</td>
<td>60.06</td>
</tr>
<tr>
<td>PbO</td>
<td>0.55</td>
<td>223.21</td>
</tr>
<tr>
<td>Na$_2$O</td>
<td>0.02</td>
<td>61.99</td>
</tr>
<tr>
<td>K$_2$O</td>
<td>0.04</td>
<td>94.19</td>
</tr>
</tbody>
</table>

Density 4.08 g/cm$^3$
Radiation length $X_0 = 2.36$ cm

In this composition BaO is neglected as its contribution (0.005%) is irrelevant to the development of the shower.

The computations have been made for energies of the initiating photon $E_Y$ (MeV) given in Fig. 1 for 5000 simulated shower events at each energy. In our calculations initial photons are assumed to impinge perpendicularly on the plane surface of the target, which is divided into cylindrical shells extending longitudinally from $t$ to $t+\Delta t$ and $t=i-1)\Delta t$, where $\Delta t=0.5 X_0$ (i = 1, 2, ..., 150) (1)

where $t$ is expressed in radiation length units ($X_0$) as in [5]. The results for SF5 are depicted in Fig. 1.

![Fig. 1. Longitudinal development of shower in SF5 obtained by Monte Carlo method using the EGS4 code [6].](image)

It has been found earlier [1] that the longitudinal distribution of shower electron ionisation loss or longitudinal shower profile (LSP) can be parameterised with sufficient good accuracy by the following gamma-like distribution function:

$$F_t(x_t | E, E_c) = a_1 t^{a_2} \exp(-a_3 t)$$

(2)
where \( x_t = t/\langle t(E) \rangle \) and \( t \) is a shower depth normalized to its average value \( \langle t(E) \rangle \) at the incident particle energy \( E \), \( E_e \) is the cut-off energy for cascade electrons (and positrons) and \( a_i \) (i=1,2,3) are parameters which are determined from experimental results. As an example Fig. 2 shows a typical longitudinal profile of shower produced in liquid xenon by gamma quanta with energy \( E = 3375 \pm 125 \text{ MeV} \) when \( E_e \) is between 1 and 1.5 MeV. The experimental data [1] are compared to the results of Monte Carlo simulation with EGS4 code [6]. In the figure is also displayed the approximating function (2) with parameters \( a_1 = 83.1 \pm 3.4 \), \( a_2 = 1.65 \pm 0.03 \) and \( a_3 = 2.62 \pm 0.03 \) at \( x_{t35} = 35.8 \) when \( x_t > 0.15 \) [1].

Finally we can draw the following conclusions:
- the results are in a good agreement with ones obtained by Longo and Sestili for the same material, i.e. SF5 lead glass [5],
- more experimental and/or Monte Carlo simulation data about showers generated in different media by particles within large energy interval and registered at different cut-off energies \( E_c \) [2-4] are needed to study quantitatively the investigated shower profiles.

Collecting data for these purposes for liquid xenon, lead, lead glass, and tungsten using the EGS4 code system [6] is in progress.

REFERENCES:
atoms in solution. When the gas atoms arrive at the grain boundaries, they precipitate to form bubbles, which can grow up to a saturation value. Then intergranular bubbles touch each other, and form inter-linked tunnels through which fission gases migrate to grain edge porosity and are consequently released to the fuel exterior. The resolution process also applies to the gas in grain boundary bubbles.

The number of gas atoms that can be held on the boundary before the saturation is a function of temperature, rating and restraint level of the fuel. It is a fundamental assumption in the model that any further gas atoms arriving at a grain boundary that is already saturated must be released from the fuel.

At temperatures below that at which significant grain growth occurs, gas transport to the grain boundaries is mainly by diffusion. Whilst at temperatures where significant grain growth occurs, the rate of arrival of gas atoms at the boundaries is increased by a contribution from grain sweeping. If temperature is high enough, grain boundary movement is able to sweep up fission gas more rapidly than they could have arrived at the boundary by diffusion.

The algorithms of the model based on the above assumptions were numerically solved and the results were compared with the experimental data. The comparison shows rough agreement.

REFERENCES:
DETERMINATION OF EFFECTIVE HE-3 AND LI-6 CONCENTRATION IN BERYLLIUM BLOCKS OF THE MARIA REACTOR

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Institute of Atomic Energy

Formulation of the problem

The MARIA reactor core is moderated by beryllium, a unique feature in research reactors. Reactor grade beryllium is characterised by a very low neutron absorption. However, when used in the core of a high flux reactor it suffers a strong irradiation leading to the (n,2n) reaction with subsequent isotope transformations:

\[ \frac{9}{4} \text{Be}(n,\alpha)\rightarrow \frac{6}{2} \text{He} \quad 0.8 \text{sec} \rightarrow \frac{6}{3} \text{Li} \]

\[ \frac{6}{3} \text{Li}(n,\alpha)\rightarrow \frac{3}{2} \text{H} \]

\[ \frac{1}{2} \text{He} (12.5 \text{y}) \rightarrow \frac{3}{2} \text{Li} \]

Both He-3 and Li-6 are strong absorbers, which change significantly beryllium absorption properties [2]. Determination of effective He-3 and Li-6 concentration in beryllium blocks of the MARIA reactor and its detailed knowledge is of prime importance for the reactor operation.

He-3 and Li-6 equations

As seen from Eq.1, beryllium is transformed practically immediately into lithium. The cross section for this transformation has a nonzero value only above 0.74 MeV. Thus, the number densities of beryllium, helium, lithium and tritium are subject to modifications following the equations (RR is the isotope reaction rate for absorption):

\[ \frac{dN_{\text{Be}}}{dt} = -N_{\text{Be}} \text{RR(Be)} \]

\[ \frac{dN_{\text{L}}}{dt} = \left[ N_{\text{Be}} \text{RR(Be)} - N_{\text{T}} \text{RR(L)} \right] dt \]

\[ \frac{dN_{\text{T}}}{dt} = \left[ N_{\text{T}} \text{RR(L)} - \lambda_{T} N_{\text{T}} + N_{\text{He}} \text{RR(He)} \right] dt \]

\[ \frac{dN_{\text{He}}}{dt} = \left[ \lambda_{T} N_{\text{T}} - N_{\text{He}} \text{RR(He)} \right] dt \]

The history of MARIA reactor operation can be divided into three periods: (1) the normal operation from 1977 until 1985, (2) a break for reconstruction, (3) normal operation since 1994.

Lithium and helium build-up during the first period of MARIA operation

For the MARIA reactor lattice the beryllium reaction rate is \(-1.8 \times 10^{-12}\), thus after the first period of reactor operation the number density of beryllium decreased by approximately \(4 \times 10^{-4}\), which can be neglected in the present analysis.

The reaction rates from Eq.2 have been calculated using the WIMSD5 code [1], at nominal power, for zero and maximum burn-up. The helium fast reaction rates are \(-2.5 \times 10^{-8}\) while the thermal are \(-1.0 \times 10^{-9}\). The lithium reaction rates for fast and thermal range are, respectively, \(-4.7 \times 10^{-9}\) and \(-1.8 \times 10^{-7}\). Taking into account the order of magnitude of the above quantities, we can derive the asymptotic formulas for number densities of He-3, H-3 and Li-6 at the end of 1977-85 period [2], making an additional assumption that \(\text{RR(He)} \gg \lambda_{T}\), since in our case RR(He) is \(-10^{-8}\) and \(\lambda_{T} = 1.78 \times 10^{-9}\):  

\[ N_{\text{L}}(t) = \left( \frac{\text{RR(Be)}}{\text{RR(L)}} \right) N_{\text{Be}} \]

\[ N_{\text{T}}(t) = N_{\text{Be}} \text{RR(Be)} \left( 1 + \frac{1}{\lambda_{T} \text{RR(He)}} \right) t \]

\[ N_{\text{He}}(t) = \left( \frac{N_{\text{Be}} \text{RR(Be)} \text{RR(He)}}{\lambda_{T}} \right) \left( \frac{1}{\sigma_{\text{He}} + \sigma_{L}} \right) \]

The number densities depend on the distance from the fuel element to the block centre, the maximum effect being approximately 25% for He-3 and 5% for Li-6.

The influence of He-3 and Li-6 contents on the fuel burn-up characteristics after 70 days of depletion has been found negligible. On the other hand, the poisoning by He-3 and Li-6, visibly depends on the flux spectrum which changes significantly with fuel burn-up.

Dependence of He-3 and Li-6 on the position of Be block

It is impossible to reconstruct the history of irradiation of each beryllium block from the operation log, therefore we could only estimate the dependence of beryllium block poisoning on its position in the reactor core.

The contents of He-3, Li-6 and H-3 is much higher in beryllium blocks situated between fuel elements than in those outside due to the relatively small dimensions of the MARIA core. To estimate this effect, a two-dimensional transport calculation has been carried out using the TRITAC code [3] for a quarter of the reactor. The average neutron flux values have been chosen and reaction rates calculated for 3 representative regions:

- adjacent to a fuel element,
- outside the core in the vicinity of the fuel element,
- outside the core in the reflector region.
Table 1. Poisoning of Be blocks at various positions in the core $\times 10^{-24}$.

<table>
<thead>
<tr>
<th>N. dens.</th>
<th>He-3</th>
<th>Li-6</th>
<th>H-3</th>
</tr>
</thead>
<tbody>
<tr>
<td>int</td>
<td>4.03E-8</td>
<td>1.89E-6</td>
<td>2.44E-5</td>
</tr>
<tr>
<td>ext 1</td>
<td>1.22E-8</td>
<td>6.07E-7</td>
<td>4.62E-6</td>
</tr>
<tr>
<td>ext 2</td>
<td>2.30E-9</td>
<td>1.23E-7</td>
<td>6.18E-7</td>
</tr>
</tbody>
</table>

Helium build-up during the break in MARIA operation

During the break in MARIA operation the amount of lithium stayed constant but tritium decayed into He-3 with the decay constant equal to 1.78E-09 sec. The He-3 build-up is shown in the figure below:

Influence of beryllium poisoning on reactor criticality

The decrease in the multiplication factor in the presence of asymptotic amounts of He-3 and Li-6 in beryllium is significant. A separate set of calculations has been carried out to estimate the effect separately for both of these isotopes. The results for the MARIA lattice with fresh fuel are given in the figure below:

REFERENCES:

Introduction

The work concerns the development of the computational code package for decision support of the MARIA reactor operator (grant No 8T10B09 95 C/2766). The package is based on the WIMSD5 [1] and TRITAC [2] codes.

There are 2 sets of criticality data for the MARIA reactor: in 1974 a critical state was achieved with 6 fuel elements and all control rods withdrawn, and in 1993 the relative reactivity weight of different core components was investigated [3].

Criticality calculations of the MARIA reactor have been realised in 3 steps presented in Table 1.

Table 1. Basic computational sequence

<table>
<thead>
<tr>
<th>Step</th>
<th>Energy groups</th>
<th>Geometrical model</th>
<th>Code</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>69</td>
<td>cell or macrocell representing an infinite lattice</td>
<td>WIMSD5 5</td>
<td>30-group cross sections for channels, followers and blocks</td>
</tr>
<tr>
<td>2</td>
<td>30</td>
<td>full 2-D horizontal cross section of the core &amp; 30 cm reflector, $B_2$ added</td>
<td>TRITAC</td>
<td>reference $k_{eff}$, 6-group cross sections for channels, followers and blocks</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>full 2-D horizontal cross section of the core &amp; 30 cm reflector</td>
<td>TRITAC</td>
<td>final $k_{eff}$</td>
</tr>
</tbody>
</table>

The first critical experiment

During the first critical experiment, the MARIA reactor achieved its criticality with 6 fuel elements. The horizontal cross section of the reactor is shown in Fig.1. All the safety and control rods were withdrawn and substituted by their followers.

The values of $k_{eff}$ calculated in 2D using the sequence of codes WIMSD5 - TRITAC are 8% higher than those from experiment, of which 1.1% has been caused by the beryllium library data and the rest may be due to the inadequate description of the leakage. It was checked on a model problem that e.g. 1.9% error results from the fuel element homo-genisation in 2D calculations. The influence of inaccuracies in material specification is too small to explain the error [6].

The Monte Carlo calculations performed using the MCNP4A code in a 3D geometry give results much closer to experimental 1.0, i.e. $k_{eff}=1.01671$. The source of the discrepancy in $k_{eff}$ may lie in the simplifications of the geometry used in MCNP, see Fig. 2, where only 7 vertical layers of materials were accounted for.
Fig. 2. The simplified model of the fuel channel, beryllium block and graphite block

Critical experiments for the second core

The set of 4 critical experiment results [3] concerns the reactor core after the 7-year break in reactor operation, one of the configurations shown in Fig 3. Two types of beryllium blocks were present in the core:
- blocks irradiated in the first period of MARIA operation, poisoned with He-3 and Li-6 [4],
- the new blocks without He-3 and Li-6.

Because of the uncertainties in Li and He poisoning [4,5], the calculations have been carried out for several He-3 contents with Li-6 number density equal to 1.9x10^{18}. The representative results are given in Table 2 where the excess reactivity evaluated from the control rod positions is compared to the calculated criticality with control rods withdrawn. The systematic error of model calculations (4.14$), was substracted from $k_{eff}$.

Table 2. Calculated and measured excess reactivity

<table>
<thead>
<tr>
<th>No.</th>
<th>Calculation N(He)=4x10^{17}</th>
<th>Calculation N(He)=1x10^{18}</th>
<th>Measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>9.03</td>
<td>3.07</td>
<td>2.99</td>
</tr>
<tr>
<td>2</td>
<td>8.49</td>
<td>2.58</td>
<td>2.49</td>
</tr>
<tr>
<td>3</td>
<td>9.12</td>
<td>3.15</td>
<td>3.03</td>
</tr>
<tr>
<td>4</td>
<td>9.42</td>
<td>3.42</td>
<td>3.26</td>
</tr>
</tbody>
</table>

The modification of the reactivity worth of the beryllium matrix (substituting beryllium by graphite or water) led to the following errors:

Table 3. Effect of configuration modifications

<table>
<thead>
<tr>
<th>N(He)</th>
<th>Control rods</th>
<th>aver_error</th>
<th>max_error</th>
</tr>
</thead>
<tbody>
<tr>
<td>4x10^{17} withdrawn</td>
<td>0.08</td>
<td>-0.12</td>
<td></td>
</tr>
<tr>
<td>1x10^{18} withdrawn</td>
<td>0.04</td>
<td>-0.08</td>
<td></td>
</tr>
<tr>
<td>4x10^{17} 2 inserted</td>
<td>0.05</td>
<td>-0.10</td>
<td></td>
</tr>
<tr>
<td>1x10^{18} 2 inserted</td>
<td>0.03</td>
<td>-0.23</td>
<td></td>
</tr>
</tbody>
</table>

Only one configuration with full experimental evidence was available for a fuel element reloading [7] with an experimental reactivity worth equal 1.8±0.5$ and calculated 1.65$.

Conclusions

The possible errors in the WIMS5 - TRITAC system can be grouped in 3 categories:
1. Old library, resulting in 1.45 discrepancy with recent libraries.
2. Tubular fuel cell homogenisation, resulting in 2.5% discrepancy with MCNP calculations.
3. Streaming effects in a small core. For the 1974 core they result in -7.5% error. For the 1993 cores, calculated with He-3 contents 1x10^{18} the discrepancy is greatly reduced. Possible explanation of this fact is that second cores are bigger and the mean free path in beryllium is reduced because of He-3 and Li-6 poisoning. Therefore highly anisotropic transport effects are less pronounced.

The 2.2% discrepancy between experiment and the Monte Carlo result may be due to geometry specification and possible impurities of beryllium blocks.

REFERENCES:
The numerical solution of large stiff systems of ordinary differential equations is very expensive and requires large and fast computers. This is painfully clear to all who attempt to solve numerically nuclear reactor kinetics equations. The discrete form may involve as much as $10^5$ ordinary differential equations and the stiffness is supplied by prompt neutrons. In this article we show that the amplitude-shape method (ASM), which takes from the quasistatic method [1,4] the representation of the solution as the product of the fast changing amplitude and slow varying shape function, can be used in the reactor kinetics. The ASM whose full exposition is given in [3], has been developed to be applicable for numerical solution of a large class of systems of ordinary differential equations and is particularly useful in case of partial differential equations describing the evolution of physical systems. Here we present the application of the ASM to the reactor kinetics equations, give some of the numerical results for model equations which, together with those from [2] show that the ASM is applicable to the reactor kinetics. From [3] it follows the ASM can be also used for nonlinear problems of nuclear reactor dynamics. Practical implementation of the ASM in reactor codes is being currently investigated under the KBN grant No. 119/T10/97/13.

