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This report was prepared by the Scientific Publications Office from contributions provided by the scientific and technical staff of ENEA's Applied Physics Division (Main collaborators in the preparation of this issue: Marisa Cecchini, Lucilla Crescentini, Lucilla Ghezzi, Carolyn Kent, Mauro Bottomei, and Peter Riske for text-composition, editing, artwork, and overall coordination; Sergio Ciarlo for photographic work.)

**Cover picture:** Visible photoluminescence from lithium fluoride films thermally evaporated on glass (left) and silicon (right) substrates and treated by a beam of electrons excited by the 458-nm line of an argon laser.
This report outlines the 1998 research activities carried out by the Applied Physics Division of the Innovation Department of ENEA.

The fields addressed and discussed include:

- optical and electro-optical technologies (chaps. 1 and 2);
- accelerator technologies (chap. 3);
- diagnostic systems for science and engineering (chaps. 4 and 5);
- theory, modelling and computational methods (chaps. 6 and 7).

The aim of the Applied Physics Division is to develop technologies and systems that can be directly applied by internal (ENEA) and external users in research (high-resolution spectroscopy, laser-generated soft-x-ray sources), production processes (laser material photoproduction, structural analysis), social, cultural and environmental sciences (laser remote sensing, modelling of ecosystems and population dynamics) and medicine (particle accelerator for radiotherapy).

Most of the work in 1998 was performed by the division's laboratories at the Frascati, Casaccia and Bologna Research Centres of ENEA; some was done elsewhere in collaboration with other ENEA units, external laboratories and industries. A good share of the activities was carried out for international projects; in particular, the IV European Union Framework Program.

I should like to stress that crucial to achieving the main objectives of the research activities was the collaboration between the division's different laboratories: the interdisciplinary approach required to carry out the work described in this report necessitates integration of a wide spectrum of expertise. The organisation of the Applied Physics Division is shown in chapter 10, while a complete list of personnel is given in chapter 11. I should also like to record that the strong and qualified support of the Technical and Administrative Services (chap. 8) was invaluable in smoothing out the course of the division's research activities.

It is hard to single out particular results or achievements. The work carried out during 1998 is amply documented in the published articles and conference papers (most of which invited) listed in sections 9.1–9.3. The division itself organised several well-attended meetings and seminars (9.4).

Finally, the continuous evolution of the division's activities and the strong interaction with national and international research institutes, universities and industries in the framework of integrated research projects—as described in this report—surely go to demonstrating the vitality of the research teams and technical and administrative services.
1.1 LASER REMOTE SENSING

Laser remote-sensing activities at ENEA Frascati are mainly devoted to developing instruments for real-time environmental monitoring of large areas. Several laser-based systems have already been constructed for remote sensing of atmospheric, terrestrial and marine constituents and for detection of heavy metals in contaminated soils. The infrared light detection and ranging/differential absorption (lidar/DIAL) facility has been extensively used to test hardware and software for range-resolved measurements of minor atmospheric gaseous components and pollutants. The mobile lidar fluorosensor laboratory is a versatile system for seawater quality measurement and was recently used in the oceanographic campaign of the XIII Italian Antarctic Expedition. New laser-induced breakdown spectroscopy (LIBS) apparatus has been developed for field analysis over large areas contaminated by heavy metals. Work has also started on designing a versatile laboratory van in which to install the atmospheric and fluorosensor lidar and LIBS apparatus for dedicated monitoring campaigns.

1.1.1 Lidar fluorosensor mobile laboratory

Today, the capability to protect the marine environment and to pick up early warnings of imminent ecological catastrophes relies mostly on the availability of diagnostic instruments that can promptly detect changes in aquatic ecosystems over large areas. These diagnostics should be able to monitor the water-quality parameters of lakes, coastal zones and open seas by revealing the presence of organic pollutants or crude oil, anthropogenic releases and, in particular, phytoplankton, the first link in the nutritional chain of zooplankton and fish. One such tool that is proving very reliable for remotely collecting information on fluorescent targets for sea and land diagnostic purposes is the spectrally-resolved local and remote laser-induced fluorescence (LIF) apparatus.

The Frascati group has already developed a number of remote lidar fluorosensors integrated with local detectors to monitor seawater quality and phytoplankton features. The latest version consists of a compact lidar fluorosensor capable of single- or dual-laser excitation of the water surface (ENEA Patent), a spectrofluorometer, a pulse amplitude modulation (PAM) fluorometer, a solar radiometer and a global positioning system (GPS) receiver. All instruments are housed in a dedicated ISO 20” container for field campaigns. In the single excitation mode, the lidar fluorosensor detects different chromophores and water impurities, while dual-laser excitation is necessary to measure the phytoplankton photosynthetic quantum yield (pump-and-probe mode). During marine campaigns, lidar data are calibrated by means of the local fluorometer at selected sites along the ship’s route and are geo-referenced through the GPS. Remotely measured LIF intensities expressed in Raman units can successively be calibrated against different pigment contents determined by standard local analytic methods. Over the last five years, the mobile lidar laboratory has been operated aboard different vessels, ranging from small boats (10 m) to the oceanographic research vessel Italica (130 m), in order
Fig. 1.1 - Mobile lidar fluorosensor laboratory on board R/V Italica. The arrow points to fixed side arm holding the large external send/receive mirror hanging from the blue container on top of the poop deck.

The mobile fluorosensor laboratory was put aboard R/V Italica in order to participate in the oceanographic campaign of the XIII Italian Antarctic expedition (1997/98). As shown in figure 1.1, the container was located in a convenient position for continuous operation along the ship's routes. Laser radiation is transmitted perpendicularly to the seawater surface by means of a large optical window and an aluminium mirror. The LIF signals are collected by a Cassegrain telescope focusing on a special fibre optic bundle coupled to a set of photomultipliers for light detection. A personal computer embedded in a Versa Module Europe (VME) bus controls the experimental settings, i.e., laser operation mode (either single or dual pulses emitted at each trigger signal) and transmitted energy, high voltage and gating of the photomultipliers, digital conversion of LIF signals and data storage. An external port is also used to acquire navigation data (GPS geo-referenced coordinates) and the overall background light intensity at the sea surface, as measured by the radiometer. Dedicated software for data acquisition and preliminary analysis in real time permits continuous automatic operation during marine campaigns.

During 1998 the lidar group concentrated mainly on analysis of the large data set collected in the Ross Sea and along the Southern Ocean transect from the Italian Station of Baia Terranova (BTN) up to New Zealand (fig. 1.2). The results were transcribed on calibrated thematic maps of phytoplankton and dissolved organic-matter concentrations, water turbidity and biomass productivity. Comparison between the laboratory determination of chlorophyll-a and the fluorescence channel at 680 nm, in seawater samples also analysed by the local fluorometer, allowed calibration of the lidar data in µg/l. Figure 1.3 shows phytoplankton blooms detected in polynya areas, particularly in front of Cape Adare (71° 20.0’ S, 170° 10.0’ E), due to upwelling along the continental slope, near Coulman Island (73° 15.0’ S, 169° 40.0’ E) and in the coastal zone near BTN (75°51.70’S 164°11.59’E).
A new proposal has been submitted to the Italian National Antarctic Programme for 1999-2001. It concerns the design, construction and operation of two new sets of apparatus for range-resolved profiling of seawater quality parameters, phytoplankton pigments and photosynthetic activity below sea level both from the ship bottom and from a remotely operated vehicle.

1.1.2 Laser-induced breakdown spectroscopy system

Laser-induced breakdown spectroscopy (LIBS) is based on analysis of emission spectra generated by atomic species present at the sample surface when a pulsed laser beam is focused on it. The high flux density vaporises the surface and causes avalanche ionisation—the so-called “breakdown” effect: the sample material passes into the plasma state, and its ionisation level and temperature depend on the energy absorbed and the sample composition. The elements in the plasma relax to ground state by losing energy in different ways, e.g., through the emission of radiation in the ultraviolet (UV) to visible range. By collecting and analysing the emission in the spectral and temporal domains, the spectral signatures assigned to specific atomic transitions can be obtained, thereby allowing qualitative identification of the species present in plasma. The corresponding line intensities can then be used for quantitative analysis.

Untreated soil samples were analysed by LIBS and by inductively coupled plasma (ICP) spectroscopy for comparison. The results for zinc determination are shown in figure 1.4. The LIBS technique still has to be fully assessed, but one of its most interesting features is that samples do not require either pre-treatment or extraction.
LIBS field apparatus is being developed. A compact laser source equipped with a focusing arm and collection optics has already been tested in the laboratory (fig. 1.5).

1.2 LASER SPECTROSCOPY MONITORING TECHNIQUES

The 1998 activities addressed two main research lines: high-resolution absorption spectroscopy based on low-power tuneable diode lasers operating in the infrared (IR); and nonlinear four-wave mixing techniques based on high-power dye lasers tuneable in the visible and UV. Significant examples of results obtained for each method are presented in the following.

1.2.1 Infrared high-resolution linear spectroscopy

An experiment for absolute measurement of OH concentration in a reference cell has been built and operated in the framework of the European Project OHDETA. A controlled source of OH radicals was designed and installed at ENEA Frascati in collaboration with the Chemistry Department of Perugia University. The OH radicals are produced in a flow tube after microwave (MW) discharge from the reaction $H + NO_2 \rightarrow OH + NO$.

An attempt was made to detect spectroscopically either OH or NO for absolute calibration of the flow system. High-resolution IR absorption measurements were performed on a multipass cell designed and operated in collaboration with the Consiglio Nazionale di Ricerca - Istituto Materiali Speciali (CNR-IMS). The NO and OH concentrations are closely related, if quenching with the buffer gases and wall losses is neglected. The experimental setup is shown in figure 1.6.

The mechanism of the reaction between NO$_2$ and the atomic hydrogen produced in the MW
1.2.2 High-resolution molecular spectroscopy

Self- and foreign broadening and shifts of a few transition lines of ammonia near 900 cm$^{-1}$ have been measured at temperatures between 200 and 400 K. These measurements, now under accurate analysis, are an important innovation in line-shape studies of pressure-induced effects because of their high precision and temperature dependence. Usually, they are only available, when they exist at all, at room temperature.

Figure 1.8 shows a typical example of the aQ(9,9) transition broadened and shifted by H$_2$. Note that the shift (difference between the centre-frequency of the narrow and broad lines) is visible to the naked eye. This was a complete surprise as it is usually so small that its value can be extracted only through complex analog and/or digital mathematical analysis. In the present case, it was possible to reduce the experimental errors to 1% and 10% for broadening and shift, respectively, which is significant when carrying out comparison with theories (e.g., the Anderson-Tsao-Curnutte [ATC] theory).

Preliminary results (figs. 1.9 and 1.10) show that
while the ATC theory describes self-broadening very well, it has some limits for self-shift.

It is worth noting that the shift of the aP(6,0) line changes sign at a certain temperature, which is the first time this effect has ever been observed. Moreover, the effects of foreign gas, with the sole exception of N$_2$, cannot be described at all by the ATC theory and require alternative theoretical approaches.

Complete analysis of these measurements is still in progress and the final results, probably with new surprises, will be reported in due time.

### 1.2.3 Nonlinear visible-ultraviolet spectroscopy

Methods based on coherent multiphoton spectroscopy are widely used as diagnostics of excited gases, flames and plasmas. Techniques such as coherent anti-Stokes Raman scattering (CARS) and degenerate four-wave mixing (DFWM) are particularly suitable for temperature measurements and/or trace detection of atoms and molecules in flames. In both cases the interaction in the gas phase involves at least two laser beams and a resonant process in the medium third-order susceptibility ($\chi_3$). While the resonant process in CARS is a Raman active vibration, in DFWM an optically allowed transition has to be excited. In both cases, a laser-like beam is generated according to the energy conservation equation involved, at the anti-Stokes frequency in CARS and at the same pump frequency in DFWM. Momentum constraints in the chosen geometry of interaction determine the direction of the signal beam. Resonant conditions are usually matched in the spectra by high-resolution scanning of either the Stokes laser wavelength in CARS or the pump laser wavelength in DFWM.