We take a very simple model of reactor kinetics with one group of delayed neutrons, which in the discretized form is represented by the system of ordinary differential equations:

\[
\begin{align*}
\frac{du}{dt} &= Du + Au + (1 - \beta)Fu + \lambda w, \\
\frac{dw}{dt} &= -\lambda w + \beta Fu. 
\end{align*}
\]

We use the following notation:

- $u$ - prompt neutron density vector
- $w$ - delayed neutron precursor density vector
- $D$ - leakage rate matrix
- $A$ - absorption rate matrix
- $F$ - fission rate matrix
- $\beta$ - delayed neutron yield
- $\lambda$ - average decay constant of delayed neutron precursors

For simplicity we assume that both vectors $u$ and $w$ are of the same dimension $n$ and all the matrices are square and of dimension $n \times n$. The usual value of the time constant characterizing the prompt neutrons is $10^3 - 10^4$ and $\lambda = 10^3$ so that the system (1) is highly stiff and explicit finite-difference schemes cannot be used. In 60' Ott and Meneley [4] put forward an idea to represent each of the vector functions $u$ and $w$ as products of scalar amplitudes and vector shape functions:

\[
\begin{align*}
u(t) &= \phi(t)v(t), \\
w(t) &= \psi(t)z(t).
\end{align*}
\]

Such representation makes sense only if the vector shape functions $v$ and $z$ are indeed slowly varying with time. To achieve this we take fixed vectors $p$ and $q$ and postulate that

\[
\begin{align*}
(Pv)(t) &= \sum_{i=1}^{n} p_i v_i(t) = \alpha_1, \\
(Qz)(t) &= \sum_{i=1}^{n} q_i z_i(t) = \alpha_2.
\end{align*}
\]

where $\alpha_1$ and $\alpha_2$ are some constants. As the immediate consequence of (3) we have
\[ \begin{align*}
P \frac{d v(t)}{dt} &= \frac{d}{dt} (P v(t)) = 0, \quad (4) \\
Q \frac{d z(t)}{dt} &= \frac{d}{dt} (Q z(t)) = 0.
\end{align*} \]

Substituting (2) into (1) we obtain

\[ \begin{align*}
\frac{d \phi}{dt} + \frac{d v}{dt} &= \phi C v + \lambda \psi z, \\
\frac{d \psi}{dt} + \frac{d z}{dt} &= -\lambda \psi z + \beta \phi F v,
\end{align*} \]

where \( C = D + A + (1-\beta) F \). Operating on these equations with \( P \) and \( Q \) yields the equations for the amplitudes

\[ \begin{align*}
\alpha_1 \frac{d \phi}{dt} &= \phi P(C v) + \lambda \psi P z, \\
\alpha_2 \frac{d \psi}{dt} &= \beta \phi Q(F v) - \alpha_2 \lambda \psi,
\end{align*} \]

and for the shape functions

\[ \begin{align*}
\frac{d v}{dt} &= \left( C - \frac{1}{\alpha_1} P(C v) \right) v + \lambda \psi \left( z - \frac{1}{\alpha_1} P z \right) v, \\
\frac{d z}{dt} &= \frac{\beta \phi}{\psi} \left( F v - \frac{1}{\alpha_2} Q(F v) z \right).
\end{align*} \]

For simplicity we introduce the notation \( \chi = (\phi, \psi) \) and \( y = (v, z) \) and rewrite (6) and (7) in an abbreviated form

\[ \begin{align*}
\frac{d \chi}{dt} &= \gamma(\chi, y, t), \\
\frac{d y}{dt} &= g(\chi, y, t),
\end{align*} \]

where the possibility that the coefficients in the kinetic equations are explicitly dependent on time, is taken into account.

The initial conditions for (8) will depend on the normalization in (3). We have taken

\[ \begin{align*}
\alpha_1 &= P(u(0)), \\
\alpha_2 &= Q(w(0)),
\end{align*} \]

from which it follows that

\[ \begin{align*}
\phi(0) &= 1, \quad v(0) = u(0), \\
\psi(0) &= 1, \quad z(0) = w(0),
\end{align*} \]

There are many ways of selecting the numerical scheme for solving (8). We choose a mixed implicit-explicit Runge-Kutta scheme of the second order. It has the form

\[ \begin{align*}
\chi_{k+1} &= \chi_k + \frac{h}{2} \left[ \gamma(\chi_k, y_k, t_k) + \gamma(\chi_{k+1}, y_{k+1}, t_{k+1}) \right], \\
y_{k+1} &= y_k + \frac{h}{2} \left[ g(\chi_k, y_k, t_k) + g(\chi_{k+1}, y_{k+1}, t_{k+1}) \right].
\end{align*} \]

The scheme is explicit with respect to \( y \) and the time consuming inversion of large matrices is avoided.

As a numerical example we choose a slab homogeneous thermal reactor characterized by the following parameters: slab width \( a = 40 \), streaming rate \( 8.844 \times 10^4 \), fission rate \( 2.53 \times 10^4 \), \( \beta = 7.22 \times 10^3, \lambda = 4.93 \times 10^3 \). The spatial variable \( x \) is discretized by the mesh with \( N \) points and the central difference approximation is used for the streaming term. The tridiagonal matrix \( D \) is evaluated using the zero boundary condition for the neutron density. The remaining two matrices \( A \) and \( F \) are assumed to be diagonal.

The full set of numerical results is given in [2]. Here we quote only those for a nearly critical reactor with the absorption rate equal to \( 2.4754 \times 10^3 \) and \( N=81 \). We choose highly asymmetrical initial conditions

\[ \begin{align*}
u(0) &= \left( \frac{2\pi}{a} \right)^3 \sin \frac{\pi x}{a}, \\
w(0) &= 370 \left( \frac{2(a-x)}{a} \right)^3 \sin \left[ \pi \left( \frac{a-x}{a} \right) \right].
\end{align*} \]

We see that after 25 sec the solution becomes fully symmetrical as it would have been expected.

The results of numerical calculations show that the newly developed amplitude-shape method can be successfully applied in the nuclear reactor kinetics. It can be made to handle large systems of kinetic equations without necessity of performing costly static calculations resulting in inverting large matrices. There should be no limitations in including all types of nonlinear effects in large power reactors.

REFERENCES:
CALCULATION OF THE DRY STORAGE FOR SPENT REACTOR FUEL
AT THE INSTITUTE OF ATOMIC ENERGY

Krzysztof Andrzejewski, Teresa Kulikowska
Institute of Atomic Energy

Introduction
Criticality calculations of the second version of the dry spent fuel storage located in the shaft of the decommissioned EWA reactor have been performed. The calculations for the first version [1] showed that the distance between the storage channels can be reduced. As previously, storing of four types of fuel from the research reactors located at Świerk is envisaged. They comprise EK-10, WWR-SM, WWR-M2 and MR-6 type fuel elements. The elements will be placed in steel tubular capsules stacked on one another. According to the general rules of safety report evaluations, the calculations were performed assuming temperature of 20° C, fresh fuel and possibility of accidental storage flooding with water. In addition variations in concrete and water densities were taken into account.

Calculational models
The dry storage is a cylindrical concrete block with radius of 115 cm. It contains 7 concentric rings of vertical storage channels surrounding one central channel. Average distance between the channels is 13 cm. The radius of the equivalent cylindrical macrocell is 7.543 cm. The geometry of the macrocell for two versions of the storage channel is given in the table below.

<table>
<thead>
<tr>
<th>Material layer</th>
<th>Outer radii</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>cm</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>3.995</td>
<td>fuel element</td>
</tr>
<tr>
<td>2</td>
<td>4.445</td>
<td>steel</td>
</tr>
<tr>
<td>3</td>
<td>4.900/5.200</td>
<td>void</td>
</tr>
<tr>
<td>4</td>
<td>5.400/5.700</td>
<td>steel</td>
</tr>
<tr>
<td>5</td>
<td>7.543</td>
<td>concrete</td>
</tr>
</tbody>
</table>

Schematic view of the channel is given in the figure.
The radial buckling was evaluated as: 4.10^-4 cm^2. The height of the stacked fuel ranges from 724 to 780 cm, and the corresponding axial buckling varies from 1.6.10^-5 to 1.9.10^-5 cm^2.
The calculations have been performed with two codes. The WIMS code was used mainly to calculate emergency situations with the storage channel and the capsule flooded with water. The Monte Carlo MCNP code was used to calculate cases with the storage in operating conditions and to confirm results of WIMS calculations. The advantage of application of two codes is elimination of possible input errors.
Determination of the most reactive fuel

\( k_{\text{op}} \) values for the four fuel types are given in the table below.

<table>
<thead>
<tr>
<th>Code →</th>
<th>MCNP dry</th>
<th>MCNP flooded</th>
<th>WIMS flooded</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel type↓</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MR-6, 80%</td>
<td></td>
<td></td>
<td>0.741</td>
</tr>
<tr>
<td>MR-6, 36%</td>
<td>0.762</td>
<td>0.856</td>
<td>0.834</td>
</tr>
<tr>
<td>WWR-M2</td>
<td>0.476</td>
<td>0.565</td>
<td>0.579</td>
</tr>
<tr>
<td>WWR-SM</td>
<td></td>
<td></td>
<td>0.536</td>
</tr>
<tr>
<td>EK-10 (40 el.)</td>
<td>0.745</td>
<td>0.706</td>
<td>0.803</td>
</tr>
<tr>
<td>EK-10 (43 el.)</td>
<td>0.765</td>
<td>0.735</td>
<td>0.807</td>
</tr>
</tbody>
</table>

As it can be seen, the IAEA safety criteria, i.e. \( k_{\text{op}} < 0.95 \), are fulfilled. The worst case is MR-6, 36% enriched fuel, and further analyses were performed for this fuel only.

Sensitivity analysis

The estimates by WIMS have lead to the following conclusions:
- The system is very sensitive to the thickness and composition of the steel capsules; maximum effect is observed for EK-10 fuel where 20% decrease in the steel density leads to +4.4% increase in reactivity.
- Increase of void fraction in concrete causes increase in \( k_{\text{eff}} \) of the system.
- Decrease in the flooding water density causes a strong increase of the system reactivity.

Final results by Monte Carlo code MCNP

The final results obtained with the MCNP code for the most reactive 36% MR-6 fuel are shown in the table below:

<table>
<thead>
<tr>
<th>Capsule</th>
<th>Inside of the capsule</th>
<th>Space capsule-channel</th>
<th>Outside of the channel</th>
<th>( k_{\text{eff}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Old 4,9/5,2 cm</td>
<td>void</td>
<td>void</td>
<td>concrete</td>
<td>0.762</td>
</tr>
<tr>
<td></td>
<td>void</td>
<td>void</td>
<td>void</td>
<td>0.898</td>
</tr>
<tr>
<td></td>
<td>void</td>
<td>void</td>
<td>water</td>
<td>0.594</td>
</tr>
<tr>
<td></td>
<td>water</td>
<td>water</td>
<td>void</td>
<td>1.021</td>
</tr>
<tr>
<td></td>
<td>water</td>
<td>water</td>
<td>concrete</td>
<td>0.856</td>
</tr>
<tr>
<td></td>
<td>water</td>
<td>water</td>
<td>concrete 40%</td>
<td>0.945</td>
</tr>
<tr>
<td></td>
<td>water</td>
<td>water</td>
<td>water</td>
<td>0.617</td>
</tr>
<tr>
<td>New 5,4/5,7 cm</td>
<td>void</td>
<td>void</td>
<td>concrete</td>
<td>0.812</td>
</tr>
<tr>
<td></td>
<td>void</td>
<td>water</td>
<td>concrete</td>
<td>0.681</td>
</tr>
</tbody>
</table>

It can be seen that the only system with \( k_{\text{eff}} \) exceeding the value 0.95 is with water inside the capsule, void outside, which has to be considered as unrealistic. The subcriticality of the proposed configuration has been fully confirmed.

REFERENCES:

The safe operation of nuclear power plants must begin already at the design stage. In this phase all problems influencing safety should be pointed out and dealt with in the best possible way. Of these Critical Heat Flux (CHF) seems to stay in the centre of interest of scientists in all countries.

The fuel rod bundle can be arranged in various ways. Most popular are rod bundles with a hexagonal or square matrix. Wire wraps, grids and other internal constructions all influence the value of CHF. The problem is in what way all these geometrical factors change the presumed value of CHF.

In this work presented are general parameters describing two-phase flow, the pool boiling process and boiling in channel flow. Next, a general description of CHF is presented with the stress put on boiling in a vertical single tube. This part of the work is based on [1]. Next, presented are some problems in tube bundles, which should be dealt with.

In a fuel bundle it is not possible to exactly foresee the place at which CHF could occur. This means that CHF occurring locally becomes the value for CHF for the whole bundle.

Depending on the type of fuel matrix, the subchannels can vary in shape. In the hexagonal and square matrix it is possible to divide all the subchannels into 3 groups: edge, wall and central. Although they have the same name the shape of the subchannels varies - see Fig. 1. This means that at this point it is necessary to state the exact type of geometry of a subchannel when performing calculations in which subchannel analysis can be used.

One possibility of performing a subchannel analysis would be an extrapolation of the results received for annular geometry. But this even intuitively proves to be not right. There are 3 possible ways of performing a subchannel analysis [2]:

(a) assuming mean values for the whole bundle and assuming that all subchannels are equal;
(b) assuming that all subchannels are different and do not interfere with each other and performing an analysis for each subchannel independently.
(c) performing a relatively exact analysis for each type of subchannels

An exact subchannel analysis raises the problem of interchannel mixing - this means the problem of finding the mass, momentum and energy movements. Also here are various types of mixing possible e.g. diversion crossflow in which the movements are a result of natural pressure differences between the subchannels. In some cases it is possible to introduce new parameters e.g. the mixing coefficient which included in equations could help to evaluate the amount of mass, momentum and energy mixing. Nevertheless a subchannel analysis, in which it is possible to describe the wall, edge and centre subchannels might be worthwhile.

This work is at present at a preliminary phase and is a continuation of [1].

REFERENCES:
THE EVALUATION OF THE EXPERIMENTS ON BOILING PERFORMED IN THE WIW-300 INSTALLATION

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The experiments performed in a test section in the WIW-300 installation are the basis for drawing conclusions about different phenomena observed in boiling process.

The test section was an assembly of two coaxial pipes with a 2.5 mm gap between them. The test section was electrically heated and some effects related to two phase flow were registered. There were over one hundred experiments performed. In thirty of them the results were similar and it is possible to formulate some conclusions.

1. In the test section an increase of inlet pressure was observed. It was the beginning of a specific thermohydraulic phenomenon which led to burnout effect. There was a simple relation between heating $P$ [kW] and discharge of cooling water - flow intensity $G$:

$$ P = k \times G $$

where $k$ is a constant with values $42 \div 64$ [kWh/m$^3$] and $G$ is flow intensity [m$^3$/h].

2. The phenomenon was initiated by 0.3 sec increase of inlet pressure and could be qualified by changes of differences between inlet and outlet pressure. In the next 2 seconds there were observed several thermohydraulic phenomena like: changes of flow intensity, pressure oscillations and wall temperature changes. They were difficult to qualify because of lack in instrumentation (no void fraction nor outlet velocity of flow was measured). Probably these phenomena were connected with the increase of bubbles and with changes in hydraulic structure of the flow (bubble flow, Taylor bubbles, mist flow).

3. Specially interesting because of burnout effect, was choking the test section with saturated or overheated steam. It was recorded in experiments in which a bypass of the test section has been used. This phenomenon was observed for almost three seconds, the flowmeter indicated a decay of flow at that time. Choking test section with steam and pressure oscillations indicated the manifestation of the Leddineg's instability. The detected oscillations could be estimated with equations which designate the Helmholtz wave in compressibility wave model.

4. Heat exchange between walls and cooling mixture (steam and water) has been changing at the time of observed phenomenon. Generally the value of heat transfer coefficient monotonously decreased to the value ten times smaller than at the beginning. More detailed information were presented in [1].

REFERENCES:
CHF INVESTIGATIONS IN WIW-300 TEST FACILITY

Elżbieta Borek-Kruszewska
Institute of Atomic Energy

The experimental investigations of the Critical Heat Flux parameters for water cooling in annular geometry of MARIA reactor fuel channel have been performed in WIW-300 test facility under the program of the aim project nr 8T10B008 95 C/2767 partially financed by KBN.

The test section and measurement system is shortly described in our previous presentation in this Report. Detailed information can be found in report [1].

The algorithm of CHF experiments run assumed that at the fixed inlet parameters of temperature, pressure and maximum power supply, the critical conditions in the test section were approached by slow decreasing of the flow according to a given curve from the PC computer.

In the case of boiling crisis detection, the measurement system emits a signal which causes termination of the experiment when inlet coolant pressure increase during 1 second exceeds the value of 0.25 MPa.

The experiments with CHF detection were performed at the maximum power supply for both tubes heated and for internal tube heated. It was impossible to obtain CHF parameters during experiments when only the external tube was heated.

The results from two typical experiments are graphically presented below in Fig. 1 and Fig. 2.

Fig. 1 presents experimental results for both tubes heated and Fig. 2 for internal tube heated.

It was observed that before CHF a sudden increment of inlet pressure occurs and these parameters were stored as CHF parameters.

Data analysis and computer calculations of CHF parameters for some correlations were done.

The Moldysz, Knoebel, Griffel, Mirshak, and Katto correlations were chosen to calculate the CHF. Comparison of the computational and experimental results is presented below in Table 1.

It was stated in the conclusion of performed experiments and data analysis that the experimental parameters before CHF approached to Katto correlation.

The next step in the calculations will be definition of a new correlation for experimental data.

REFERENCES:

Table 1. Critical Heat Flux for chosen correlations and experimental data

<table>
<thead>
<tr>
<th>( \rho_w )</th>
<th>( T_{in} )</th>
<th>( T_{out} )</th>
<th>( P_{in} )</th>
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<td>MPa</td>
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Fig. 1. Experimental results for both tubes heated

Fig. 2. Experimental results for internal tube heated
EXPERIMENTAL RESEARCH IN WIW-300 TEST FACILITY ACCORDING TO A GIVEN PROCEDURE

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The experimental research in 1997 in the WIW-300 test facility with the new test section described below were performed under the program of the aim project nr 8T10B008 95 C/2767 partially financed by the KBN.

The investigations in annular geometry of the MARIA reactor MR6 fuel channel during the loss of flow accident should be the basis of the safety analysis important for the reliable operation of the reactor under the increased nuclear power level in a fuel element.

The new test section which approximately models the MARIA reactor channel has been designed according to the technical assumptions of the project. The test section has been constructed as an assembly of two concentric pipes with 30/25 mm O/I diameter and with 1000 mm length. The 2.5 mm gap was filled with water coolant. As the heating element an internal and external tubes made of stainless steel have been used. Nuclear heating was simulated by the Joule effect from the DC generator of 300 kW power. The loss of flow accident was simulated by the digital control of regulation valve on the bypass of the pump according to the setting curve from PC computer. This setting curve was adjusted exactly to reactor pump flow curve after damage of reactor pump power supply.

The test section has been equipped with NiCr-Ni thermocouples of 1 mm diameter placed on the inside and outside of the pipes. As the data acquisition system the OITECH Daq-Board 200A system with two DBK19 thermocouple cards have been used.

The detailed information about the test section and measurement system are included in [1] and [2].

The procedure of the experimental run assumed that at the fixed inlet coolant parameters of temperature, pressure and power supply, the flow was decreased according to the setting curve from PC computer.