Multiplex CARS, where a broadband dye laser emits a set of Stokes frequencies and the corresponding anti-Stokes radiation is dispersed on an optical multichannel analyser, allows single-shot temperature measurements of the major flame constituents (e.g., N$_2$ in air), which are particularly interesting in the characterisation of turbulent combustion. The typical limit of broadband CARS is, however, the low sensitivity, which is not sufficient to trace minor components in a combustion process. As a third-order completely resonant process, DFWM has the sensitivity to detect transient species formed at low concentration levels. The principle of multiplex DFWM has already been demonstrated in different geometries. A system based on folded-forward geometry has been developed for application to industrial burners characterised by turbulent phenomena during combustion. It is suitable for single-shot temperature determination in a flame using the Q$_1$(10) and P$_1$(6) lines in the (1,0) A-X vibrationally excited band of OH. A typical broadband OH spectrum measured on a lean iso-butane/air laboratory flame is shown in figure 1.11. The peak ratio $I(Q_1(10))/I(P_1(6))=4.1\pm0.2$ gives a temperature $T=1700\pm50$ K, in full agreement with independent CARS measurements performed on N$_2$ at the same flame location.

![Broadband DFWM spectrum of OH radical](image)

**Fig 1.11** - Broadband DFWM spectrum of OH radical $X^2\Pi(v'=0)$ - $A^2\Sigma^+(v'=1)$ branch measured on a lean flame at the top of the inner blue cone (about 40 mm above the burner)

### 1.3 LASER PROCESSING AND DIAGNOSTICS

#### 1.3.1 Laser synthesis of nanometric powders

Laser-assisted synthesis of nanosized particles has been researched at ENEA Frascati for many years. In particular, silicon-based ceramics (e.g., SiC) suitable for structural materials in industrial applications have been prepared.

Since the discovery of strong room-temperature photoluminescence from
Porous silicon, a lot of interest has been directed towards nanoscale silicon structures because of their potential applications in Si-based opto-electronic devices. What appears an ideal method for growing silicon nanosized particles in a controlled and reproducible way is to produce ceramic powders through heating gaseous precursors by a CO$_2$ laser. In addition, through laser-assisted synthesis the desired morphological and chemical properties of powders can be obtained by adjusting the reaction parameters. Although the variations in powder characteristics have been widely studied in the past, it is still quite difficult to characterise particle-size scaling vs the reaction parameters.

**On-line scattering diagnostics**

To obtain silicon powders with very small diameters (<10 nm) and luminescence spectra above the band gap of bulk silicon, a system has been developed for measuring in situ particle diameter and number density to provide real-time measurements of nucleation and growth kinetics in the reaction zone.

These diagnostics are based on He-Ne light scattering and transmittance measurements throughout the particulate plume. Data were analysed according to the Lorentz-Mie theory of scattering by a spherical, homogeneous particle, by assuming that each particle scatters separately with no optical interference between scattering.

As the intensity of scattered light is a complex convolution of particle size, density and refractive index, an analytical technique was applied to separate the particle parameters and determine particle size and particle density evolution along the reaction flame. The laser-synthesised silicon particles were characterised by Brunauer, Emmett and Teller (BET) specific surface measurement, transmission electron microscopy (TEM) and small-angle neutron scattering (particle-size distribution, see sect. 4.2) in order to check the values obtained by the scattering-extinction technique.

Scattering-extinction and temperature measurements were performed on laser-heated silicon powder synthesis reactions under a range of process conditions. Figure 1.12 reports particle radius and particle number density $N$ as a function of position above the reactant gas nozzle. These data are representative of other runs. The plots show that the embryos of the particles are nucleated before the reactant gas stream reaches the laser beam, and the particle number density remains almost constant at the beginning of the reaction zone. This means that the first stage of particle growth is due to accretion of embryos already formed from gaseous precursors, with a consequent increase in silicon mass density in the reaction zone. When the silane is totally consumed, as the particles

![Graph showing particle radius evolution and particle number density](image)

Fig. 1.12 - Particle radius evolution a) and particle number density b) along the reaction flame for different experimental conditions: $p=0.7$ atm, laser power 700 W (red square); $p=0.4$ atm, laser power 700 W (orange cross); $p=0.4$ atm, laser power 350 W (blue cross); $p=0.2$ atm, laser power 700 W (green cross)
By decreasing the reaction temperature (i.e., reactor pressure and laser power), silane is totally consumed at the middle of the reaction zone and the probability of collisions between particles, and hence particle agglomeration, is reduced. The final particle size is mainly affected by the nucleation rate and silane depletion percentage (i.e., number of embryos). In these process conditions, polycrystalline silicon particles are formed. The close agreement between BET equivalent diameter and TEM observations indicates there is no void space accessible to adsorbate gas between the crystallites in the particles, confirming that particle growth mainly occurs through accretion from vapour molecules and not by agglomeration. The size distributions of particles synthesised in these process conditions (fig. 1.13, curve b) appear to be more uniform.

The emergence of a fixed number of embryos at the beginning of the reaction zone and the cessation of nucleation in the hotter part of the flame are the important features of laser synthesis revealed by the measurements. The experience gained using this technique allowed synthesis of silicon particles with diameters <10 nm, which exhibit photoluminescence spectra above the band gap of bulk silicon.

**1.3.2 Laser deposition of thin films and surface treatments**

The 1998 research activities ranged from film deposition for opto-electronics and gas sensors to surface treatments for crystal growth of solar cell elements. The major results obtained during the year are summarised in the following.

**Formation of epitaxial Si_{1-x}Ge_{x} alloy layer on Si(001) by pulsed-laser-assisted epitaxy**

The insertion of SiGe layers in Si-based integrated-circuit technology is considered a breakthrough in the fabrication of new functional microelectronic and opto-electronic devices, e.g., modulation-doped transistors, heterojunction bipolar transistors or Si-based light-emitting devices using quantum well structures. It has been demonstrated that the problems encountered in the lattice-mismatched heteroepitaxy of SiGe on Si, which limit any widespread diffusion of such systems, can be tackled by introducing a properly designed buffer layer to provide a lattice parameter that allows undisturbed growth of the active layer. Appropriate buffer layers should match the microstructural properties of standard devices and reduce production time and/or costs.

Graded Si_{1-x}Ge_{x} buffer layers were produced by pulsed-laser-assisted epitaxy (fig. 1.14) in the framework of the ESPRIT Project “Low-Cost Si-Ge Microstructures”. Si(001) substrates were heated to growth temperature and germane (GeH_{4}) and disilane (Si_{2}H_{6}) gas precursors were fluxed in order to penetrate in the laser beam there is a rapid increase in radius accompanied by a strong decrease in density number, indicating that growth proceeds through the aggregation of smaller particles by collision.