In the case of boiling crisis detection, the measurement system emits signal which causes termination of the experiment when inlet coolant pressure increase during 1 second exceeds the set value 0,1-0,25 MPa.

The experiments were performed at the following inlet coolant parameters:
- inlet pressure: 0,9±1.3 MPa;
- inlet temperature: 70±115 °C;
- inlet flow: 5,6 m³/h;
and in three various series where there were heated
- both tubes, internal and external
- internal tube only,
- external tube only.

About 260 experiments were successfully performed. The results from two of them are graphically presented below in Fig. 1 and Fig. 2.

Fig. 1 presents the measured parameters for an experimental run for two tubes heated.

Fig. 2 presents experimental results for only internal tube heated.

In none of the experiments performed according to a given procedure, the CHF parameters were measured. More detail information about research and experimental results are presented in [3].

The analysis of the experimental data showed that the nuclear power level in the fuel element of the reactor MARIA can be increased to 2.4 MW.

REFERENCES:
Fig. 1. The measured parameters for an experimental run for both tubes heated.

Fig. 2. The measured parameters for an experimental run for internal tube heated.
In the paper [1] the systematic analysis of convergence conditions, used in comparison theorems proven for a few types of matrix splittings representing a large class of applications, is presented. The central idea of this analysis is the scheme of condition implications, derived from the properties of regular splittings of a monotone matrix $A = M_1 - N_1 = M_2 - N_2$ [2], shown below.

An equivalence of some conditions as well as an autonomous character of the conditions $M^{-1}_2 \geq M^{-1}_1 \geq 0$ and $A^{-1}_1 N_2 \geq A^{-1}_1 N_1 \geq 0$ are pointed out.

Conditions ensuring that a splitting of a nonsingular matrix $A = M - N$ will be convergent are unknown in a general case. However, general properties of a splitting of $A$ (not necessary convergent), useful in proving many comparison theorems, are given in the following lemma.

**Lemma.** Let $A = M - N$ be a splitting of $A$. If $A$ and $M$ are nonsingular matrices, then the matrices $M^TN$ and $A^TN$ commute, and the matrices $NM^{-1}$ and $NA^{-1}$ also commute.

**REFERENCES:**
[1]. Z.I. Woźniacki: Matrix Splitting Principles. Submitted to *Linear Algebra and its Applications*. (The main results of the paper have been presented in the invited paper in XII Conference on Applied Mathematics, Palic, Yugoslavia, September 8-12 1997).
CONDITIONS FOR CONVERGENCE AND COMPARISON

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Comparison theorems, proven under different conditions for different types of matrix splittings representing a large class of applications, play an essential role in the convergence analysis of iterative methods for solving linear systems.

The analysis presented in the paper [1] is based on condition implications derived from the properties of regular splittings.

The decomposition \( A = M - N \) is called a regular splitting of \( A \), if \( M \) is a nonsingular matrix with \( M^{-1} > 0 \) and \( N > 0 \).

It is easy to verify that for regular splittings of a monotone matrix \( A \) (i.e., \( A^{-1} \geq 0 \)),

\[
A = M_1 - N_1 = M_2 - N_2
\]

the assumption

\[
N_2 \geq N_1 \geq 0
\]

implies the equivalent condition

\[
M_2 \geq M_1
\]

but the last inequality implies the condition

\[
M_1^{-1} \geq M_2^{-1} > 0
\]

This condition can be expressed, as follows

\[
(1 + A^*N_2)^{1/2} A^{1/2} \geq A^{1/2} (1 + N_2A^*)^{1/2}
\]

which, after relevant multiplications, is equivalent to

\[
A^*N_2A^{1/2} \geq A^{1/2} N_1A^{1/2} \geq 0.
\]

From the above inequality, one obtains

\[
A^*N_2A^*N_1 \geq (A^*N_1)^2 \geq 0
\]

and

\[
(A^*N_2)^2 \geq A^*N_1A^*N_2 \geq 0.
\]

Hence,

\[
\rho^2(A^*N_2) \geq \rho(A^*N_1A^*N_2) = \rho(A^*N_1A^*N_1) \geq \rho^2(A^*N_1)
\]

which gives us

\[
\rho(A^*N_2) \geq \rho(A^*N_1).
\]

Since

\[
\rho(M^*N) = \rho(A^*N/(1 + \rho(A^{-1}N))),
\]

the inequality

\[
\rho(M_1^{-1}N_1) \leq \rho(M_2^{-1}N_2)
\]

can be deduced.

REMARKS ON SOME RESULTS FOR MATRIX SPLITTINGS

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The paper [1] is an extension of the former version. The subject of the paper is devoted to the discussion of aspects related mainly to the use of proper conditions in splitting definitions in order to avoid a confusion in the interpretation of comparison theorems. For instance, one of such questions is a confusion caused by the use of different definitions of weak regular splittings.

In the case of the strict inequality in (4), similar considerations lead to the strict inequality in (11).

On the other hand, from the inequality (2), one obtains

\[
A^*N_2 \geq A^*N_1 \geq 0,
\]

which implies the inequalities (6), (7) and (8), and additionally

\[
A^*N_1A^*N_2 \geq (A^*N_1)^2 \geq 0,
\]

and

\[
(A^*N_2)^2 \geq A^*N_2A^*N_1 \geq 0.
\]

The inequality (3) gives us that

\[
A^*M_2 \geq A^*M_1 \geq 0,
\]

since for each regular splitting of \( A \)

\[
A^*M = I + A^*N,
\]

hence, it is evident that both conditions (12) and (15) are equivalent.

Each of the above conditions, except (8) and (14), leads to the inequality (11). However, as can be shown on simple examples of regular splittings the reverse implications is not true. Thus, the above inequalities are progressively weaker conditions which used as hypotheses in comparison theorems provide successive generalizations of results.

REFERENCES:


The orginal definition of weak regular splitting of \( A = M - N \), introduced by Ortega and Rheinboldt [2], is based on three conditions: \( N \geq 0, M^*N \geq 0 \) and \( NM^* \leq 0 \). Some authors ignore the last condition which implies weakening this definition and some comparison theorems, proven for regular splittings, do not carry over.
The definitions of splittings, with progressively weakening conditions and consistent from the viewpoint of names, are here collected.

Let $M, N \in \mathbb{R}^{m \times n}$. Then the decomposition $A = M - N$ is called:

(a) a regular splitting of $A$ if $M \geq 0$ and $N \geq 0$,
(b) a nonnegative splitting of $A$ if $M \geq 0$, $M^\top N \geq 0$, and $NM \geq 0$,
(c) a weak nonnegative splitting of $A$ if $M \geq 0$ and either $M^\top N \geq 0$ (the first type) or $NM \geq 0$ (the second type),
(d) a weak splitting of $A$ if $M$ is nonsingular and either $M^\top N > 0$ (the first type) or $NM \geq 0$ (the second type). In particular a given weak splitting can be both types,
(e) a convergent splitting of $A$ if $\rho(M^\top N) < 1$.

Another question discussed in the paper is the analysis of additional conditions for the hypotheses used by Beauwens, which ensure the correctness of his results [3].

The following result represents the modified version of Beauwens' theorem.

**Theorem.** Let $A = M_1 - N_1 = M_2 - N_2$ be two convergent weak splittings of $A$ the same type, that is, either $M_1^\top N_1$ and $M_2^\top N_2$ or $M_1 N_2$ and $N_2 M_2$ are nonnegative matrices. Then anyone of the following assumptions

(a) $(A^\top N_1 - A^\top N_1) A^\top N_1 \geq 0$
(b) $(A^\top N_2 - A^\top N_1) A^\top N_2 \geq 0$

implies $\rho(M_1^\top N_1) \leq \rho(M_2^\top N_2)$.

Thus, Beauwens' results, as they are given in [3], are correct if the matrix $N_2$ is nonsingular in the case of the assumptions (b) and (d) of his theorem.

**REFERENCES:**

[1]. Z.I. Woznicki: Remarks on Some Results for Matrix Splittings. The paper, after the announcement in NA-digest net, is distributed in Internet - the LaTeX input file is available via anonymous ftp on cxl.cyf.gov.pl (148.81.40.10), file: pub/woznicki/axel.tex, (1997).

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**THERMAL PROBLEMS WHILE IRRADIATING THE TARGET MATERIALS IN MARIA REACTOR**

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One of the major goals of MARIA reactor is production of radioisotopes for medical and industrial use. Possibility of neutron flux increase due to its upgrading allows to obtain the higher specific activities of the irradiated target materials. The neutron flux increase is accompanied by an augmentation of heat generation in these materials caused mainly by emission of gamma radiation. The basic materials to be considered are sulphur (S), tellurium dioxide (TeO$_2$) and iridium (Ir).

Preparation of sulphur for irradiation by melting it and pouring into an aluminium can of an outer diameter of $d = 15$ mm and wall thickness of $\sigma = 0.6$ mm. On closing the can and checking its tightness it is placed in one out of eight vertical isotope channels of diameter $18$ mm made in a special aluminium block. In the course of irradiation the cooling water is flowing through the annular gap and removing the heat generated in cans and aluminium block. Fig. 1 presents the radial distribution of temperature in the can for heat generation rate $q_m \approx 5$ W/g, water at the inlet of the isotope channel $T_w \approx 50^\circ$C and a flow velocity in annular gap $v = 1.5$ m/s [1].

**Fig. 1. Radial distribution of temperature in the can**
Due to its small thermal conductivity the sulphur is in a liquid state in the first zone of the can. For the assumed values of the heat generation rate, the thickness of layer in the solid state adjacent to the can wall doesn’t exceed $\sigma \approx 0.5 \text{ mm}$, hence for the radius value less than $r_s \approx 0.4 \text{ mm}$ the sulphur is in the liquid state.

Assumed heat generation rate $q_m \approx 5 \text{ W/g}$ in the isotope channel corresponds to the reactor power $P \approx 20 \text{ MW}$.

To have all sulphur in solid state the heat generation rate should be $q_m \leq 0.15 \text{ W/g}$. This value is about 33 times smaller than the assumed one in the calculation. The sulphur in the can begins to melt when the reactor power is equal $P \approx 0.6 \text{ MW}$. To avoid the can cracking due to the rise of stresses caused by the thermal expansion of sulphur the amount of its mass to be placed into the can should be limited.

Tellurium dioxide is used for iodine production (I-131). The melted TeO$_2$ is poured into the aluminium can of an outer diameter $d = 25 \text{ mm}$ and wall thickness $\sigma = 0.6 \text{ mm}$. On closing the can and checking its tightness it is placed in one of the isotope channels of a diameter $d = 28 \text{ mm}$. The cans and channel wall are cooled by water flowing through an annular gap with a velocity $v \approx 1.5 \text{ m/s}$. Water temperature at the inlet of isotope channel is $T_m \approx 50^\circ \text{C}$. Fig. 2 shows the radial temperature distribution in the isotope channel for several values of the heat generation rate ($q_m = 1, 2, 3$ and $4 \text{ W/g}$). In the course of tellurium dioxide irradiation its melting ($T_{\text{mel}} = 733^\circ \text{C}$) should be avoided.

The iridium is irradiated in aluminium cans of an external diameter $d = 25 \text{ mm}$ and wall thickness $\sigma \approx 0.6 \text{ mm}$. Iridium targets are made of foil with a thickness $\sigma = 0.2 \div 0.5 \text{ mm}$ and diameter up to $d = 3 \text{ mm}$ or of wire with diameter up to $d = 1 \text{ mm}$ and length $l \leq 5 \text{ mm}$.

Inside the can there is a holder made of a material with good thermal conductivity. Aluminium or graphite is used as the structural material for the holder. Holder elements are formed with annular segments which are a joined by a central mandrel. In these annular segments special cylindrical sockets for placing the iridium targets are made.

After inserting the holder with targets to the can it is tightly closed and loaded into the isotope channel. In order to attain the large specific activities the channels for iridium irradiation are placed in beryllium matrix of the reactor core.

Heat generation rate in those spots achieves values of $q_m \approx 10 \text{ W/g}$ and larger. Fig 3 shows the radial temperature distribution in the isotope channel for iridium irradiation ($q_m = 10 \text{ W/g}$).

The values of temperatures in the holder, targets and mandrel depend on the gas gaps. In order to attain the temperature decrease inside the can those gaps should be diminished as much as possible. In the case when $q_m > 10 \text{ W/g}$, it is necessary to apply the graphite holders. They prevent the targets to be sunk into the holder what could have happened if the holder had been fabricated of aluminium ($T_{\text{mel}} = 660^\circ \text{C}$).

REFERENCES:
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[2]. W. Bykowski: „Thermal analysis of the can with tellurium dioxide target material during irradiation“, IAE, B-29/97.
[3]. W. Bykowski: „Thermal analysis of the can with iridium target material during irradiation“, IAE, B-33/97.
THE NEUTRON EMISSION METHOD FOR DETERMINATION OF FISSILE MATERIALS WITHIN THE SPENT FUEL - EQUIPMENT OPTIMIZATION

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2 Research Reactor Centre, Institute of Atomic Energy

A nondestructive assay method using neutron emission technique has been proposed and designed for the determination of the fissile isotopes distribution along the irradiated fuel assemblies of MARIA reactor. The method is based on detection of fission neutrons emitted from external neutron source and multiplied by fissile isotopes: U-235, Pu-239, and Pu-241 within the spent fuel.

Neutrons emitted from the spent fuel originate mainly from fission induced in the fissile material and the source neutrons penetrating the fuel rod without interaction. Additionally, the neutrons from spontaneous fission of actinide isotopes contribute to the population of emitted neutrons.

The Monte Carlo code [1] has been used for the geometrical simulation and optimization of the measuring equipment (Fig. 1), i.e. neutron source, moderating container, collimator, and the neutron detector.

Two objective functions were used in optimization process: the thermal neutron flux integrated with fission cross-section for U-235 (flux cross-section integral), and the thermal neutron current integrated with fission cross section (current cross-section integral). The first criterion has been applied to optimize the moderating container, and fuel-detector geometry; the second one in collimator simulation. All the simulations were performed for the fresh fuel assembly and for its mock-up made of aluminum to separate the "fission component" from the total signal.

The results of calculation show [2] that the moderating container having dimensions Ø32cm x 30cm, and collimator of 26cm x 6.8cm x 2cm constitute the optimal configuration. In Fig 2 are shown the results of Monte Carlo simulation of the fuel assembly - neutron detector geometry. The flux - cross-section integral is plotted versus distance between the fuel and the detector. The maximum ratio of detector output signal for fuel and mock-up (signal to background ratio) was found for the distance of 4.5 cm.

![Fig. 1. Scheme of measuring equipment](image)

![Fig. 2. Fuel - neutron detector geometry optimization](image)

In the real experimental procedure at least two calibration points have to be used: detector count rates for fuel element and its mock-up, representing the nominal amount of fissile material and zero content. For the intermediate region the linearity between the output signal and fissile material content within the fuel is assumed.

REFERENCES
The fuel clad is a main barrier against fission product release and the thermal safety limits are being so established as to maintain its integrity. Most typical are maximum clad temperature and heat flux transferred from the clad to the coolant.

The main thermal limits are not directly measurable but certain derived thermal parameters (e.g. inlet/outlet coolant temperature, coolant flow rate and pressure, reactor power, peaking factor) allow calculating of the maximum clad temperature and heat flux. One of the calculation uncertainties in such procedure comes from the global fluctuations of coolant flow and reactor power.

The power spectral density (PSD) of coolant flow, measured for MARIA reactor is shown in Fig. 1. A very distinct oscillating mode has been observed with characteristic frequency of $\omega_0 = 1.57$ radians/sec (0.25 Hz), and the relative amplitude of about 1%.

Assuming, that the fluctuating component of coolant flow $\delta Q$, and the maximum clad temperature perturbation $\delta T_c$ constitute the input and output to the system respectively (see Fig.2), one can express the system response in terms of transfer function $G_T(\omega)$.

For dominant frequency $\omega_0$, and relative amplitude of coolant flow oscillation equal 1%, the amplitude of maximum clad temperature was calculated as 0.4 deg.

Similar analysis has been performed for the maximum heat flux on the fuel surface. Phase shift between the maximum temperature and heat flux oscillations is constant, and equal $5\pi/4$. Maximum amplitude of heat flux oscillation for characteristic frequency $\omega_0$ was estimated as 0.9 W/cm$^2$ (0.5 % of nominal value).

REFERENCES:
AUTORADIOGRAPHY OF PAINTINGS - NEUTRON ACTIVATION FACILITY AT MARIA REACTOR

Krzysztof Pytel, Ludwik Dąbkowski, Małgorzata Wierzchnicka, Alina Koziel, Leonard Strzalkowski, Beatrycze Pytel
Research Reactor Center, Institute of Atomic Energy

One of nondestructive testing methods enabling the examination of pigments in paintings is a neutron activation followed by successive autoradiographies. In conventional neutron activation autoradiography technique a painting is exposed to a beam of neutrons emitted by the thermal column or neutron guide tube from research reactor. Such neutron sources are not available at MARIΑ reactor. Also direct activation of paintings on existing neutron beams was inadmissible due to intensive gamma radiation and fast neutron components in the beam.

A novel technique has been proposed and developed for the purpose of painting activation on MARIΑ reactor. A painting is exposed to thermal neutrons scattered from the main beam by means of a scattering block (see Fig.1) what reduces drastically undesirable gamma and fast neutron radiation. The crucial point of technique was a proper distribution of scattering medium density along the neutron beam allowing to obtain the homogeneous intensity of scattered neutrons. The maximum dissipation of incident beam by means of a scattering block was the second objective of the project.

It turned out that with certain simplifications one can find analytical solution for the scattering medium density distribution [1]. For the polyethylene foil used as a scatterer the density varies from 1.7 mg/cm² at the beginning of block (adjacent to the beam hole) to nominal one at the end (see Fig. 2).

Activation facility has been designed, manufactured and installed on the beam hole H-8 of MARIΑ reactor. The scattering blocks are partially (except the side adjacent to painting) surrounded by three layers: 120 mm thick graphite, playing the role of neutron reflector, 1 mm cadmium absorber and 100 mm lead shield. The effective cross section of scattered neutron field is of 2000 mm x 280 mm. To allow activation of paintings of height over 280 mm the irradiation facility has been equipped with scanning device in vertical direction.

Final distribution of scattered thermal neutron flux along the horizontal axis is shown in Fig. 3. The only small correction of theoretical density distribution was required to achieve the homogeneity of neutron flux of order 10%. Almost 94% of incident neutrons undergo scattering within the block.

This work was supported by the State Committee for Scientific Research in the frames of KBN research contract No. 1H01E 001 96C/3009.

REFERENCES:
THE NTD TECHNIQUE AS A METHOD FOR PRODUCING OF HOMOGENEOUS SINGLE CRYSTALS WITH PRECISELY CONTROLLED CHARACTERISTICS

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Neutron transmutation doping (NTD) is the technology to produce the doped semiconductor materials (such as based on GaAs) with highest homogeneity.

The method features on avoiding the introduction of other atoms into monocrystal. Dopands are formed directly from the host atoms by radiative capture reactions under thermal neutron irradiation.

The following reactions occur:

\[
\begin{align*}
69\text{Ga}(n,\gamma) & \rightarrow 70\text{Ge} + \beta \\
71\text{Ga}(n,\gamma) & \rightarrow 72\text{Ge} + \beta \\
75\text{As}(n,\gamma) & \rightarrow 76\text{Se} + \beta 
\end{align*}
\]

Isotopes Ge and Se behave as doping donors.

Special rotary channel has been constructed, at MARIA reactor (Fig. 1), to imply the NTD method.

During irradiation, the monocrystal rotates along the vertical axis in the channel. Entire monocrystal GaAs as well GaAs wafers were irradiated in this way.

After irradiation and deferral time the samples were examined by the following methods:

- Hall effect,
- photoluminescence,
- examination of deep levels by means of nonstationary photocurrent spectroscopy (PITS),
- measurements of carriers concentration by means of electric break down,
- examination of local vibrating modes in the infrared absorption (determination of carbon concentration).

It has been revealed that carriers concentration for monocrystals doped by NTD method is characterised by a fluctuation of 3-4 times smaller than for monocrystals produced by Czochralski method.

Material doped by NTD method is also characterised by a high purity.

Fig. 1. Rotary channel construction
DECOMMISSIONING OF EWA REACTOR

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Research Reactor Centre, Institute of Atomic Energy

This report describes the following tasks:

1. Surveillance on the permanently shutdown reactor facility.
2. Elaboration of technology for reactor decommissioning.
3. Dismantling the reactor structural components.
4. Dosimetric surveillance of EWA reactor decommissioning process.

In the reported period (01.01.97-31.12.97) some of the technological systems of EWA reactor were operating to ensure the safety of the facility in compliance with requirements of the Permit no.2/95/EWA issued by the Chairman of the National Atomic Agency. Beyond that, basing on the Permit no. 1/97/EWA of 23 May 1997 the dismantling works of the reactor first cooling circuit were carried out.

The assessment of state of reactor facility being permanently excluded from operation based on its technological and operational data as well as failures, events and disturbances occurred in reported period. There have also been estimated:
- system of the physical protection of the facility;
- state of nuclear materials protection;
- staffing of the service teams.

To ensure the safety of reactor facility the selected devices and technological systems were operated continuously, among them the power supply system, ventilation system, dosimetric system, etc.

There have been controlled:
- pumping station of the primary cooling circuit,
- indications of the devices measuring water levels in reactor vessel biological shield and AR spent fuel storage facility,
- state of low liquid radwastes sump tank fill (R-1),
- state of the spent fuel storage facilities (19, 19A),
- stand - by of warning signalling,
- stand - by of power generation set in the reactor emergency supply system.

In compliance with the safety report and operational quality assurance requirements some technological parameters have also been periodically controlled. These included:
- chemical and radiological analyses of water samples from reactor and biological shield tanks, spent fuel and AR storage facilities;
- laboratory measurements of dosimetric filters operating in the dosimetry control system of air released to the atmosphere through stack.

Due to the worsening of water chemical parameters in AR fuel storage facility water has been exchanged.

It should be stressed that no inefficiencies or emergencies happened.

To ensure safety of EWA reactor facility and of its spent fuel storage pools, the continuous around the clock surveillance was kept by one person.

In general, the EWA Reactor Operation Department has sufficient and experienced staff for conducting the dismantling work and providing operational service and safety of the spent fuel storage facilities.

Within the task No. 2 including the preparation of technology for reactor decommissioning the following works have been completed:

1. In February 1997 fresh nuclear fuel was dispatched from EWA reactor (it concerns MR and EK-10 fuel) to the store situated in MARIA reactor facility.
2. The technical design was done and three shielding containers for intermediate radioactive waste from the selected reactor internals were constructed.
3. All the experimental apparatus and all kinds of biological shields of the horizontal neutron beams have been removed from the reactor hall and transmitted for further use by physicists. All other structural materials e.g. various sorts of spectrometer bases made of steel and some steel-water shields, were transferred to a metallurgical plant as a scrap (overall mass of removed components ca. 120 tons).
4. Materials and decontamination ingredients as well as technical outfit and equipment necessary for dismantling were collected.
5. On requirement from the NAEA Nuclear Safety and Radiation Department inspectors a supplementary documentation to the Plan of EWA Reactor was elaborated.
6. ,,The technology - operational instruction for dismantling of pumping station of EWA reactor first circuit - DEMEWA no. 1/97” was written.
7. An efficiency examination of the full decontamination for some components of primary cooling circuit installation in compliance with technology highlighted in the
8. Intermediate radioactive waste from dismantling the reactor internals such as isotope channels, ionisation chamber and control rods channels (dismantled in December of 1996) were reloaded from AT fuel pond into three shielded containers of diameter 100 mm, length 1250 mm and a mass of 200 kg and transferred to the Radioactive Waste Management Department along with low radioactive waste contained in three standard containers (barrels of 0.2 m³).

9. The following documents have been produced:
   - SHAPE
     - „The system and procedure of dosimetric control of structural elements arising from EWA reactor dismantling”;
     - „The control system of decontamination efficiency of EWA reactor structural elements”;
     - Technology of dismantling of EWA reactor vessel and thermal column components”.

10. A training program has been elaborated for personnel participating in dismantling works and the dismantling groups have been trained. The major work has been carried out within the task no. 4. It comprised:
   - A special tub with outfit for complete decontamination of structural elements obtained during dismantling operations has been installed. The tub was connected to the exhaust ventilation.
   - At first the preliminary works have been done. Those included:
     - dismantling of secondary cooling circuits heat exchangers;
     - filtration of water in the primary cooling circuit by means of stationary ionite filter;
     - all the electrical devices in the pumping station were disconnected from their power supply;
     - water from the primary cooling circuit was drained to the low level radwaste tank;
     - the reactor vessel was separated from pumping station equipment by dismantling some pieces of main pipes (suction and delivery) which were localised in the compartment no. 30;
     - the flanges of the pipes from the vessel side were plugged and the reactor vessel was filled with mineral water.

   Having completed the preliminary works the dismantling of pumping station installation of primary and secondary circuits localised in compartment no. 39 has been accomplished.

   The following equipment has been dismantled and decontaminated:
   - four sets of heat exchangers (additionally they have been cut up into smaller pieces, decontaminated again and transferred into scrap),
   - 19 valves of various size,
   - main circulation pumps (4 pc.),
   - suction and delivery pipes of the primary cooling circuits,
   - installation of thermal column cooling system,
   - installation of experimental water loop,
   - components of the secondary cooling system situated in compartment no. 39,
   - electrical and measurement instrumentation.

   All the dismantled elements (with exception of heat exchangers separators) of the pumping station compartment after receiving dosimeter certificates have been transferred into scrap.

   The scope of dismantling in the pumping station of primary cooling circuit and of some elements of the secondary cooling circuit localised in compartment no. 39 foreseen in the dismantling plan for 1997 has been fully accomplished.

   The assessment of decontamination effectiveness has been performed according to the requirements included in relevant domestic and EU documents and the specific activity value was assumed to be 1 Bq/g which is ten times lower than the pre-set by law limit value.

   From the accurate dosimeter measurements done for the dismantled stainless steel elements one can state that after decontamination while transferring them for scrap the loose surface contamination level was substantially lower than allowed 0.4 Bq/cm² for β and γ - irradiation isotopes and 0.04 Bq/cm² for α emitters.

   As an example a table with measure data is attached below.

   After dismantling the pumping station equipment there has been released for scrap:
   - stainless steel 1H18N9T 26 920 kg
   - carbon steel St35 12 870 kg
   - lead in steel lining 5 600 kg
   - electric motors 1 800 kg

Table 1. Segment of pipe on delivery side of 09-1-97 pump
   (swab from an area of 100 cm²)

<table>
<thead>
<tr>
<th></th>
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<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>Ce-144</td>
<td>185</td>
<td>&lt; 1.80</td>
<td>&gt; 103</td>
</tr>
<tr>
<td>Sb-125</td>
<td>50</td>
<td>&lt; 0.78</td>
<td>&gt; 64</td>
</tr>
<tr>
<td>Ru-106</td>
<td>120</td>
<td>&lt; 4.0</td>
<td>&gt; 30</td>
</tr>
<tr>
<td>Cs-137</td>
<td>20</td>
<td>&lt; 0.67</td>
<td>&gt; 30</td>
</tr>
<tr>
<td>Zn-65</td>
<td>11.5</td>
<td>&lt; 1.1</td>
<td>&gt; 10</td>
</tr>
<tr>
<td>Co-60</td>
<td>240</td>
<td>&lt; 0.7</td>
<td>&gt; 343</td>
</tr>
<tr>
<td>in average</td>
<td>6.3 Bq/cm²</td>
<td>&lt; 0.09 Bq/cm²</td>
<td>&gt; 70</td>
</tr>
</tbody>
</table>

During dismantling of pumping station the following quantities of low level radwastes have been produced:
a) liquid effluents:
- water from the primary cooling circuits drained before beginning of the dismantling – 22.0 m$^3$,
- decontamination solution used in the decontamination process (after neutralisation) – 3.2 m$^3$,
- technical water used in rinsing process of elements decontaminated – 35.0 m$^3$;
b) solid wastes:
- installation elements not treated by decontamination (measurement sensors, pulse tubes, small size valves etc.) 5 barrels of total volume 1.0 m$^3$,
- four heat exchangers of dimensions $\phi$ 190x2100 mm from the thermal column cooling system (total volume 0.25 m$^3$),
- auxiliary materials used for decontamination (gloves, lignin, tampons etc.) totally 22 buckets (capacity of a bucket 50 l), in total 1.10 m$^3$.

It should be especially stressed that the dosimetric monitoring has been done during the entire process of dismantling and decontamination of the reactor pumping station.

Before releasing the materials for scrap there have been performed measurements which comprised:
- spectrometric measurements of samples taken from swabs of contaminated surfaces before and after decontamination;
- measurements of gamma irradiation doses on decontaminated elements;
- measurements of $\beta$-radiation contamination on decontaminated elements (direct method and by means of swabs).

All the measurement results have been recorded in the Dosimetric Measurement Record and special protocols.

PREPARATION OF Fe$_{3-x}$Mn$_x$Si (for x=0.05) SINGLE CRYSTALS FOR POLARIZING NEUTRON MONOCHROMATORS

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In Crystal Growth Laboratory of the Institute of Atomic Energy in Świeck, the single crystals of Fe$_{2.95}$Mn$_{0.05}$Si compound, useful for neutron polarizing monochromators, are grown among other types of crystals.

Preparation of Fe$_{2.95}$Mn$_{0.05}$Si single crystals, of high structural quality is very difficult. It is because of molten material supercooling during crystallization process and the strong tendency to form low angle grains in the growing crystal.

A special technique with elements of Bridgman and Stockbarger methods was used to grow the crystals. Using that procedure single crystals of Fe$_{2.95}$Mn$_{0.05}$Si compound of about 70 mm in diameter and 120 mm long, have been obtained.

The best crystals were selected and next cut into plates using electroerosion spark machine. To improve the structure quality (to remove the structure of low angle grains), some plates were annealed in temperatures closely to the melting point of Fe-Mn-Si compound. The lowering of a number of low angle grains in the crystal and the increase in peak maximum of rocking curve were observed in the most of annealed plates. The observed change of the shape of rocking curve measured before and after crystal annealing is shown in Figs. 1a and 1b

The mosaic spread (FWHM) of the crystals, neutron reflectivity and also homogeneity of the neutron reflectivity (using neutron topography and scanning technique) have been measured. In such a way the big, single crystal plates, up to the size 70 x 30 x 10 mm$^3$, were selected. The faces of every plate were parallel to (111), (211) and (110) crystallographic planes. The mosaic spread (FWHM) measured in small areas of the plates (cross section of neutron beam - 5mm x 10mm) was 4-5 minutes of arc. The mosaic spread (FWHM) measured using neutron beam 20mm x 30mm, was found to be 13.8 minutes of arc. Beside such small mosaic value, the neutron reflectivity of Fe$_{2.95}$Mn$_{0.05}$Si compound was high (20-30 %) and similar to that of Heusler (Cu$_2$MnAl) alloy crystal. It appear a real perspective to improve the reflectivity of...
Fe_{2.95}Mn_{0.05}Si polarizing neutron crystal monochromators, increasing their mosaic.

The preliminary experiment performed in our laboratory has shown, that reflectivity measured for Fe_{2.95}Mn_{0.05}Si single crystal plate after termomechanical treatment was about two times higher than the reflectivity of not treated Fe_{2.95}Mn_{0.05}Si crystals, characterized by low mosaic spread. The neutron reflectivity from Fe_{2.95}Mn_{0.05}Si single crystal plate after termomechanical treatment, measured with the use of 1mm pin-hole diaphragma, is shown in Fig. 2.

The further work with Fe_{2.95}Mn_{0.05}Si single crystal growth and also improvement of those crystals neutron reflectivity are planned.

Fig. 1. Rocking curves measured for Fe_{2.95}Mn_{0.05}Si single crystal plate (a) before and (b) after annealing. Transmission geometry, reflection from (111) crystallographic plane.

Fig. 2. Results of Fe_{2.95}Mn_{0.05}Si single crystal sample reflectivity measurement (using pin-hole of 1 mm in diameter).
TWO SUBMODIFICATIONS OF $\gamma$-TYPE $\text{Al}_2\text{O}_3$ OCCURRED IN THE RESULT OF PLASMA SPRAYING PROCESS

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These works are performed within the research cycle concerning coating materials and coatings protecting surfaces of engine and machine parts in the high temperature region [1,2].

The aim of these works is the choice of new improved compositions to high temperature resistant coatings. Particular attention is directed to coating materials of high resistance to short time temperature changes and thermal shocks. Such materials are suitable to coatings of thermal barrier type [3,4].

Some research results obtained in the last year for the coatings containing materials from the $\text{Al}_2\text{O}_3$ - $\text{SiO}_2$ and $\text{Al}_2\text{O}_3$ - $\text{ZrO}_2$ systems are described earlier [5].

Now an effect revealed recently during experiments with plasma spraying of some materials based on $\text{Al}_2\text{O}_3$ will be presented.

Two X-ray diffraction patterns slightly differing each other have been obtained. Both show the presence of metastable alumina of $\gamma$ type. In the first pattern for the coating sprayed on metallic substrate we can observe crystalline phase of $\gamma$ type with two strong diffraction peaks and few weaker slightly diffuse, with medium level of background (Fig. 1b). In the second pattern for the same material as previously, sprayed into water we can observe only two strongest peaks of $\gamma$ type of $\text{Al}_2\text{O}_3$ with slight background growth in a few places (Fig. 1c). Other visible difference between these two patterns is higher intensity of strongest diffraction peak in the second pattern. For comparison on fig. 1a diffraction pattern of thermodynamically stable crystalline modification of $\alpha$ - $\text{Al}_2\text{O}_3$ (corundum) is presented. There is no doubt that pattern from Fig. 1a present entirely different crystalline modification than those from Fig. 1b and 1c.

The patterns from Fig. 1b and Fig. 1c show occurring of two submodifications in metastable alumina of $\gamma$ type differing in ordering of atoms and probably in crystallite sizes. Difference in strongest peak intensity may be connected with some kind of polytypism. In order to find the reasons of the presented differences between diffraction patterns from Fig. 1b and 1c the characteristic features of plasma spraying process should be taken into consideration. This process is characterised mainly by short time (range of ms) of material flight by high temperature region and resulting high cooling rate (range of mega K/s). These conditions are favourable to phase transitions with forming of metastable phases which are not encountered in conditions nearer to thermodynamic equilibrium. The second factor to take into consideration is the difference in cooling and heat exchange conditions between plasma spraying of coating on substrate and spraying into water. In the case of such ceramic materials as alumina which is rather heat insulator spraying into water, when each grain of material is cooled separately, give higher cooling rate than in the case of coating, when cooling is going through neighbouring grains of the same insulating material. Therefore it may cause some differences in ordering and microstructure which are visible on X-ray diffraction patterns.

Further experiments and works on such problems are still in progress.

REFERENCES:
Fig. 1. Diffraction patterns of the Al$_2$O$_3$

- a - corundum powder, b - coating sprayed on substrate, c - material sprayed into water.

**MONITORING SYSTEM FOR INDUSTRIAL E-BEAM FLUE GAS TREATMENT PROCESS**

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The results of reliable and precise measurements of gas composition in different key points of electron-beam installation are necessary for its proper operation and control. Only the composition of flue gas coming into installation is adequate to composition of flue gas emitted from coal-fired boiler. At other points of e-b installation the gas composition is strongly modified by conditions of the process therefore specific measuring systems (sampling, conditioning and set of gas analyzers) for its determination are required. The system for gas composition measurement at inlet and outlet of e-b installation is described in the paper.