The relative duration of these phases depends on the process parameters. At high reaction temperature (i.e., reactor pressure >0.5 atm and high laser power), silane is totally consumed at the beginning of the reaction zone and growth proceeds by coagulation. The residence time of the particles in the laser beam, the silane mass density in the flame and the number of collisions determine the final particle size. If the temperature exceeds the silicon melting point, the particles can coalesce by a viscous flow process, and large monocrystalline silicon particles (r > 25 nm) are observed by TEM. The size distribution of these particles is characterised by inhomogeneous broadening on the right side, due to a coagulation process (fig. 1.13, curve a).
to deposit a SiGe layer by chemical vapour deposition (CVD). During CVD growth, a 4 mm\textsuperscript{2} area of the sample was irradiated by the homogenised beam of a KrF laser (248 nm, FWHM 20 ns). Graded buffers with Ge concentration increasing from 0–10% and thickness ranging between 300 and 500 nm were deposited at 530–570°C by fluxing GeH\textsubscript{4}:Si\textsubscript{2}H\textsubscript{6}=1:1 mixtures and irradiating the sample at 0.5 J/cm\textsuperscript{2} at 1 Hz. Rutherford backscattering analysis revealed that the resulting layers had good epitaxial properties. High-resolution x-ray diffraction (XRD) characterisation showed that for a similar Ge concentration all the buffer layers were fully strained.

To obtain the strain relaxation required for application in microdevice fabrication, both the Ge content and the layer thickness were increased. Strain relaxation was observed by high-resolution XRD reciprocal space maps in layers deposited by fluxing pure GeH\textsubscript{4} at 600°C, while maintaining the same irradiation conditions. In this case Ge concentrations exceeding 50% and layer thicknesses close to 1 mm were estimated. These results and the optimal epitaxial quality exhibited by the layers confirmed pulsed-laser-assisted epitaxy as a flexible and powerful growth technique for application in SiGe-based microdevice technology.

Growth of poly-Si films by laser-assisted chemical vapour deposition

Large-grain poly-Si films are required to improve the performance of solar cell devices. In the framework of the FOTO Project, poly-Si films were grown by laser-assisted CVD (fig. 1.15) on Corning glass substrates and on Si(001) wafers covered by an 800-nm-thick SiO\textsubscript{2} layer. CVD was obtained by fluxing disilane (Si\textsubscript{2}H\textsubscript{6}) at a pressure of 1 mTorr, while substrates were heated to 550–600°C. During growth, the films were exposed to KrF excimer laser pulses (248 nm) at 350 mJ/cm\textsuperscript{2} (Corning substrates) and 450 mJ/cm\textsuperscript{2} (SiO\textsubscript{2}/Si substrates).

The typical bands at 375 and 300 nm in the reflectance spectrum demonstrated the formation of a polycrystalline phase in the Si films. Scanning electron microscopy (SEM) analysis after dry etching showed the formation of grains with maximal lateral dimensions of the order of 0.8 μm. Although
these results are preliminary, they appear quite encouraging for the achievement of optimal poly-Si film by laser-assisted CVD.

Epitaxy of Ge on Si(001) in the presence of surfactant elements studied by high-resolution photoemission spectroscopy with synchrotron radiation

The addition of appropriate elements, such as As, Sb, Bi, H, which act as surfactants may assist the epitaxy of Ge on Si and solve the problems caused at the interface by lattice mismatch between Si and Ge.

High-resolution core level spectroscopy with synchrotron radiation was used to study the growth of Ge at 350°C on Si(001)c4x2 in the presence of one monolayer (ML) of Sb or Bi. The experiments were performed at the vacuum ultraviolet (VUV) beamline of ELETTRA (Trieste) in collaboration with the CNR Istituto Struttura della Materia. Analysis of the Si2p and Ge3d core levels demonstrated the superior capability of Sb in assisting the growth and in promoting a nearly perfect bulk-like arrangement of the Si atoms at the Si-Ge interface. The same result is not achieved when using Bi as its saturation coverage of 0.7 ML leaves a fraction of the Si substrate uncovered, where pure Ge epitaxy on Si, without surfactant assistance, takes place.

**1.3.3 Material characterisation**

X-ray diffraction

New x-ray diffraction (XRD) methodologies based on analysis of the diffraction peak shape have been developed as support to the research on the production and photoluminescence (PL) properties of silicon nanopowders. Particular attention was paid to the particle-size distribution function and to analysis of the particle oxidation state. A Monte Carlo fitting algorithm originally developed for analysis of heavily strained materials was modified for determination of the particle-size distribution. The method was further tested on a sample of silicon nanopowder produced by laser synthesis and the results compared with those of transmission electron microscopy (TEM). Figure 1.16 shows the size distribution function obtained from XRD shape analysis and derived by particle counting in TEM images.

The comparison confirmed the validity of the method. The main advantages of XRD are that it is nondestructive and easy to carry out.

Knowledge of the oxidation state of Si nanoparticles is extremely important in PL studies of silicon nanocrystals. Indeed, the degree of particle oxidation has a strong influence on the PL characteristics. As the oxide layer has an amorphous structure and the nanoparticles crystalline, XRD can easily distinguish between the two. The dependence of the mean particle size was investigated as a function of the degree of oxidation. To model the oxidation process, a shell-wise oxidation of spherical particles with a log-normal distribution (LND) was assumed, which approximates the distribution measured by TEM (see fig. 1.16) quite well. The size distribution is modified after several steps of shell removal from the crystalline nuclei (fig. 1.17).
Figure 1.18 reports the relative decrease in the mass mean crystalline sphere radius $R_M$ as a function of the corresponding relative decrease in the total mass $M$ of the crystalline size. It can be observed that with increasing oxidation the decrease in mean size depends strongly on the polydispersity of the starting distribution, expressed by the variance $\sigma$ of the LND. Note in the present case ($\sigma=1.2$) that to reduce the crystallite size to half that of the starting material requires a 95% oxidation.

High-resolution electron microscopy (see fig. 1.19) has confirmed the adopted model, and the studies so far developed have given useful indications for technological applications of the powder, e.g., fabrication of aerogels with nonlinear optical properties.

**Optical properties of nonlinear materials**

One of the greatest challenges in optics is to develop a computer based on all-optic photonic switches in the place of electronic transistors. Nonlinear optical materials are the key ingredients of functional photonic devices. Candidate materials systems include metal or semiconductor doped glass, which exhibit high nonlinearities. All-optic devices require some kind of laser source coupled to nonlinear optical elements. Optical amplification and laser action were recently observed in rare-earth-doped glass. In spite of the first promising results, this field is only in its infancy. Many performance constraints have to be satisfied before these materials can be truly useful for applications. Hence, understanding the correlation between material fabrication and processing with nonlinear optical properties is especially critical in the upgrading of advanced nonlinear materials for photonic devices.

Activities in 1998 were focussed on optical characterisation of nonlinear optical materials (metal nanoclusters embedded in glass) and optically active materials (rare-earth-doped glass) for applications in photonics. Spectroscopic properties of doped glass were investigated by detecting optical absorption, emission and excitation spectra of the systems, whereas nonlinear optical properties were studied by a Z-scan setup (based on a mode-locked Nd:glass laser delivering 4-ps single pulses). A Q-switched Nd:YAG laser (10-ns pulses with intensity up to 1 J/cm²) was used for studying sample stability and/or modifications under laser irradiation.

**1.4 LASER METROLOGY, ARTIFICIAL VISION AND DIGITAL HOLOGRAPHY**

The year 1998 was mostly devoted to developing laser applications in artificial vision and optical metrology, with advanced industrial spin-offs. Both coherent and incoherent sensors were investigated. Particular consideration was given to the latter, which are designed to map 3-D targets with millimetre...
resolution (topological radar) at distances of tens of meters over real large surfaces. These sensors could be used both in heavy-industry environments and in the conservation of cultural and archaeological remains. What is required is an optical radar capable of 3-D submillimetre-resolution mapping of real surfaces some square meters in dimension, at distances ranging from 3 to 20 m. Recent measurements have given useful results; an operative demo unit has been developed that shows that the required performance can be achieved and that the overall task is feasible.

1.4.1 Incoherent sensor

The demo unit consists of an incoherent diode laser sensor equipped with a scanning camera, fully designed and developed at the Frascati laboratories. A modulated beam sounding technique is used for applications at medium or low distances because the heterodyne technique employing current frequency down-conversion allows indirect measurement of the round-trip time delay of the sounding beam through measurement of the phase retardation of the signal photocurrent.

As the sensor should be able to work in any environmental conditions, the undesired background light expected in a non-structured environment, collected by the receiving optics and reaching the detector, should be minimised. This has been obtained by introducing an interferential filter with a 10-Å bandwidth, combined with an iris that restricts the instantaneous field of view to the dimensions of the beam spot on the remote target. The amplitude of the sinusoidal signal generated by the avalanche depends on the reflectivity of the scene and the phase depends on the distance. Part of the modulated beam is reflected by a beam splitter and two prisms onto a photodiode that generates a sinusoidal signal with constant amplitude and phase and acts as a reference for the instantaneous phase measurement of the current signal from the detector.

This sensor is operated in combination with a scanning camera that sounds the scene with a collimated and focused modulated beam raster synchronised with an analog-to-digital converter and an acquisition system. The sensor has been used to obtain both range pictures and depth maps by probing the elements of the scene (pixels) in sequence. After suitable filtering, this mapping is independent of environmental illumination and the reflective properties of the surface. Results are summarised in figures 1.20–1.22.
Laser in-vessel viewing system

Along with the laser radar prototype described previously, a mockup of an amplitude-modulated (AM) laser viewing system for use in machines for controlled thermonuclear studies has been developed. Thermonuclear fusion research machines, such as the Joint European Torus (JET) and the International Thermonuclear Experimental Reactor (ITER), have a very complex structure and the components inside the vacuum vessel have to withstand severe thermal, electric and mechanical loads both in normal and in abnormal (disruptions) plasma phases. Hence, the in-vessel components have to be periodically inspected for damage and to schedule maintenance activities.

A laser in-vessel viewing system (LIVVS) with a ranging capability of ~1 mm has already been demonstrated and an improvement will be tested at ENEA Frascati using an AM coherent beam configuration. If development of the diode laser source, acousto-optic-modulator unit and radar electronics devices proceeds as expected, submillimetric ranging accuracy should be achieved well in time for application on ITER. As submillimetric accuracy is required to assemble in-vessel components (e.g., divertor tiles), some form of ranging apparatus is needed in addition to the availability of a high-resolution in-vessel viewing system. During machine construction, very accurate metrology can be performed using laser interferometer apparatus. Unfortunately, present commercial systems cannot withstand the in-vessel operating conditions after a D-T plasma phase so hard radiating apparatus has to be developed.

In the mockup laser radar scheme, the laser beam amplitude is modulated (up to some tenths of MHz). Both intensity and phase shifting of the reflected beam (with respect to the launched one) are simultaneously detected: a high-accuracy image of the target is obtained (with lateral resolution of 1 mm at 10 m) from the intensity signal and target ranging can be performed using the phase shifting.

The AM system has been designed so that its components (acousto-optic modulator; diode laser sources; electronics, etc.) can be modified such as to achieve substantial improvements in its ranging performance (~100 μm at 10 m). The LIVVS consists of the following components:

Active optics module (AOM). This unit is located outside the bioshield and hence not affected by neutron or gamma fluence. The laser beam is generated by a 200-mW, 840-nm, single-mode diode; it is collimated to a diameter of 2 mm and then focused up to a 80-μm-diameter spot inside the AOM. The module is based on a TiO₂ crystal and is used to modulate the beam amplitude up to 30 MHz for ranging purposes, as no directly modulated high-power diode laser is available yet. When only viewing is required, the amplitude is modulated at 1 MHz using the laser driver. The AOM output is focused onto the iris plane, which transmits only the first diffraction order of the optical field. A fraction of this beam, split by a polarising corner cube, is sent to an amplified wide-band silicon photodiode that generates the phase reference signal to be processed by the radar electronics (RE) unit located close the active module. To assure a diffraction-limited focusing condition on the target, the main output beam is collected in a single-mode 5.5-μm optical fibre and transmitted to the passive optics module. The power transmitted through the optical fibre is about 50 mW, well below the maximum allowable value (100 mW). An amplified silicon avalanche photo diode (APD) located inside the active module transduces the backscattered beam, coming from the passive module, into a rf signal. This signal is then processed together with the phase reference signal by the RE in order to generate the signals required for performing the amplitude and range images of the target.