**Process monitoring system (PMS)**

Process monitoring system should ensure the continuous measurement of parameters which exert a direct influence on the effectiveness of SO$_2$ and NO$_x$ reduction and on the e-b process itself. A simplified diagram of PMS and localization of measuring points are shown in Fig. 1. Two types of extractive measuring systems are applied for the process monitoring. The main type is designed for monitoring the continuous operation (CEM) of e-b installation. This system is based on the gas analyzers. Other system is designed for occasional off-line measurements and called grab sample.
Continuous emission monitoring (CEM) system

Process inlet

A normal composition of flue gas emitted from coal-fired boiler and dedusted by ESP is analyzed at the installation inlet. The following flue gas parameters should be continuously measured: concentrations of $SO_2$, $NO/NO_x$ and $O_2$, humidity, volumetric rate of flow, temperature, pressure and fly ash loading. The measured values make possible to determine:

- the required efficiencies of $SO_2$ and $NO_x$ removal from flue gas,
- flue gas irradiation dose,
- amount of water to be added to flue gas in the humidifier,
- amount of ammonia to be added to flue gas before its entry to the process vessel.

The following types of gas analyzers are preferable for measuring the above mentioned concentrations: $SO_2$ concentrations - analyzers based on the principle pulsed fluorescence or NDUV analyzers, $NO/NO_x$ concentration - chemiluminescence analyzers, $O_2$ concentration - paramagnetic analyzer. Volume flow rate of flue gas is the main parameter characterizing the cleaning installation. Its value is directly used to calculate the required irradiation dose, water and ammonia feed rates. The annular flow meters with automatic correction for flue gas temperature and pressure as well as with periodic cleaning of sensor are preferable. The $SO_2$ removal efficiency strongly depends on the flue gas humidity at process vessel. Flue gas humidity increases to level of 10+14% (V) in an evaporative spray cooler.

At the installation outlet

At this point, efficiencies of $SO_2$ and $NO_x$ removal from flue gas in the installation and the ecological noxiousness of leaving gas should be determined. In this connection, continuous measuring of the concentrations of $SO_2$, $NO/NO_x$, $NH_3$ and $O_2$, particulate loading and temperature are anticipated.

The basic factors which may adulterate the measurement of gas composition are as follows:

- low gas temperature (60 to 90 C) and its high absolute humidity (at the level 10 + 14% (V)),
- the presence of unreacted ammonia,
- gas leaving the process vessel contains the particles of final products which are hygroscopic and have submicron size.

The specific chemiluminescent ammonia analyzer with two converters is preferred for measurement the concentration of $NO/NO_x$ and $NH_3$ in the gas leaving the installation.

Grab sample system

Grab sample system is based on the manual wet chemical methods for determination of special components concentration in the flue gas [1]. These methods are used occasionally in the following cases:

- for checking the readings of the CEM system. Measuring points for both system are close one to another. Such measurements are provided for: $SO_2$, $NO_x$ and $NH_3$ concentration,
- for calibration of the in-situ type gas analyzers - measurements of: particulate loading, humidity and volumetric flow rate of flue gas,
- for measurement of the component concentrations which are not measured by CEM - $N_2O$ concentration and aerosols size distribution.

In recent years the sampling train for $N_2O$ concentration measurement was modified [2].

Conclusion

The process monitoring system should ensure successful operation of the e-b installation. For these purpose two types of measuring systems are applied. Both systems have been tested at pilot plant at EPS Kaweczyz. Now both of them are recommended for industrial e-b demonstration plant at EPS Pomorzany in Szczecin.

REFERENCES:
The main purpose of the experimental and designed works was to obtain a long-term and stable operation of the laboratory installation. Many modifications were introduced to the plasmatron construction. Finally, the three experiments have been carried out, each of four hours duration. The stable operation of installation was achieved. The final design of the plasmatron is presented in the paper [1].

On this base, the project of semi-industrial scale installation for quick pyrolysis of coal powder in the stream of hot gases from arc plasmatron was developed (Fig. 1). Its basic components are: the arc plasmatron with powersupply system, combustion chamber (pyrolyzer) and coal feeding system. The arc plasmatron with a long electric arc in the cylindrical channel blown off by axial vortex air flow, consists of two water-cooled electrodes insulated from each other and separated by a gap where the air is introduced. Typical operating parameters are: electric power 110–120 kW, heat efficiency 0.90–0.92, air feed rate 12–13 kg/h, nitrogen feed rate 3.5–4.0 kg/h (for cathode protection).

The combustion chamber consists of a water-cooled cylinder with a tangential air inlet, lined internally with concrete. The plasmatron is located on the axis of the head of combustion chamber. The powdered coal is transported to the two injectors located in the head of the combustion chamber.

The operating parameters are: coal feed rate 300–500 kg/h, secondary air feed rate 400–700 kg/h. Since the combustion chamber is operated fuel-rich, the swirling hot gas is rich in CO, H₂ and coke. Investigations show that the unique design of the new type of burner (plasmatron + pyrolyzer) provides good prerequisites for rapid ignition and stabilised combustion of pulverised coal and air mixture.

This technology may be used for ignition and stabilisation of combustion in coal-fired boiler in the power plant and to eliminate the combustion of high-sulphur oil for this purpose.

REFERENCES:
Inorganic cements are favoured in radioactive waste solidification as immobilization media because of their low cost, ease of processing and resistance to fire and radiation damage. Potential disadvantages are their permeability and low strain.

The addition of organic additives, such as polymers, to cement at the mixing stage produces a polymer modified cement which can have reduced permeability and increased mechanical properties. A considerable amount of research has been carried out [1] for development of polymer modified cements for civil engineering applications.

The objectives of the work were: to assess more thoroughly the properties of polymer modified cements as matrices for evaporator concentrates; to optimise the composition of the mixes; and to determine any problems which might arise in scaling-up a pilot plant scale.

A simulated evaporator concentrate was used for our studies. The composition of the concentrate was similar to those of chemical laboratory drain radioactive waste at Świerk. In contrary to evaporator bottoms from nuclear power plants there was no boric acid. The main waste component were sulphates that constituted nearly 50% of all chemical components by weight. Commercially available organic polymers (styrene-butadiene latex and epoxide resin - epidian 53, commonly proposed additives for modification of mortars), and inorganic sorbents (bentonite and silica-gel, usual used as a mineral improved admixtures in concrete) were used with loadings up to 20% for polymers and 5% for sorbents by weight of the additive medium to dry cement powder.

Portland cement of type P-35N from the factory at Chelm was selected from among of six another cements. Samples made with cement and
additives were evaluated to investigate the effects of evaporator concentrate loading, waste-to-cement ratio, and water-to-cement ratio. The results of the experiments were interpreted in terms of observed mechanical (compressive strength) and chemical stability (leachability) of solidified products.

The main conclusions of this work are:

1. The overall effects of organic polymer and inorganic sorbents additives on mechanical properties are complicated but in general mechanical strength tends to increase. Most of solidified products with concentrate and additives indicated better compressive strength, near to 30% compared with the products without additives. Silica-gel and latex are the least satisfactory additives for this property.

2. The additives produced little reduction in leach rates for $^{137}$Cs at polymer to cement ratio of around 0.2.

3. It is stated, that compression strength in the range of 14-19 MPa for solidified products maybe satisfying, in respect of the structural stability criterion of radioactive wastes for disposal, but the improvement of leaching properties is insufficient. The most of samples of modified cements had lower leach rates than that of unmodified cements. Cumulative fraction release for $^{137}$Cs was between 20-37% in distilled water after 21 days.

REFERENCES:
INVESTIGATIONS OF THE SULPHUR CONCRETE PROPERTIES BEFORE AND AFTER IRRADIATION IN AN ACCELERATOR

Ewa Hajewska, Antoni Malczyk, Zygmunt A. Wojciechowski, Martyna Przyborska
Institute of Atomic Energy

Concrete used for immobilization of radioactive wastes can be enriched with ion exchange resins added in order to prevent transportation of contaminants from the radioactive waste forms to the environment by an aqueous medium and with retarders particulary useful for offsetting the effects of high temperature occurring in containers during the setting and hardening [1] of Portland cement.

Other helpful additive was sulphur [2]. The concrete with supplementary sulphur [3] has the numerous advantages:

- high compressive strength,
- high resistance against water, acids and oils,
- good isolation properties,
- short time of solidification,
- possibility of recycling,
- easy application of access aggregates, like sand, glassfibers, calcite etc.,

as well as some disadvantages, among them:

- high costs,
- necessity of using increased temperature (about 140°C) in the production and application.

The sulphur concretes found the application in the industry and marine architecture [4] and in the protection of nuclear objects, for example in the Tchernobyl power station [5].

The specimens of the concrete made with polymeric sulphur, water and addition of barytes and amphibolite were prepared in the Radioactive Waste Management Department of IAE.

The compressive strength and microstructure of sulphur concrete with different additions were investigated [6] using these specimens, among them 60 samples before irradiation and 33 after irradiation in an accelerator.

Measurements of compressive strength were made, according to Polish Standard (PN) [7] on samples without salts and with the addition of NaCl and Na₂SO₄ from 9,1% to 60%. After the compressive tests the crack surfaces were observed in the electron scanning microscope.

The shapes and the dimensions of specimens are made as cylinders Ø80mm, height 80mm and Ø50mm, height 50mm or as cuboid with dimensions 50x50x40mm and 50x50x40mm. The majority of tests were performed with cuboid specimens 50x50x30mm.

In the Table 1 the medium values (each from 4 specimens) of compressive strength of different kind of concretes are given. The results of compressive tests showed that the irradiation in accelerator has an influence on the compressive strength of concrete. It caused the increase of R_c for concretes with the addition of salts, and the decrease of R_c for the concretes without the salts. This dependence was observed for all kinds of concretes being under examination.

The crack surfaces of some specimens after compressive tests were observed in the scanning electron microscope.

On Fig.1 and 2 the examples of crack surfaces are presented: on Fig.1 the specimen of sulphur concrete without addition before and after irradiation and on Fig.2 the crack surfaces of the specimens of sulphur concrete with barytes without and with addition of salts.

Table 1. Medium value of compressive strength $R_c$ [MPa] of the concrete

<table>
<thead>
<tr>
<th>No</th>
<th>Composition of specimen</th>
<th>$R_c$ [MPa] before</th>
<th>$R_c$ [MPa] after</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sulphur + 40% Na₂SO₄</td>
<td>20,0</td>
<td>26,9</td>
</tr>
<tr>
<td>2</td>
<td>Sulphur + 40% NaCl</td>
<td>19,0</td>
<td>21,9</td>
</tr>
<tr>
<td>3</td>
<td>Sulphur + 54,5% amphibolite + 9,1% Na₂SO₄</td>
<td>31,8</td>
<td>41,2</td>
</tr>
<tr>
<td>4</td>
<td>Sulphur + 54,5% amphibolite + 9,1% NaCl</td>
<td>32,2</td>
<td>40,4</td>
</tr>
<tr>
<td>5</td>
<td>Sulphur + 54,5% barytes + 9,1% Na₂SO₄</td>
<td>31,4</td>
<td>40,2</td>
</tr>
<tr>
<td>6</td>
<td>Sulphur + 54,5% barytes + 9,1% NaCl</td>
<td>34,2</td>
<td>39,1</td>
</tr>
<tr>
<td>7</td>
<td>Sulphur + 84,7% amphibolite</td>
<td>48,5</td>
<td>35,6</td>
</tr>
<tr>
<td>8</td>
<td>Sulphur + 89,3% barytes</td>
<td>48,6</td>
<td>32,6</td>
</tr>
<tr>
<td>9</td>
<td>Sulphur + 60% barytes</td>
<td>29,2</td>
<td>33,7</td>
</tr>
<tr>
<td>10</td>
<td>Sulphur</td>
<td>11,6</td>
<td></td>
</tr>
</tbody>
</table>

REFERENCES:
[6]. E. Hajewska, A. Małczyk, Z.A. Wojciechowski, M. Przyborska: Badania własności betonów siarkowych przed i po napromienieniu w akceleratorze, Raport IEA Nr: B-36/97

Fig. 1. Specimen of sulphur concrete, 1500x.
a - before irradiation, b - after irradiation

Fig. 2. Specimen of sulphur concrete with 54,5% of barytes, 1500x.
a - without addition of salt,
b - with 9,1% Na₂SO₄,
c - with 9,1% NaCl
INVESTIGATION OF IMPACT STRENGTH AND CRACK TOUGHNESS OF 13HMF STEEL USING RECONSTRUCTED CHARPY SPECIMENS

Witold Szteke, Ewa Hajewska, Waldemar Bilous, Martyna Przyborska, Tadeusz Wagner, Jan Wasiak, Mariusz Wieczorkowski, Zygmunt Andrzej Wojciechowski

Institute of Atomic Energy

The re-use of specimens is an issue that, due to its importance has elicited an increasing interest since the middle of the eighties. The re-use may be accomplished by two methods: miniaturization and reconstruction of test samples.

In the Material Research Laboratory of the Institute of Atomic Energy a technique of reconstructing Charpy specimens of low-alloy steel 13HMF using welding method was developed.

Charpy U specimens made according to the standard PN-79/H-04370 (Fig.1) and Charpy V specimens (Fig.2), after tests, performed with Wolpert pendulum system WP 15/30, were reconstructed using HBS welding equipment. The results of impact tests - KCU2 on specimens before and after reconstruction are given in Table 1 and the results of crack toughness investigations - KId in Table 2.

![Fig. 1. Charpy U specimen used for impact tests](image1)

![Fig. 2. Charpy V specimen used for toughness tests](image2)

<table>
<thead>
<tr>
<th>Table 1. Results of impact tests before reconstruction</th>
<th>after reconstruction</th>
</tr>
</thead>
<tbody>
<tr>
<td>No of sample</td>
<td>KCU2 [J/cm]</td>
</tr>
<tr>
<td>UOHC4</td>
<td>63.62</td>
</tr>
<tr>
<td>UOHC5</td>
<td>74.97</td>
</tr>
<tr>
<td>UOHC8</td>
<td>50.47</td>
</tr>
<tr>
<td>UOHC10</td>
<td>66.46</td>
</tr>
<tr>
<td>UOHC12</td>
<td>63.66</td>
</tr>
<tr>
<td>UOHC15</td>
<td>75.23</td>
</tr>
<tr>
<td>mean x</td>
<td>65.73</td>
</tr>
<tr>
<td>std.dev. σn</td>
<td>9,14</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2. Results of crack toughness tests before reconstruction</th>
<th>after reconstruction</th>
</tr>
</thead>
<tbody>
<tr>
<td>No of sample</td>
<td>KId [MPa m1/2]</td>
</tr>
<tr>
<td>WOHC11</td>
<td>42,00</td>
</tr>
<tr>
<td>WOHC13</td>
<td>46,10</td>
</tr>
<tr>
<td>WOHC14</td>
<td>43,70</td>
</tr>
<tr>
<td>WOHC16</td>
<td>44,70</td>
</tr>
<tr>
<td>WOHC17</td>
<td>48,20</td>
</tr>
<tr>
<td>WOHC18</td>
<td>43,70</td>
</tr>
<tr>
<td>mean x</td>
<td>44,73</td>
</tr>
<tr>
<td>std.dev. σn</td>
<td>2,17</td>
</tr>
<tr>
<td>mean x</td>
<td>62,77</td>
</tr>
</tbody>
</table>
The impact tests were performed according to the standard PN-79/H-04370 and the toughness tests according to the standard PN-88/H-04366 and ASTM E 24.01. The fatigue crack \((\alpha/W=0.45+0.55)\) were performed on the Instron 8501 system. \(K_{\text{id}}\) integral were determined using Wolpert pendulum system WP 15/30. The crack surfaces of the specimens after tests were observed in scanning electron microscope. The examples of diagram of impact tests and the fractography are given on Fig. 3 (impact strength) and on Fig.4 (crack toughness tests).

![Diagram](image1)

![Diagram](image2)

Fig. 3. The diagrams of impact bend tests and fractography of 13HMF steel (impact strength study)
\(a\) - before reconstruction,  \(b\) - after reconstruction
Fig. 4. The diagrams of impact bend tests and fractography of 13HMF steel (toughness study)
a - before reconstruction,  b - after reconstruction

The results of impact tests (KCU2) as well as of fracture mechanics investigation (Ktc) shows that the technology of reconstruction of Charpy specimens by welding is satisfactory. The mean values of KCU2 and Ktc for the specimens before and after reconstruction have the appropriate standard deviations.

REFERENCES:

INVESTIGATION OF THE STATIC COMPRESSIVE STRENGTH OF MAGNETIC ALLOYS Fe - Cr - Co

Witold Szteke, Jan Wasiak, Waldemar Bilous, Tadeusz Wagner,
Martyna Przyborska, Antoni Malczyk
Institute of Atomic Energy

Working out the method of production of plastic permanent magnets from Fe-Cr-Co alloys is of great importance for practice.

In theory it was associated with selecting the optimal chemical composition of the alloy in which during the process of heat treatment it occurs a strain hardening of solid solution by the precipitating ferro- and paramagnetic phases [1].

In practice the influence of the chemical composition and heat treatment on the plastical properties Fe-Cr-Co alloys was examined.

The following mono and polycrystalline specimens of this alloys were used:
- Fe, 23% Cr, 15% Co, 2% V - polycrystalline,
- Fe, 23% Cr, 15% Co, 3% Mo - monocristalline,
- Fe, 23% Cr, 15% Co, 5% Mo - monocristalline.
Samples with dimensions 5x5x10 mm were prepared in the I.P. Bardin Central Research Institute for Iron and Steel Industry - Moscow, Russia.

The compression tests were carried out on the INSTRON 8501 Dynamic Testing System. In order to meet the requirements of research programme a special equipment for these tests were designed and made. It made possible running the tests with accuracy 0.5% of the maximal range of extensometer.

The strain measurements of 25 samples in the range 0 to 2.5 mm were performed.

The tests results in the form of diagrams are shown in Figure 1.

Fig. 1. The compressive stress versus strain for sample nr M9854-2/Z (computer id: CR 18).

The calculated results of the static compressive strength are given in the Table 1.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Heat treatment</th>
<th>$R_{10}$ [MPa]</th>
<th>$R_{0.2}$ [MPa]</th>
<th>Twinning</th>
</tr>
</thead>
<tbody>
<tr>
<td>M9854-1</td>
<td>500°C/6h</td>
<td>939</td>
<td>1054</td>
<td>+</td>
</tr>
<tr>
<td>M9854-2</td>
<td>650°C/30min</td>
<td>432</td>
<td>510</td>
<td>-</td>
</tr>
<tr>
<td>M9854-4</td>
<td>650°C/30min</td>
<td>374</td>
<td>478</td>
<td>-</td>
</tr>
<tr>
<td>M9854-5</td>
<td>500°C/6h</td>
<td>868</td>
<td>1017</td>
<td>+</td>
</tr>
<tr>
<td>M404-1</td>
<td>550°C/40min</td>
<td>808</td>
<td>972</td>
<td>-</td>
</tr>
<tr>
<td>M404-2</td>
<td>550°C/40min</td>
<td>856</td>
<td>1079</td>
<td>-</td>
</tr>
<tr>
<td>M404-3</td>
<td>650°C/15min</td>
<td>644</td>
<td>716</td>
<td>-</td>
</tr>
<tr>
<td>M404-4</td>
<td>650°C/15min</td>
<td>590</td>
<td>732</td>
<td>-</td>
</tr>
<tr>
<td>M404-5</td>
<td>626°C/15min</td>
<td>610</td>
<td>649</td>
<td>-</td>
</tr>
<tr>
<td>M404-6</td>
<td>626°C/15min</td>
<td>561</td>
<td>638</td>
<td>-</td>
</tr>
<tr>
<td>M404-7</td>
<td>600°C/30min</td>
<td>578</td>
<td>756</td>
<td>-</td>
</tr>
<tr>
<td>M404-8</td>
<td>600°C/30min</td>
<td>657</td>
<td>734</td>
<td>-</td>
</tr>
<tr>
<td>M404-9</td>
<td>550°C/1h</td>
<td>1070</td>
<td>1183</td>
<td>+</td>
</tr>
<tr>
<td>M404-10</td>
<td>550°C/1h</td>
<td>835</td>
<td>1030</td>
<td>+</td>
</tr>
<tr>
<td>M404-11</td>
<td>500°C/10h</td>
<td>1015</td>
<td>1026</td>
<td>+</td>
</tr>
<tr>
<td>M404-12</td>
<td>500°C/10h</td>
<td>918</td>
<td>1018</td>
<td>+</td>
</tr>
<tr>
<td>M404-13</td>
<td>500°C/10h</td>
<td>943</td>
<td>1109</td>
<td>+</td>
</tr>
<tr>
<td>M9854-3</td>
<td>Z</td>
<td>158</td>
<td>487</td>
<td>+</td>
</tr>
<tr>
<td>M9854-2</td>
<td>Z</td>
<td>570</td>
<td>781</td>
<td>+</td>
</tr>
<tr>
<td>M9854-4</td>
<td>650°C/15min</td>
<td>622</td>
<td>875</td>
<td>-</td>
</tr>
<tr>
<td>M9854-5</td>
<td>600°C/30min</td>
<td>989</td>
<td>1159</td>
<td>-</td>
</tr>
<tr>
<td>M9854-6</td>
<td>550°C/40min</td>
<td>1032</td>
<td>1613</td>
<td>-</td>
</tr>
<tr>
<td>M9854-7</td>
<td>550°C/40min</td>
<td>978</td>
<td>1603</td>
<td>+</td>
</tr>
<tr>
<td>M9854-8</td>
<td>626°C/15min</td>
<td>723</td>
<td>840</td>
<td>-</td>
</tr>
<tr>
<td>M9854-8</td>
<td>500°C/10h</td>
<td>1223</td>
<td>1444</td>
<td>-</td>
</tr>
</tbody>
</table>

The samples after compression tests and the obtained results were passed to the Bardin Institute - Russia for further investigations.

REFERENCES:
DAMAGE MICROSTRUCTURES AND ITS ROLE ON YIELD STRESS IN AUSTENITIC STAINLESS STEEL IRRADIATED TO LOW DOSES WITH 124 MeV Xe AND 225 MeV Ar IONS

Andrzej Hofman
Institute of Atomic Energy

Initial process of microstructure evolution in austenitic stainless steel 00H17N14M2 irradiated at low doses by heavy ions at temperature range 373K - 873K have been studied and compared with yield stress data. The microstructure induced by radiation was examined by a transmission electron microscope. In all cases the dislocations loops of interstitial type were observed. The density of the dislocations loops was high and showed a strong temperature dependence (Fig. 1).

In general the size of irradiation-induced defects decreases with decreasing irradiation temperature due to lower mobility of point defects and higher interaction among them (Fig. 2).

In all series of irradiations at various temperatures, the loop density saturates at a certain dose level, beyond which it decreases. For higher temperatures the loop density saturates at lower dose and its level is higher. The decrease of density is due to loop-loop coalescence.

From the electron microscopic observation it can be inferred that the tiny defects formed by heavy ions are interstitial type dislocations loops. At 373K the density of the dislocation loops was extremely high. Strong contrast of images at weak beam condition suggests that loops have a stacking faults. It is clear that besides these interstitial clusters the same amount of vacancies are also accumulated in the specimens; many of the vacancy clusters may be too small to be resolved.

The stress of a metal is sensitive to its irradiation-induced microstructure. In order to clarify the correlation between the observed small dislocation loops and the yield stress change the yield stress change is plotted against the defect density in Fig. 3.

According to the theory of hardening, the yield stress change due to dislocation loops, \( \Delta \delta_y \), is expressed by following equation:

\[
\Delta \delta_y = 2 \cdot \alpha \cdot \mu \cdot b (N \cdot d)^{1/2},
\]

where \( \alpha \), \( \mu \), \( b \), \( N \) and \( d \), mean barrier strength of obstacles, shear modulus, Burger's vector, density of dislocation loops, respectively. Fig. 3 shows plotting of \( \Delta \delta_y \) against \( N^{1/2} \). It is clear that \( \Delta \delta_y \) is proportional to \( N^{1/2} \).

From these results in can be concluded that the yield stress in 00H17N14M2 austenitic stainless steel irradiated by heavy ions to relatively low fluences at 373K was qualitatively in good agreement with the dispersed barrier
model of radiation hardening. The major defects which increase yield stress were the observed tiny interstitial type dislocation loops. The role of the accumulated vacancies on yield stress is probably minor. [1, 2].

REFERENCES:
MAJOR INDUSTRIAL ACCIDENTS

Mieczysław Borysiewicz ¹, Adam Markowski ²
¹Institute of Atomic Energy
²Technical University of Łódź

The basic differences between accidents and routine operations, in terms of their potential pressures on the environment and human populations, relate to: the toxicity of discharges, volume and rate of release, and flammability and explosiveness.

The damage pathways are often very complex, involving direct and indirect effects to more than one environmental medium. The resulting damage can differ from that associated with routine activities in a number of ways. For example, the development of unexpected, uncontrollable conditions in a chemical process plant could result in the production of large quantities of toxic compounds. If the safety systems and emergency facilities fail, this could result in release to the environment of large quantities of toxic gases and/or fire and explosion. Depending on the prevailing weather conditions and the sensitivity of the surrounding environment, a single event such as this could cause considerable short- and long-term damage to natural resources (groundwater, rivers, soils), to terrestrial and aquatic ecosystems and to humans.

Technology-related major accidents are of concern also due to their interrelated characteristics: unpredictability of when and exactly how they will occur (and hence perceived lack of control), uncertainty over environmental pathways and impacts, and unforeseen interactions (human and technical) in the source facility. These features of major accidents justify treating them as a significant source of social and environmental risks for the purpose of assessment and management. Risk, in this sense, is defined as the probability of an undesired effect.

The human health and environmental risks associated with accidents vary according to the location and inherent safety of industrial installations or other hazardous activities.

Accident risk management therefore focuses on the two basic elements of risk: the magnitude of the consequences of an accident strongly dependent on location and the probability that these will occur (mainly dependent on the safety of the operation). In practice, risk management requires a combination of source-oriented and impact-oriented measures, involving the operator of the hazardous activity, the relevant public authorities and services and members of the public.

A number of the above issues of major industrial accidents were analysed and described in the monograph [1]. They are:
- sources and relevance of information on past accidents;
- methods of hazards identification and risk assessment;
- principles of risk management;
- classification of severe chemical accidents;
- physical phenomena of severe chemical accidents and methods of their calculations;
- principal factor influencing the onset and development of accident scenarios of chemical process installation;
- major accidents of energy generation systems;
- catastrophes in hard coal mining;
- catastrophes of inland transport, sea transport and offshore installations involving dangerous substances.

REFERENCES:
ENHANCEMENT OF THE EU DECISION SUPPORT SYSTEM RODOS AND ITS CUSTOMISATION FOR USE IN POLAND

Mieczyslaw Borysiewicz, Andrzej Furtek, Slawomir Potempski, Henryk Wojciechowicz, Roman Żelazny
Institute of Atomic Energy

In the beginning of 1997, within the European Union INCO-Copernicus programme, a new project started on „Enhancement of the EU Decision Support System RODOS and its Customisation for Use in Eastern Europe”. The following groups of tasks are being performed:
• installation of the RODOS system in Emergency Centre,
• translation of the RODOS user interface into Polish,
• collection of geographical data and transfer into RoGIS (RODOS Geographical Information System),
• connection to radiological networks,
• connection to meteorological networks,
• collection consequence and emergency management data,
• adequacy of the food chain transfer and dose models and the corresponding data sets of the RODOS module ECOAMOR with respect to their validity in Poland,
• definition of criteria for division of Poland into radioecological macro-regions,
• collection of the data required for each radioecological region and their integration in RODOS,
• essential food chain model customisation for use in Poland,
• adaptation and/or modification of models, databases and criteria used in the RODOS module FRODO for quantifying agricultural countermeasures,
• collection of data sets relevant for countermeasure evaluation and ranking.

The paper [1] describes the current status of the RODOS customisation in Poland.

REFERENCES:

ADAPTATION OF THE NUMERICAL WEATHER FORECAST SYSTEM RAMS FOR USE IN POLAND

Mieczysław Borysiewicz ¹, Andrzej Gałkowski ², Slawomir Potempski ¹, Barbara Żelasińska ³,
Roman Żelazny ¹

¹ Institute of Atomic Energy
² Institute of Plasma Physics and Laser Microfusion
³ Warsaw University

In case of major nuclear or chemical accidents a Decision Support System (DSS) should be available to crisis management team to support the decision making during both the first hours of an accident and also in the longer terms. Its principal task is to give the real time assessment of the extent of the accident, the size and the position of the area affected and calculation of the number of people involved or affected. It necessitates timely numerical weather diagnosis and prediction and the simulation of the atmospheric pollutant transport. The speed and accuracy of such calculations is essential for effectiveness of the DSS.

Atmospheric dispersion phenomena can be naturally divided according to time and space scales. To cover all scales of interest for the DSS two approaches are possible:
- integration of different programmes developed for different scales
- application of a programme with built-in features of multi-scale handling with interactive nesting procedure allowing to specify any number of telescoping grids or even moving while calculating transport of dispersion and accounting for phenomena such as the propagation of thunderstorms.
The feasibility of the second approach rests heavily on the performance of the Numerical Weather Prediction Model for the area of concern. The application of Global or Continental Scale Prediction Systems is of limited use due to its coarse grid and limited orographic and land-use details in such a grid system. Thus there is a need to apply a Limited Area Model (LAM), that using detailed topography data, land-use information and other parameters, enables much more accurate and reliable weather forecasts in the area of interest. LAM are being embedded in the Global Weather Prediction System.

In Poland it is planned to use the Regional Atmospheric Modelling System (RAMS) [1], acquired from the Colorado State University, as a LAM, dedicated to the National DSS for Nuclear Emergencies (NDSS), being developed in cooperation with the programme RODOS of the Commission of the European Union.

RAMS represents the state-of-the-art, general purpose regional, mesoscale and cloud-scale atmospheric simulation and prediction software. RAMS resulted from the merger of the cloud-scale, non-hydrostatic model developed by William R. Cotton with the mesoscale primitive equation code developed by Roger A. Pielke. RAMS has been widely used, tested and documented in over 500 technical publications including studies of land/sea breezes, convective storms, weather modification, soil-vegetation-atmospheric interactions, air pollution dispersion and emergency response, mesoscale temperature forecasts, large eddy simulations and air flow over complex terrain. RAMS currently also serves as an operational regional, mesoscale and local weather prediction system.

Model configurations include 1-2 or 3 dimensions, numerous (>40 if needed) layers in the vertical, detailed planetary boundary layer representations, two-way multiple nested interactive grids (in both the vertical and horizontal). Horizontal grid sizes can range from < 2 m (simulating flow around building) to > 100 km (global circulation modelling). RAMS has hydrostatic or non-hydrostatic modes, and can employ uniform or available land use, topography, roughness, soil moisture and water temperature. There are selectable options for turbulence closure, finite difference schemes, geographic coordinate systems, upper and lateral boundary conditions and more.

RAMS generates basic atmospheric state variable (wind, temperature, pressure, moisture) at each model grid point and time step. From these a wide variety of parameters can be derived, including turbulence, vorticity, stability indices, sound propagation, air density, refractive indices, cloud liquid water, precipitation rate, etc.

Initializing data can be as minimal as a single local rawinsonde or profiler. Alternately, RAMS initialization can use an entire mesoscale data base or, more commonly, nest within grid point fields provided by NMC or other global models providing non-homogeneous initial and non-stationary boundary conditions. Four dimensional data assimilation (4DDA) is available.

RAMS has been implemented in the HP 735 software environment and adapted to serve as a front end to application modules of the transport of radionuclides in atmospheric flows, over distances of different scales (local, mesoscale and regional) for the purposes of NDSS/RODOS. An interactive graphic system, supported by NCAR and AVS packages, can be used to display and animate RAMS generated fields in a variety of formats.

A three level nested grid model has been developed and relevant geographical and land use data collected for an area of the Central and Eastern Europe, embedding Poland. Making use of this model, a successful experiment was carried out to provide 24 hour numerical weather forecast for Poland during a ten days period, basing on data, acquired in quasi real time mode and on-line from the European Centre for Medium Range Weather Forecast to set up the initial-boundary conditions for that model.

REFERENCES:
In case of a nuclear emergency a number of important decisions have to be undertaken by crisis management team basing on the currently available information, coming from radiological and meteorological real-time monitoring networks and taking into account predictions of development of radiological situation. Typically this information is not precise and may change in time rapidly. In order to support process of decision making appropriate uncertainties should be considered. These uncertainties come mainly from the following sources of information:

- source term,
- prediction of meteorological fields,
- dose assessment.

Supporting process of decision making means also taking into account possible benefits and disadvantages of undertaken decisions, preferences of decisions’ makers, impact on sociological and economical situation and, first of all, availability of technical means for crisis management team. Some techniques based on Bayesian approach are proposed as a basis for implementation of decision support system in case of a nuclear emergency in Poland [1]. Such an approach in natural way handles with all types of uncertainties mentioned above.

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19. I. A. Malakhov, B. Slowiński (invited lecture): Experimental investigation of cumulative phenomena using the 4π spectrometer SPHERE. Cairo, Egypt, 15-19 November 1997


21. Moustafa S. El-Koliel, M. Szuta: A Theoretical model for analysis of fission gas release from UO₂ fuel under irradiation conditions.. Al-Azhar Engineering Fifth International Conference, Cairo, Egypt, December 1997


25. J.R. Mika: (invited lecture) Amplitude-shape method: the quasistatic method revisited. 15th International Conference on Transport Theory, Goeteborg, Sweden, 1-7 June 1997 (J.R. Mika was invited as the member of the Programme Committee of the Conference and the chairman of one of the Sessions)


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40. **M. Szuta**: *Algorithm of fission gas release from UO₂ fuel during low and intermediate temperature irradiation*. International Workshop on Fuel Rod Modelling and the Use of TRANSURANUS, München, Germany, 29 - 30 April, 1997

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2. P. Czerski: Analiza zmian oporów przepływu w warunkach zachodzącego zjawiska wrzenia. Raport IEA B-2/97,-in Polish

3. K. Pytel: Efekty zatruciowe w reaktorze MARIA. Raport IEA B-3/97,- in Polish


7. R. Janczak: Porównawcza analiza kosztów wytwarzania energii elektrycznej dla różnych technologii z uwzględnieniem wpływu na środowisko (Comparative assessment of electricity generation costs for various sources including environmental impact). Raport IEA C- 7/97


10. K. Andrzejewski, T. Kulikowska: Obliczenia współczynników mnożenia paliw jądrowych w II-jej wersji suchego przechowalnika (Calculations of multiplication factors for the second version of a dry spent fuel storage). Raport IEA C- 10/97, -in Polish


13. K. Andrzejewski, T. Kulikowska: Parametryzacja stałych mareriałowych paliwa reaktora MARIA w trakcie wypalania (Parameterization of material constants for MARIA reactor burn-up calculations). Raport IEA B- 13/97,- in Polish


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17. B.Filipiak, Z. Haratym, K. Mlicki: System i procedury kontroli dozymetrycznej elementów konstrukcyjnych pochodzących z demontażu reaktora EWA (System and radiation protection control procedures for the construction elements from the decommissioning of EWA reactor). Raport IEA B-17/97, -in Polish

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21. W. Bykowski, K. Lewicki: Technologia montażu, zaladunku i rozładunku obrotowego kanału izotopowego (The assembling, packing and discharging of rotary isotope channel). Raport IEA C-21/97, -in Polish


24. K. Pytel, L. Dąbkowski: Optymalizacja bloku rozpraszającego do celów autoradiografii obrazów w reaktorze MARIA (Optimization of scattering block for the purpose of paintings autoradiography on MARIA reactor). Raport IEA C-24/97, -in Polish

25. W. Bykowski: Analiza cieplna zasobnika z siarką jako materiałem tarczowym w trakcie napromieniania (Thermal analysis of the can with sulphur target material during irradiation). Raport IEA B-25/97, -in Polish


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31. J. Ozimkowski, J. Suwalski: Magnetyczna struktura monokryształu perowskitu strontowo-
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calculations of the MARIA reactor based on the configuration data base). Raport IEA B-35/97, -in Polish