Passive optics module (POM). As this module has to be placed on the JET limb, it is exposed to neutron and gamma radiation. Hence, only hard-rad components are adopted and all the optics are manufactured using fused silica, which maintains good transparency at 840 nm even in JET/ITER operating conditions. A collimating beam expander transmits the beam through the probe and the scanning head in order to have a 1-mm spot at 15 m from the POM. The receiving optics is also located inside the POM and subtends the maximum solid cone angle allowed by the probe geometry. The receiving optics consists of a fused silica plano convex lens with 100-mm diameter (collecting aperture limited to 32 mm because of the probe inner diameter) and 150-mm focal length. The collected beam is transmitted back to the active module through a 600-μm-diameter optical fibre.
LIVVS probe. A remotely controlled beam alignment system allows the laser beam to reach the scanning head inside the vessel. The JET probe is basically composed of two AISI 304 steel rotating coaxial pipes, each operated by its own remotely controlled stepping motor. At the bottom end of the probe, the tiltable outer pipe is shaped like a pinion engaging the rotation movement gear of the prism, which rotates at about 1 rps in the tilt direction and at a few rph in the pan. The rotation speed ripple is controlled by means of a microstep control unit that drives the motor up to 50,800 steps per shaft revolution and by very accurate gearing and a gear play recovery system. High-precision ceramic miniature bearings are used to reduce friction—which for mechanisms operating in vacuum and at high temperature can lead to seizure—and to comply with dimensional specifications. Taking into account the stepper features and the tilt & pan overall gear ratio, one has 1,411 microsteps per degree for tilting and 14,111 for panning. The prism position is detected through two optical encoders modified to meet vacuum and radiation specifications. The rotation encoder disk is fixed to the prism, while the revolution encoder disk is fixed to the inner pipe. Both are placed inside the vacuum chamber. The encoder disk will be read by means of optical fibres that carry the light signal 120 m away from the probe, where the laser source and electronics are also located. By properly decoding the two signals coming from each encoder, it is possible to know the position of the scanning head up to 72,000 times for a single pan revolution and up to 10,000 times for a tilt rotation. Figure 1.23 shows the LIVVS scanning head and the results of viewing tests performed at ENEA Frascati.

Control, data acquisition and imaging. All electronics is located in a control room outside the bioshield, about 120 m from the probe, and includes the following: a) A radar unit that decodes the photo receiver electric signals and extracts amplitude and phase information from the backscattered beam. The unit has an accuracy of 0.1% and operates at 4 MHz below 58 dB on the dynamics of the input signal. b) The VME control unit. c) The imaging system, based on specifically designed software running on a Silicon Graphics Work Station.

1.4.2 Holographic and speckle interferometry

Holographic and speckle interferometry activities are mainly directed to developing suitable techniques for nondestructive testing (automated systems for industrial on-line quality control) and structural and modal analysis (procedures for highly reliable validation of
finite-elements models for complex structures and components).

During 1998, activities were carried out for the University Satellite (UNISAT) Project, a research programme involving several Italian universities. The project aim is to design, build and launch a microsatellite. In this context, a finite-elements model (FEM) of the structure of the UNISAT microsatellite was validated and a multipurpose bus is under development.

The experimental design is based on a multitray modularity concept that enables all the subsystems to be accommodated on a suitable tray (fig.1.24). Each tray is assigned to a particular (or cluster of) subsystem(s) so that manufacturing and testing can be done separately. Current design procedures for aerospace structures rely on FEMs built at the beginning of the design phase in order to certify that all the requirements are satisfied. These models have to be verified by means of experimental techniques. Electronic speckle pattern interferometry is a powerful tool for finite-elements model validation as it provides high-resolution information on the dynamic behaviour of the structure. The operational shapes of the structure under test can be experimentally detected and the results compared with the features numerically evaluated by the FEM to test its reliability. Experimental measurements were performed dynamically, exciting the microsatellite by means of a piezo-electric actuator. Figure 1.25 shows results relative to one rectangular panel; figure 1.26, those relative to the top octagonal plate.

![Fig. 1.24 - UNISAT microsatellite based on a multitray modularity concept. a) Internal structure; b) view of the external shell](image)

![Fig. 1.25 - Speckle fringes showing a modal pattern of the lateral plate of the UNISAT microsatellite](image)

![Fig. 1.26 - Speckle fringes showing a modal pattern of the top octagonal plate of the UNISAT microsatellite](image)
panel. The dark and bright 'fringes' (speckle correlation fringes) visible in the figures correspond to the iso-amplitude of the vibration component along a “measuring direction”, which is defined by the optical setup, and hence provide direct visualisation of the dynamic displacements of the microsatellite surfaces.

Electronic speckle pattern interferometry was also used for nondestructive testing (NDT) of laser welds on specimens of structural steel panels used in the production of platforms for heavy-duty marine and truck construction. The specimens were 60x40cm² 10-cm-thick panels made of two outer skins welded on an inner Ω-shaped Greek fret core. To set up a NDT procedure suitable for on-line investigation in industrial environments, measurements were performed on panel specimens that had imposed defects with the typology and dimensions typically found during panel production. Results show that a reliable NDT procedure for production control can be defined. Figure 1.27 shows a specimen panel in the test fixture and a view of the inner Ω-shaped Greek fret core; laser beam welds correspond to the thin black segments parallel to the shorter side of the panel. Figures 1.28 and 1.29 show the behaviour of two specimens after thermal excitation applied by a heater (black arrow at the bottom of the image). Thermal excitation causes the outer skin to dilate, as shown by the dark and bright fringes (speckle correlation fringes), which correspond to the loci of points undergoing the same displacement. In figure 1.28, two defect-free welds steadily constrain the outer skin to the Greek fret, as shown by the fringes that bend and run parallel to the welds. In figure 1.29, the weld on the left is defect free (fringe behaviour is the same as in fig. 1.28); the weld on the right is clearly defective (the fringes cross the welding without bending, thereby showing that the outer skin is not structurally bound to the Greek fret).

Fig. 1.27 - a) Specimen panel in the test fixture; b) inner Ω-shaped Greek fret core

Fig. 1.28 - Speckle fringes showing panel displacement due to thermal stress: symmetric fringe patterns mean defect-free laser welds

Fig. 1.29 - Speckle fringes showing panel displacement due to thermal stress: asymmetric fringe patterns mean defective laser welds
1.5 OPTICAL COMPONENTS

1.5.1 Thin-film coatings and devices

Thin-film technology has numerous applications. At ENEA Casaccia, studies on film materials and thin-film coating production are mainly devoted to optical applications. The types of coatings and optical components recently produced are narrow-band transmission filters, coatings on plastic, laser mirrors and electrochromic devices. Optical thin films and components (oxide and fluoride films, glazing for buildings, etc.) are characterised using various techniques. Some of the standard methods (ellipsometry) have been modified in order to improve their performance.