36. E. Hajewska, A. Malczyk, Z.A. Wojciechowski, M. Przyborska: Badania własności betonów
siarkowych przed i po napromienieniu w acceleratore (Investigations of the sulphur concrete
properties before and after irradiation in the accelerator). Raport IEA B-36/97, -in Polish

37. E. Fuksiewicz, T. Kozlowski, M. Wójcik: Instalacja do szybkiej pirolizy pyłu węglowego
(Installation for the quick pyrolysis of coal-dust suspension). Raport IEA B-37/97, -in Polish

38. E. Borek-Kruszewska, W. Bykowski: Program badań w instalacji WIW-300 (Experimental
program for WIW-300 test facility). Raport IEA B-38/97, -in Polish

39. P. Czerski: Analiza możliwości określenia oporów przepływu w kanale paliwowym reaktora MARIA
na podstawie doświadczeń przeprowadzonych na instalacji WIW-300 w 1995 roku (The estimation of
experiments performed in 1995 on WIW-300 installation in designation flow resistances in nuclear
fuel channel used in MARIA reactor). Raport IEA B-39/97, -in Polish

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proton implanted silicon). Raport IEA B-40/97

41. K. Wieteska, W. Wierzchowski, A. Turos, W. Graeff, R. Grötzschel: Rentgenowskie badania
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eksperymentów według zadanej algorytmu (Software for experiment control according to a given
algorithm) Raport IEA B-43/97, -in Polish

44. E. Borek-Kruszewska, W. Bykowski: Charakterystyki układu pomiaru i regulacji natężenia
przepływu chłodzącego przez odcinek badawczy (Static and dynamic characteristics of coolant flow
and control systems for test section). Raport IEA B-44/97

45. Borek-Kruszewska, W. Bykowski: Przeprowadzenie eksperymentów w instalacji WIW-300 z
detekcją krytycznej wymiany ciepła według zadanej algorytmu (Experimental research of critical
heat flux in WIW-300 test facility according to a given algorithm). Raport IEA B-45/97, -in Polish

47. Borek-Kruszewska, W. Bykowski: Opracowanie wyników badań eksperymentalnych (Experimental data analysis). Raport IEA B- 47/97, -in Polish


49. Z. Rusinowski: Badania dozymetrycznego miernika promieniowania mieszanego w polu impulsowym (Tests of the dose equivalent meter of mixed radiation in pulsed field). Raport IEA B- 49/97, -in Polish

50. Z. Rusinowski, N. Golnik: Testy rekombinacyjnego miernika równoważnika dawki przestrzennej we wzorcowym polu promieniowania mieszanego wielkiej energii w CERN (Tests of the IAE dose equivalent meter in radiation field of High Energy Calibration Facility at SPS- CERN). Raport IEA B- 50/97, -in Polish

51. N. Golnik: Mikrodozymetryczna metoda wyznaczania przestrzennej równoważnika dawki w polach promieniowania mieszanego za pomocą komory rekombinacyjnej (Determination of the ambient dose equivalent in mixed radiation fields by recombination chamber - microdosimetric approach). Raport IEA B- 51/97, -in English


53. E. Hajewska, W. Szteke: Prace naukowo-badawcze dla zleceniodawców zewnętrznych (Research works for the external institutions). Raport IEA B- 53/97, -in Polish

54. A. Hofman, T. Kochański, A. Malczyk: Badania wpływu oddziaływania produktów rozpadu na koszulkę elementów paliwowych (Influence of the fission products on the cladding material of fuel elements). Raport IEA B-54/97, -in Polish


59. T. Wagner, W. Szteke, E. Hajewska: Instrukcja technologiczno-dozymetryczna rekonstrukcji próbek świadków metodą łączenia doczołowego w Laboratorium Badań Materiałowych (The dosimetric instruction for welding technology of reconstruction Charpy specimens in the Material Research Laboratory of IAE). Raport IEA D- 59/97, -in Polish

61. S. Ligenza, J. Ozimkowski: Mössbauer studies of magnetic oscillators in Li-Ti-Zn induced by external magnetic field. Rapport IEA B- 61/97,-in Polish


63. J. J. Milczarek, J. Jankowska-Kisielińska, K. Mikke, B. Henion: Anisotropy of the generalised susceptibility in Mn(38%Ni) alloy in the magnetic phase transition region. Rapport IEA B- 63/97

64. W. Bykowski: Experimental results on migration of corrosion products in a cooling loop of the MARIA reactor. Part 1 - Start-up phase. Rapport IEA B- 64/97,-in Polish

65. P. Marks, A. Koziel: Experimental results on migration of corrosion products in a cooling loop of the MARIA reactor. Rapport IEA C- 65/97

66. Ł. Strugalski, E. Strugalska-Gola, A. Wojciechowski: Quantitative characteristics of nucleons emitted in various stages of nuclei spallation. Rapport IEA B- 66/97,-in Polish

67. S. Bednarski, M. Ślepowroński, K. Siemensmeyer, A. Gukasov: Growth of Fe3(x)Mn(x)Si (x=0.05) single crystals of high structural quality and improvement of parameters of polarizing neutron monochromators prepared from those crystals. Rapport IEA B-67/97,-in Polish


70. K. Józefowicz: Improved determination of neutron ambient dose equivalent H*(10)n in standard fields of isotope neutron sources in IAE. Rapport IEA B- 70/97,-in English


72. V. P. Voronov, A. Rajewska: Neutron scattering in 2,6 lutidine confined in porous glass. Rapport IEA B- 73/97
74. B. Paluchowska, J.K. Maurin, J. Leciejewicz: Dimeryczne cząsteczki związków kompleksowych kobaltu i cynku z kwasem 2-furanokarboksylowym stabilizowane systemem wiązań wodorowych typu C-H \_\text{woda} - H\_\text{furan} O\_\text{woda} - H \_\text{n}(Dimetric molecules of Co(II) and Zn(II) complexes with furan 2 carboxylic acid stabilized by the system of interconnect C - H\_\text{water} O\_\text{water} - H\_\text{furan} O\_\text{water} - H \_\text{n} hydrogen bonds). Raport IAEA B- 74/97

75. S. Ligenza: O sprzężeniu oscylatorów w samoorganizującej się magnetycznej strukturze komórkowej w ferrycie \text{Li-Ti-Zn} (On the oscillator coupling in self-assembled cellular magnetic structure in \text{Li-Ti-Zn} Ferrite system). Raport IAEA B- 75/97


OTHER ACTIVITIES

Seminars at the Institute of Atomic Energy

GENERAL SEMINARS


2. I. Malachov Prof, G. L. Mielkumov Ph.D (JINR Dubna): Research plans of the Laboratory of High Energy in Dubna ................................................................. 24 April 1997

3. Natalia Golnik Ph.D: Wykorzystanie reakcji \text{^{10}B(n,a)^7Li} do celów medycznych (BNCT) (Boron neutron capture therapy) ................................................................. 8 May 1997

4. Rostislav Mach Ph.D (Nuclear Physics Institute, Řež, Czech Republic): Research and development of modern nuclear technologies: recent program in the Czech Republic ........................................ 14 October 1997

5. M. Diaczenko Ph.D (JINR Dubna): Experimental activity in frame of ENERGIA program in Dubna, .................................................................October 1997

SEMINARS ON THE SOLID STATE PHYSICS


3. Andrzej Czachor Prof. Ph.D., D.Sc: The IAEA meeting on neutron beam research, Lisbon. .................................................................20 November 1997

4. Krzysztof Maletka M.Sc.: Phase transitions in selected compounds containing U\text{\textsuperscript{4+}}: .................................................................4 December 1997

5. Housni Al-Wash, (Zagazig University, Cairo, Egypt): Thermodynamic functions of the model antiferromagnet with identical coupling between all spins ......................................18 December 1997
JOINT SEMINARS ON RADIATION PROTECTION AND MEASUREMENTS
-Institute of Atomic Energy (IAE)
-Soltan Institute for Nuclear Studies (INS)
-Radioisotope Center (RC)

1. Aleksander Polański, Ph.D. (INS): Źródła promieniowania przy wytwarzaniu energii z wykorzystaniem akceleratorów (Radiation sources accompanying the energy production with the use of the accelerators). .......................................................... 5 February 1997


SEMINARS ON NUCLEAR REACTOR PHYSICS AND ENGINEERING (IAE RESEARCH REACTOR CENTRE)


2. Tadeusz Matysiak B.Sc.: Projekt koncepcyjny suchego przechowalnika wypalonego paliwa jądrowego w szybie betonowego bloku reaktora EWA. (The preliminary project of the dry storage facility for spent fuel in the concrete shaft of EWA reactor) .......................................... 11 March 1997


4. Stefan Chwaszczewski Prof.Ph.D.,D.Sc.: Zastosowanie wysoko wzbogaconego paliwa jądrowego do zmniejszenia zagrożenia środowiska od składowania wypalonego paliwa. (Application of high enriched fuel for minimalisation of the environmental hazard during storage) ................................................ 8 April 1997


6. Mr. A. A. El-Kafas (Egypt): Research Reactors in Egypt - present status and future. 2 October 1997

7. Mr. Attya A. Abou-Zaid (Egypt): Proposed method for the spent fuel burn-up determination. ......... 30 October 1997

SEMINARS GIVEN BY IAE SCIENTIST
abroad

1. Z.I.Woźnicki Ph.D.: Construction of pre-factorization algorithms for different geometries of point mesh. University of Novi Sad, Yugoslavia .......................................................... 16 September 1997

2. Z.I.Woźnicki Ph.D.: Recent results in the development of efficient iterative methods. University of Santa Clara, California, USA ...................................................... 28 October 1997
3. Z.L.Woźniak Ph.D.: Some results of study monotonicity problems and a high reliability of symmetrical solutions obtained by means of prefactorization algorithms. UCLA (University of California, Los Angeles), Los Angeles, USA 3 November, 1997


5. M.Zieleński Prof.Ph.D., D.Sc.: Recombination Methods for the Dosimetry of Mixed Radiation. Ionizing Radiation Division of the National Institute of Standards and Technology, Gaithersburg, Maryland, USA 30 October 1997

in Poland

1. S.Chwaszczewski Prof.Ph.D., D.Sc.: Nuclear Power in Poland; Prospects and Conditions. Institute of Experimental Physics, Warsaw University 10 January 1997

2. S.Chwaszczewski Prof.Ph.D., D.Sc.: Nuclear Power in Poland; Environmental Impacts. Institute of Experimental Physics, Warsaw University 25 February 1997


4. B Paluchowska M.Sc.: Metody koordynacji metali ziem alkalicznych przez aniony 2- i 3-furankarboxylanowe - obliczenia kwantowomechaniczne a wyniki badań strukturalnych. Referat na seminarium Pracowni Krystalchemii Wydziału Chemii Uniwersytetu Wrocławskiego (Coordination of alkaline earth metals with 2- and 3-furancarboxylate anions - quantum mechanical calculations and crystallographic data) April 1997

5. J.K.Maurin Ph.D: (referat zaproszony) Zależna od konformacji wydajność reakcji glutarimidów z fenyllitium. Seminarium Sekcji Krystalchemii Polskiego Towarzystwa Chemicznego, (Conformation related reaction efficiency of glutarimides with phenyllithium; Invited lecture at Seminar of Crystallochemistry Section of Polish Chemical Society) May 1997

6. J.K.Maurin Ph.D: Wiązanie wodorowe oksy- karboksyl: Preferowane oddziaływania determinujące upakowanie w kryształach "karboksyl-oksymów". Pracownia Krystalchemii Wydziału Chemii Uniwersytetu Warszawskiego (Oxime-carboxyl hydrogen bond: the preferred interaction determining crystal packing of "carboxy-oximes". Seminar of Crystallochemistry Laboratory, Chemistry Department, University of Warsaw) 18 November 1997

7. L.Górski Ph.D: Przemiany fazowe w warunkach szybkozmiennych działań temperatury Instytut Fizyki Uniwersytetu Warszawskiego (Phase transitions at the short time high temperature action. X-ray Seminar, Physics Department, University of Warsaw) 5 November 1997


12. S. Bednarski Ph.D., M. Ślepwoński M.Sc.: Otrzymanie wysokiej jakości (dokonalności strukturalnej) monokryształów stopu Fe$_{2,95}$Mn$_{0,05}$Si i stopu CoFe (8% at.) oraz doskonalenie parametrów użytkowych polaryzujących monochromatorów neutronów wykonanych z tych kryształów. Ogólnopolskie Seminarium Rozpraszania Neutronów, Chlewiska, (Growth of high quality single crystals of Fe$_{2,95}$Mn$_{0,05}$Si compound and CoFe (8%at.) alloy and improvement neutron polarizing monochromators prepared from these crystals. Polish Neutron Scattering Lectures, Chlewiska, Poland) - in Polish, November 1997

LECTURES AT UNIVERSITIES

Rajmund Janczak Ph.D. Nuclear Energy Warsaw University of Technology
Janusz R. Mika Prof. Ph.D., D.Sc Mathematics Technical University of Łódź
Bronisław Słowiński Prof. Ph.D., D.Sc Physics Warsaw University of Technology
Zbigniew Strugalski Prof. Ph.D., D.Sc Physics Warsaw University of Technology

SCIENTIFIC AND TECHNOLOGICAL CO-OPERATION JOINT PROJECTS

BULGARIA

Joint IAE Research Project with the Institute of Nuclear Research and the Atomic Energy, Bulgarian Science Academy:
- Study of Atomic Order in Glasses and Other Amorphous Materials.
Polish side partner: E. Maliszewski Ph.D., D.Sc

CERN

Common CERN-CEC Project:
- Measurement of Dose Equivalent in Relativistic Stray Radiation Fields. (CEC FI3P-CT92-0026).
Polish side partners: N. Golnik Ph.D., Prof. M. Zielczyński Ph.D., D.Sc.

CZECH REPUBLIC

CMI Praha, dr M. Kralik
- Intercomparison of dosimetric parameters measured in standard fields of mixed radiation
Polish side partner: K. Józefowicz Ph.D.

- Protocol on the cooperation between the Institute of Atomic Energy (Świerk-Otwock) and the Nuclear Institute of the Academy of Science of the Czech Republic (Řež Republic/Prague) in:
Nuclear reactions of intermediate energy in extended heavy targets
Czech side partner: D. Sc. R. Mach
Polish side partner: B. Słowiński Prof. Ph.D., D.Sc

EUROPEAN RENEWABLE ENERGY CENTERS AGENCY (EUREC AGENCY EEIG) Contract nr. ERBJU2CT920179
- Growth of Multicrystalline Silicon Ingots for Photovoltaic by a modified Method of Electromagnetic Casting.
Polish side partner: S. Bednarski Ph.D.

EGYPT

- Protocol on the cooperation between the Nuclear Research Center (Cairo) and the Institute of Atomic Energy in:
Radiation materials investigation using beams of heavy ions, neutrons and gamma rays.
Publications

Egyptian side partners: prof. A.M. Adawi, prof. N. Comsan
Polish side partner: prof. B. Słowiński, Ph.D., D.Sc.

FRANCE

Joint IAE Research Projects with CEN SACLAY, Laboratoire Leon Brillouin, Dr B. Hennion
- Anisotropy of generalised susceptibility in Mn(38% Ni) alloy in the magnetic phase transition region.

- Temperature dependence of the parameters of the spin wave dispersion relation in Mn(38% Ni) alloy.

- Improvement of Single Crystal CoFe(8at%) Polarizing Monochromators.
Polish side partners: S. Bednarski Ph.D. M. Śleprowoński M.Sc

GERMANY

Joint IAE Research Project with Neutron Physics Division of the Physicalisch - Technische Bundesanstalt Braunschweig dr. H. J. Brede:
- Development and Test of Recombination Method for Dosimetry in Mixed Radiation Fields.
Polish side partner: N. Golnik Ph.D.

Polish-German Cooperation
Joint IAE Research Project with DESY-HASYLAB, Dr. W. Graef
- Topographic Studies of Planar Structures and highly Doped Crystals.
Polish side partner: K. Wieteska Ph.D. (Polish-German Gouvernements Co-operation 244/R96/R97/R98 N-1000 95 BO)

Associated Contract to the EC-Contract No F14P-CT95-0007 Contractor: Forschungzentrum Karlsruhe GmbH, Technik und Umwelt
- RODOS; a real time on-line decision support system for off-site emergency management in Europe.
Polish side partner: M. Borysiewicz Ph.D.

GREAT BRITAIN

NPL Teddington, dr David Thomson
- Determination of dosimetric parameters of neutron + gamma fields.
Polish side partner: K. Józefowicz Ph.D.

JOINT INSTITUTE FOR NUCLEAR RESEARCH, DUBNA, RUSSIA

Common IAE Research Projects:
- Investigation of influence of Heavy Ions Irradiation on Mechanical Properties of Austenic Stainless Steel.
Polish side partner: A. Hofman Ph.D.

JINR, Laboratory of Biophysics, prof. E. A. Krasavin.
- Radiobiological and Radiation Investigations using JINR accelerators.
Polish side partner: Prof. M. Zielczyński Ph.D., D.Sc. N. Golnik Ph.D.

Laboratory of Nuclear Problems, JINR, Dr. O. V. Savchenko
- Radiotherapy with the JINR Phasotron Beams.
Polish side partners: N. Golnik Ph.D., Prof. M. Zielczyński Ph.D., D.Sc, Z. Rusinowski M.Sc.

JINR, Laboratory of High Energy, prof. A. Malachow.
- Experimental and theoretical investigations of the electronuclear methods of energy production - and radioactive waste transmutation - project ENERGIYA.
Polish side partner: Prof. Z. Strugalski Ph.D.
IAEA

International Atomic Energy Agency (IAEA), Vienna, Austria,

- **Design of the measuring systems for industrial demonstration plant for electron beam flue gas treatment, according with the requirements of the ISO, ECD, EPA and JIS standards.**

Project leader: dr Massoud Samei, Head Europe TC Divisions IAEA
Polish side partner: Janusz Licki M.Sc.

JAPAN

Japan Atomic Energy Research Institute (JAERI), Takasaki Radiation Chemistry Research and Establishmment (TRCRE) Takasaki,

- **Experimental optimization studies of the radiation technology for SO₂ and NOₓ removal from flue gases carried out at pilot plant at EPS Kawęczyn, according to the bilateral programme and with the participation of a Japanese specialist.**

Project leader: dr Okihiro Tokunga, Director Department of Radiation Research for Environment and Resource TRCRE
Polish side partner: Janusz Licki M.Sc.

REPUBLIC of SOUTH AFRICA

Scientific cooperation with the University of National, Durban: **Numerical Analysis.** Polish side partner: Prof. J.R. Mika, Honorary Research Fellow of the University of Natal.

RUSSIA

Scientific Technological Cooperation Joint Project: IAE with State Technical University and Institute of Metal Physics (Moscow)

- **Investigation of atomic and magnetic microdynamics, structural peculiarities close to martensitic phase transition and kinetic of the decomposition, connected to physico-mechanical features of 3d metal alloys.**


Technological Cooperation Joint Project of IAE with Institute of Metal Physics, Moscow:
- **The Studies of the Physical Basis of Technological Processes of Developing High Damping Alloys with Peculiar Elastic Properties**


SWEDEN

Scientific Technological Cooperation Joint Project IAE with Studsvik Neutron Research Laboratory:
- **Investigation of Magnetic Materials by Polarized Neutron Diffraction Method.**

Polish side partner: K. Blinowski Ph.D.

YUGOSLAVIA

Scientific Co-operation with University of Novy Sad (Prof. Ljiljana Cvetković)

- **Numerical Mathematics.**

Polish side partner: Z. I Woźnicki Ph.D.
LONG TERM VISITS OF IAE STAFF MEMBERS TO FOREIGN COUNTRIES

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<td>A.Hofman</td>
<td>Joint Institute for Nuclear Research Dubna</td>
<td>February 1995 - February 1999</td>
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FELLOWSHIPS at the IAE

Fellowships granted by Polish National Ministry of Education on the basis of the Agreement on Cultural and Technical Cooperation between the Governments of Egypt and Poland:

- Mr Al-Wahsh Housni Awad Alla Awad Alla Ph.D., student from Egypt; period of study 4 years, starting from 1 November 1994, supervisor prof. A.Czachor

- Mr Moustafa Saleh Moustafa El-Koliel Ph.D., student from Egypt; period of study 4 years starting from 15 September 1995, supervisor prof. S.Chwaszczewski

- Mr Ahmed Attya Abou Bakr Ph.D., student from Egypt; period of study 4 years starting from 1 April 1996, supervisor prof. S.Chwaszczewski

D.Sc. and Ph.D Theses

D.Sc THESIS

Marcin Szuta Ph.D.: Processes of Fission Gas Release from Uranium Dioxide During Neutron Irradiation. Warsaw University of Technology 16 October 1997

Ph.D THESSES

Beata Paluchowska: Coordination of 2- and 3-furanocarboxylate anions by alkaline earth metals. Instytut Energii Atomowej, Świerk 30 June 1997

Nabendru Paramasur: Amplitude-shape method for the numerical solution of ODES. Durban-Vestville University. Supervisor: Prof. J.R. Mika February 1997

STRATEGIC GOVERNMENT PROJECT

1. Radioactive Waste and Spent Fuel Management
(SPR-4); November 1997-December 1999
Research part of the project co-ordinated by IAE; Co-ordinator J.J. Milczarck M.Sc.
GRANTS
Granted by State Committee of Scientific Research

1. **Recombination Method for Microdosimetry**.
   Chief Investigator: Natalia Golnik Ph.D.,
   grant No. 4 P05D 033 11; November 1996 - September 1999

2. **Decision Support System in Case of Nuclear Emergency**.
   Chief Investigators: Mieczyslaw Borysiewicz Ph.D., Prof. Roman Żelazny Ph.D., D.Sc.,
   grant No 4109294 C/1598; January 1995 - December 1997

3. **Heteroring Oxygen in the Process of Coordination of Alkaline Earth Metals**.
   Chief Investigator: Beata Paluchowska M.Sc., PhD grant, Supervisor Prof. A. Czachor
   Ph.D., D.Sc.
   grant No 3T09A12210; January 1996 - June 1997

4. **Optimisation Study of the Electron Beam Process for Removal SO\textsubscript{2} and NO\textsubscript{x} from Flue Gas with High Concentration of SO\textsubscript{2}**.
   Chief Investigator: Janusz Lacki M.Sc., PhD grant, Supervisor Prof. A. Chmielewski
   Ph.D., D.Sc.
   grant No 3T09C 02610; January 1996 - June 1997

5. **Mössbauer Spectroscopy of Fullerites**.
   Chief Investigator: Zbigniew Kucharski Ph.D.
   grant No. 7T08A01610; April 1996 - December 1997

6. **Package of Computational Programs for Increased Operational Safety of the MARIA reactor**.
   Chief Investigator: Krzysztof Andrzejewski Ph.D.
   grant No 8T10B009 95 C/2766; May 1996 - November 1998

7. **Safety Research of the MARIA Reactor Fuel Assembly Operation at Increased Power**.
   Chief Investigator: Elżbieta Borek-Kruszewska M.Sc.
   grant No 8 T10B008 95C/2767; July 1996 - July 1998

8. **Transport and activation of corrosion products in a nuclear reactor with independently operating multi-loop cooling**.
   Chief Investigator: Piotr Marks M.Sc., PhD grant, Supervisor Prof. A. Chmielewski
   Ph.D., D.Sc.
   grant No 8 T 10 13014 12; January 1997 - July 1998

9. **Application of amplitude-shape method to reactor kinetics**.
   Chief Investigator: Prof. Janusz Mika Ph.D., D.Sc.,
   grant No N8T 10B 05513; July 1997 - December 1998

10. **Magnetic inelastic scattering in the antiferromagnetic Mn(12%Ge) alloy**.
    Chief Investigator: J. Jankowska-Kisieliriska M.Sc.,
    grant No 2 P03B 071 13; January 1997 - December 1998

11. **Hydromechanical study of flow boiling phenomena in nuclear MARIA reactor**.
    Chief Investigator: Piotr Czerski M.Sc., PhD grant, Supervisor Associated Prof. A. Rasmus
    Ph.D., D.Sc.
    grant No 8 T10B 024 12; January 97 - June 1998

12. **Study of magnetic properties of some rare earth compounds with AuCu\textsubscript{3}-type structure by elastic and inelastic scattering of neutrons**
    Chief Investigator: Prof. Andrzej Murasik Ph.D., D.Sc.,
    grant No 466/PO3/97/12; March 1997 - June 1999

13. **Phase transition in some ionic conductors containing uranium U\textsubscript{4+}**.
    Chief Investigator: Krzysztof Maletka M.Sc., PhD grant, Supervisor Prof. A. Murasik
    Ph.D., D.Sc.
    grant No 465/PO3/97/13; March 97 - January 1998
   Chief Investigator: Assoc. Prof. Witold Szteke M.Sc.,
   Project No 7 7845 95 C/2504, Contract No 1442/C.T08-7/95 ; January 1996 - December 1997

15. Longterm safe storage of the used medical radiation sources emitting radon in the tight closed steel containers.
   Chief Investigator: Assoc. Prof. Witold Szteke M.Sc.,
   Project No 7 7846 95 C/2503, Contract No 1586/C.T08-7/96 ; May 1996 - August 1997

RESEARCH PROJECTS GRANTED BY EUROPEAN UNION

Enhancement of the EU Decision Support System RODOS and its customisation for use in Eastern Europe. (Ulepszenie Systemu Unii Europejskiej Wspomagania Decyzji RODOS i jego przystosowanie do wykorzystania w Europie Wschodniej)
Chief Investigator Mieczyslaw Borysiewicz Ph.D., grant F14 P-CT96-00XY; Coordinator FZK Karlsruhe Germany K.W.E. Kontrakt Nr ERBJC15 CT 96 0318, January 1997-June 1999
Decision Support System for Nuclear Emergency in Europe (System wspomagania decyzji w zakresie postępowania w kraju po wypadku jądrowym w ramach programu UE Copernicus).
Chief Investigator: Mieczyslaw Borysiewicz Ph.D., January 1995 - June 1999

Przygotowanie projektu w programach badawczych Unii Europejskiej pt. Ocena właściwości mechanicznych materiałow konstrukcyjnych przed i po napromienieniu z zastosowaniem próbek odzyskiwanych i mikroprobek PHARE PL-09/95/04.02 1/135
Chief Investigator: Assoc.Prof. E.Hajewska PhD.
(Preparation of the project to the one of the European Comission research programme „Estimation of mechanical properties of construction materials before and after irradiation using the reconstructed specimens and micro-specimens”. PHARE PL-09/95/04.02 1/135
Chief Investigator: Assoc.Prof. E.Hajewska PhD.)
CONFERENCES ORGANISED BY IAE AND WITH IAE COOPERATION

IV SEMINAR
"MATERIALS INVESTIGATION FOR POWER STATIONS AND POWER INDUSTRY"
18-20 June 1997, Zakopane

CHAIRMAN:
E. Hajewska

SCIENTIFIC PROGRAM COMMITTEE
E. Hajewska, Świerk
S. Chwarszewski, Świerk
A.J. Tkacz, EuRoPol GAZ S.A.
K. Wieteska, Świerk

ORGANIZING COMMITTEE
W. Szteke - chairman
J. Wasiak - secretary
W. Bilous
M. Przyborska
J. Wojciechowska
B. Zubowski

This was the fourth seminar on the subject covering a wide range of applications implemented the operation and maintenance of power plants including the pipelines, heat exchanger and other process equipment as well as the operation of gas transport pipelines. There were three sessions on:
- Materials in Power Industry,
- Gas Transport Pipelines,
- Diagnostic Methods.

The full papers were published in Raport IAE-26/A and the short presentations in the second part of the proceedings.

The seminar was organized by Material Research Laboratory IAE.

PROGRAMME

Lectures

1. J. Bielanik, J. Wawszczak, J. Żukowski: Application of the Polish Steel Grade 0H14N5MCuNb for Production of Rotor Disks for Turbocompressors by Means of Vacuum Soldering Technology
2. J. Okrajni, J. Woszczek, K. Mutwil, M. Ciesla: The Pipeline Effort and Life Assessment
5. N. Pikor: Hydraulic Pressure Test of Transit Gas Pipeline Jamal-Europe
6. G. Wiśniewski: Development of the Gas Pipeline Systems European Standards and Codes in the Sphere of their Construction
7. J. S. Michalik: Provision of International Law Regulations on the Control of Major Chemical Accident Hazards Regarding Liquid and Gaseous Fuel Transportation through Pipeline Systems
8. C. Dybiec, S. Janowski, S. Włodarczyk: The Control of Stress and Structure Changes by the Eddy-Currents Method
Short presentations

1. C. Dybiec, S. Wlodarczyk: Estimation of Retained Austenite by Eddy-Currents Method
2. W. Bokszczanin: Anticorrosive Protection of Steel Construction Exposed at the Elevated Temperatures
3. L. Golaski, M. Biel Golaska: Estimation of the Pressure Vessel Strength on the Bases of FAD Diagram

WORKSHOP

FORECASTING OF MESOSCALE PHENOMENA
2 - 13 June 1997

organized by:
Institute of Geophysics, Warsaw University
Interdisciplinary Center for Mathematical and Computational Modelling, Warsaw University
Institute of Meteorology and Water Management
Institute of Atomic Energy

Lectures
1. K. Haman: From history of NWP
2. B. Jakubiak: Mesoscale Forecasting with UKMO model: Polish Experiences
3. B. Jakubiak: Output from Model at ICM UKMO
4. Zb. Sorbjan: Modelling of Atmospheric Boundary Layer
5. Craig Tremback: The Use of Parallel Computer Platforms for Operational Mesoscale Weather Forecasting
6. Craig Tremback: An Emergency Response System Using an Operational Mesoscale Model
7. P. Grabowski: Modelling of Thermodynamical Processes with Precipitation
8. L. A. Smith: Nonlinear Dynamics Models and Systems
10. L. Rontu: Problems of HIRLAM Radiation Parameterization in Cloudy Cases
12. P. Grabowski: Cloud Resolving Modelling of Convection
15. P. Benard: Non-hydrostatism as a Switchable Option in "Classical" Primitive Equations Modelling: Laprise Coordinate Implementation in ALADIN
16. L. Lobocki: Visualization Tools for PC
17. Stuart Bell: General Description of Unified Model Parallel Version of the Analysis Assimilation, New Correction Observation Processing and Quality Control System
18. P. Andrews: The development of an Operational Variational Data Analysis Scheme
19. B. McPherson Assimilation od Cloud/rain Data in MOPS System
20. D. Salmon: Experiences with the Parallelization of the Code for HIRLAM and Operational Models in the T3E Environment
21. V. Grubisic: The Basic Analytic Equations and Numerical Approximations of the EULAG Model
22. V. Grubisic: Applications of the EULAG Model to Dry and/or Moist Orographic
23. I. Zawadzki: Integration of Model and Remote Sensing in Nowcasting
24. Lex Wolters: Automatic Code Generation
25. K. Nowinski: Visualization with AVS
26. L. Lobocki: Overview of NCEP, Atmospheric Models with the Short Description of the ETA Model
27. M. Niezgodka: Perspectives of Mesoscale Modelling in ICM
INFORMATION ACTIVITY

1. N. Golnik as the Editor of the Proceedings of the Symposium "Consequences of Polonium and Radium Discovery for Medicine, Radiological Protection and Medical Industry", Polish Journal of Medical Physics and Engineering, Vol. 3, No.9, 1997

2. P. Jaracz, N. Golnik, J. Jabłońska: Fizyczne podstawy techniki rentgenowskiej, dozimetrii i ochrony radiologicznej. Podstawy programowe. (Physical principles of the X-ray techniques, of the dosimetry and radiological protection - proposed scope of an educational programme) Raport Nr 8, Dział Szkolenia i Doradztwa Instytutu Problemów Jądrowych, Świerk, 1997


EXPERT ACTIVITY

EXPERT OPINIONS MADE IN MATERIALS RESEARCH LABORATORY

Witold Szteke, Ewa Hajewska, Waldemar Bilous, Jan Wasiak, Tadeusz Wagner, Mariusz Wieczorkowski, Zygmunt A. Wojciechowski, Antoni Maleczyk

Institute of Atomic Energy

In 1997 in Material Research Laboratory 15 expert opinions were made for external customers. Most of them were complex and relative to the investigations of the chemical composition of materials, mechanical and corrosion properties as well as structure. The properties of the main steam pipelines after long time exploitation including the welding joints were investigated, especially its toughness, impact and structure changes, and the materials of gas transport pipelines were tested. Material Research Laboratory has the Certificate of Testing Laboratory Accreditation Nr L 25/1/95 and the II Degree Certificate of Recognition of the Office of Technical Inspection Nr L-II-001/95. These certifications give MRL the license to prepare expert opinions and reports for materials. All work is carried out according to the Quality Assurance Program described in the Quality Books, General and Operating Procedures.
POPULARIZATION ACTIVITY OF NUCLEAR SCIENCE AND TECHNOLOGY

Klemens G. Kruszewski
Institute of Atomic Energy

Institute of Atomic Energy continuously active in the field of popularization. In the year 1997 the permanent popularization activity was continued. 3216 visitors (secondary schools, universities, civil defence) have visited the Świerk centre and got acquainted with its nuclear research facilities.

During the last weekend of October 1997 the research centre at Świerk was for the fourth time thrown open to the public. Those "open house" days were organized by the Institute of Atomic Energy, the Andrzej Soltan Institute for Nuclear Studies and the Radioisotope Centre POLATOM together with the National Atomic Energy Agency in response to permanent great concern expressed by the public at large and to meet the demand of our scientific community insisting on giving people better information about nuclear research and technology and benefits and risk connected with the application of nuclear techniques.

The Świerk centre was open to all but special invitations were sent to over four hundred primary and secondary schools of Warsaw and Warsaw province.

At the Institute of Atomic Energy
- The high-flux research reactor MARIA.
- Neutron spectrometers and diffractometers for the investigation of crystal and magnetic lattice dynamics by means of inelastic neutron scattering.
- The management of radioactive waste originating mainly from the production and use of radioactive preparations for tumour diagnostics and therapy.
- The system of protection against ionizing radiation and the inspection of fissible materials demanded by the Treaty on the Non-Proliferation of Nuclear Weapons.
- Research in the field of solid-state physics: the measurement of Mössbauer effect of new magnetic materials and the compounds of rare earths with transition metals; the artificial growth of metal and alloy monocrystals for neutron polarizers and monochromators; the investigation of magnetic structure properties of uranium and rare earths compounds by neutron scattering technique; the X-ray examination of molecular and crystalline structure of organic compounds including those with pharmacotherapeutical activity and so on.
- The investigation of irradiated construction materials in hot cells to assure safe operation of research reactors and other nuclear facilities.

At the Institute for Nuclear Studies.
- The exhibition demonstrating Institute's activities.
- Measurement techniques and nuclear electronics including the construction of nuclear radiation detectors of the "silicon ball" type and the set of neutron detectors for the EUROBALL project. Research in the field of nuclear physics aimed at applications in medicine and environment protection for instance the measurement of cross-sections required to determine the total calcium content in man and Pb-210 content in soil.
- The compact isochronous proton cyclotron C-30; principle of operation, design, possible application.
- Research in the field of hot plasma and the possibility of its use in thermonuclear fusion and technology (e.g. to modify materials by surface hardening, to improve anticorrosive properties and so on).
- Electron accelerators and other equipment for cancer therapy.

At the Radioisotope Centre POLATOM.
The exhibition demonstrating the production of radioisotopes for nuclear medicine, industry, research and environment protection. During the two days the research centre at Świerk was visited by over 1800 visitors.

The Institute of Atomic Energy took also part in the celebration of the 130 anniversary of M. Skłodowska-Curie birthday and the centenary of radium discovery. The celebration was organized by the National Atomic Energy Agency.

To sum up, in the year 1997, the Institute of Atomic Energy received over 5700 visitors and organized their visits in both Institutes.
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