Hafnium oxide thin films

One of the materials most investigated is hafnium oxide ($\text{HfO}_2$). A high-index material in the UV spectral range, it is very promising for laser optical coatings because of its relatively high damage threshold and good thermal and mechanical stability. To optimise the film properties, different deposition techniques (sputtering, e-beam evaporation) have been studied.

Sputtering yield. The different sputtering yields of the elements composing the film modify the stoichiometry and consequently the absorption and the refractive index. In the Sigmund picture of target sputtering, an impinging ion undergoes a series of collisions with randomly distributed atoms in the target. The recoil atoms with sufficient energy can generate another series of secondary collisions. Sigmund uses the linear Boltzmann transport equation to describe the collision cascade in an infinite medium. The following relation shows the sputtering yield $Y$ at projectile energy $E$:

$$Y(E) = A \alpha N S_n$$  \hspace{1cm} (1)

$A$ contains all specific material properties and the surface state, $\alpha$ is an energy-independent function, $N$ is the target density and $S_n(E)$ is the nuclear stopping power. There is a threshold energy that represents the minimum ion energy necessary to transfer $U_Q$ (surface binding energy) to an atom of the surface target in a backward direction. Based on a few-collision-events model, a simple formula can be derived for the threshold energies $E_{th}$. The threshold energies for the materials studied are listed in Table 1.1. Figure 1.30 shows the sputtering yield measurements compared with the sputtering yield calculated by (1) for Ar on $\text{HfO}_2$ and Xe on $\text{HfO}_2$.

The low-energy sputtering yield described by the Sigmund model is in agreement with the experimental values. The preferential sputtering of oxygen atoms is related to the mass proportion of the elements constituting the oxide. The calculated partial sputtering yield can be used to find the expected stoichiometry of a thin film grown under ion bombardment.

Momentum transfer. The role of ion assistance during film growth has been extensively studied to obtain more compact, dense, adherent and stress-controlled coatings. The effect of the ion momentum transfer parameter during e-beam evaporation of $\text{HfO}_2$ films on silica substrate was considered and it was demonstrated that increasing the momentum parameter $P$ increases the density and intrinsic stress of ion-beam-assisted $\text{HfO}_2$ thin films. The momentum transfer $P$ from the ions to the incoming atoms can be defined:

<table>
<thead>
<tr>
<th>Table 1.1 - Threshold energies for different oxides</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{HfO}_2$</td>
</tr>
<tr>
<td>$E_{th}^{\text{Hf}}$ (eV)</td>
</tr>
<tr>
<td>Ar 31</td>
</tr>
<tr>
<td>Xe 44</td>
</tr>
</tbody>
</table>
where \( n_{\text{ion}} \) and \( n_{\text{atom}} \) are the ion and atom numbers, respectively, determined by measuring the rate (nm/s) and the ion current density (\( \mu \text{A/cm}^2 \)),

\[
P = \frac{n_{\text{ion}}}{n_{\text{atom}}} \sqrt{2m\gamma \cdot E}
\]

(2)

\[m \text{ and } E \text{ are the mass and the energy of ions, and } \gamma = (4m\cdot M)/(m + M)^2 \text{ where } M \text{ is the mass of evaporating atoms. The refractive index values at a 500-nm wavelength for the different } P \text{ values (fig. 1.31) reveal the densification effect of Xe ion assistance on the hafnium films. Samples deposited at different } P \text{ values were analysed by XRD in order to correlate the optical behaviour and intrinsic stress with the microstructural modifications.}

As observed in figure 1.32, the features of the diffraction patterns differ with increasing \( P \). The tensile-to-compressive stress change is not an abrupt transition from a random to an oriented phase. The random oriented nanocrystalline structure is progressively amorphised by increasing the energy
delivered to the system. Additional energy allows formation of an oriented phase with compressive stress and high density. The ion momentum transfer is a fundamental parameter for the optical and mechanical properties in ion-beam-assisted hafnium thin film and also for the microstructural evolution of the film itself.

Narrow-band transmission filters

The narrow-band thin-film filter is based on the Fabry-Perot interferometer, which consists of two identical parallel reflecting surfaces divided apart by a spacer. This device can be replaced by a complete thin-film assembly consisting of a half-wave dielectric layer (spacer layer) bounded by two high-reflecting stacks of quarter-wave dielectric layers (fig. 1.33) of alternate high and low refractive indexes. Its optical response shows a narrow region of transmission bounded on either side by regions of rejection.

The materials employed to produce the filters were selected from those with high transparency in the wavelength range of interest (i.e., low absorption coefficient) and with a high as possible ratio of the refractive indexes. Two oxides, hafnium dioxide HfO$_2$ (high refractive index $n=2.30$ at $\lambda=280$ nm) and silicon dioxide SiO$_2$ (low refractive index $n=1.48$ at $\lambda=280$ nm) were selected as closely fitting the above requirements.

The stability and reproducibility of the refractive index in optical thin films are directly related to the physical structure of the films. In fact, as already reported, thin films are usually affected by columnar structures, and the water vapour absorbed from the atmosphere can change the refractive index value with respect to that measured under vacuum.

In order to investigate the influence of ion-beam assistance on the optical stability of the Fabry-Perot, the transmittance of a set of filters deposited without ion assistance was compared with that of another set assisted by Xe ions during the evaporation process. In figure 1.34 the transmission functions of three non-ion-assisted Fabry-Perot filters with 28 layers are shown, measured as deposited (filters A) and after one year (filters B). It appears that the transmittance peak has shifted by about 2 nm; one of the filters, submitted to a thermal cycle by liquid nitrogen immersion, shows an increase in the half-bandwidth with a strong decrease in the transmittance value at the wavelength peak. The characteristics of the filters shown in figure 1.34 are summarised in table 1.11, where $T_{\text{max}}$ is the transmittance at the peak, $\lambda$ is the peak wavelength

<table>
<thead>
<tr>
<th>Filter</th>
<th>1A</th>
<th>1B</th>
<th>2A</th>
<th>2B</th>
<th>3A</th>
<th>3B</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{\text{max}}$</td>
<td>0.60</td>
<td>0.46</td>
<td>0.57</td>
<td>0.59</td>
<td>0.78</td>
<td>0.788</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>295.2</td>
<td>297.3</td>
<td>306.7</td>
<td>309.2</td>
<td>324.7</td>
<td>326.5</td>
</tr>
<tr>
<td>$w$</td>
<td>0.63</td>
<td>0.95</td>
<td>0.74</td>
<td>0.77</td>
<td>0.91</td>
<td>0.93</td>
</tr>
</tbody>
</table>
and w is the half-bandwidth. The transmittance of some ion-assisted filters is reported in figure 1.35.

Optical-response stability was tested by simulating the operating conditions of the filters (exposure to UV radiation, humidity atmosphere up to 95% and temperature from +55°C to -25°C). No humidity shift and no peeling phenomena were observed. The high transmittance peak value and bandwidth lower than 0.5 nm after testing confirm the high optical stability of ion-assisted coatings during the evaporation process.

**Coatings on plastic substrate**

Thanks to their low weight and high resistance to crushing, polymers are beginning to replace glass in optical applications. Multilayer antireflection coatings are widely used on glass substrates to reduce reflection losses and to increase transmission of optical systems. They are also suitable for application on plastic substrates, particularly in ophthalmics, but present some problems due to low environmental durability and wear resistance. The effects of different low-energy ion-beam treatments of poly-diethylene-glycol-bisallyl-carbonate (CR39) and poly-carbonate (PC) substrates on the adhesion of hard oxide coatings deposited by dual-ion-beam sputtering have been studied. Ar and Xe were used as bombarding ions to investigate the effect of different mass projectiles on the bond strength at the film/substrate interface. Practical adhesion was evaluated by environmental testing according to ISO 9211-3:1994(E) for optical coatings. Dual-ion-beam sputtering seems to be a promising technique for thin-film deposition on plastics. First of all it allows the substrate temperature to be kept low enough to minimise thermal stress at the film/substrate interface. Good packing density and structure can be achieved by energy transfer from the assisting ions to the depositing atoms. In order to get a quantitative evaluation of the adhesion, samples were subjected to a scratch test. The critical load is defined as the load at which the first tensile crack appears out of the stylus track, as tensile stress is the failure mechanism for brittle material films. Actually, the differences among the measured values of different samples can be related to thickness variations rather than to different adhesion values (see fig. 1.36).

An improvement in surface hardness was also observed, as measured by the radius size of the stylus track. Figure 1.37 shows that the values of the scratch hardness of coated samples are higher than those of untreated substrates.
Environmental tests were performed to assess the influence of different ion treatments on interface bond durability. Indeed, such practical measures of adhesion are often more successful than measurements of the forces required to separate coatings from substrates. A coating might have good adhesion to its substrate when judged by peel force measurements, but the same coating/substrate system might fail when subjected to extreme environmental conditions. The film surface status after environmental tests is reported in the table 1.3.2.

The Xe treatment in an oxygen-rich atmosphere seems to be the most effective in promoting adhesion. The observed improvement in adhesion can be tentatively explained on the basis of ion bombardment simulation, using the TRIM program. Figure 1.38 shows the distribution of vacancies produced by Ar and Xe irradiation. The total number of vacancies near the surface is the same for both treatments and depends on the values of the momentum transferred from ions to single-target atoms; nevertheless, the distribution of Ar-produced vacancies covers a large depth from the surface into the bulk.

A similar situation occurs for the distribution of recoiling atoms (target atoms moved from their original position). Hence, it can be reasonably assumed that species adsorbed from the atmosphere (oxygen in this case) are confined in a region nearer to the surface during the Xe treatment than during the Ar. Moreover, the former, with fewer vacancies and recoils, should produce less damage than the latter.

High-reflectance laser mirror

Copper is generally used as substrate material for CO\textsubscript{2} laser mirrors because of its good thermal conductivity, low cost and easy manufacture. The surfaces of copper mirrors are usually finished by polishing.

The possibility of using diamond-like carbon thin films deposited by radiofrequency (rf) sputtering as a protective multilayer for enhanced-reflectivity copper mirrors employed in infrared applications was investigated. To obtain a multilayer formed of materials with characteristics known to be suitable, zinc selenide and carbon were chosen as high and low refractive index materials, respectively (see fig. 1.39). Figure 1.40 reports the reflectance curves of coated and uncoated copper mirrors in the infrared wavelength range of interest ($\lambda=10.6$ $\mu$m).
Electrochromic devices

Electrochromic (EC) devices have numerous applications; e.g., monitors, variable-reflectance mirrors and variable-transmittance windows. However, the most prominent application is in the design of “smart windows”, large-area glazing for the variable inlet of light and solar energy into energy-efficient buildings.

Considerable progress has been made in this field, with the first smart window marketed in September 1998. Nevertheless, some requirements, such as adequate optical contrast, still have to be met.

**Device structure.** Electrochromic devices (fig. 1.41) are made up of an electronically conducting, transparent contact layer (generally indium tin oxide), a mixed conductor $W$ (mainly oxide tungsten oxide $WO_3$), an electronically blocking but ion-conducting electrolyte $E$, a second mixed conducting film (again mainly oxide) $C$ and another electronically conducting layer. The idea is that the system can switch from an optically transparent to an optically opaque state by an electrochemical redox process.

While $WO_3$ is suitable as an electrochromic cathode in EC windows, a comparatively good material to be used as counter-electrode ($C$) has not been found. ENEA Casaccia is currently studying the deposition and optical, electrochemical and structural properties of suitable thin-film materials, such as cerium oxide, mixed cerium-zirconium oxide and mixed cerium-vanadium oxide.

**Thin-film deposition and device performance.** Films are deposited by reactive rf sputtering of a target made of finely mixed powders cold pressed into a target holder. As the powders are not sintered or glued, the targets are placed at the bottom of the chamber and the substrates are clamped on the top (sputter-up configuration).

A complete device was assembled using $WO_3$ and Ce-V (deposited from the target composed of $CeO_2/V_2O_5=1$) mixed oxide thin films. Good optical contrast and high transparency in the bleached state were observed (fig. 1.42). The film deposition parameters for improving long-term performance are under investigation.

**Fig. 1.40 - Reflectance of coated and uncoated copper mirrors as a function of wavelength**

![Reflectance graph](image)

**Fig. 1.41 - Schematic of an EC window. A current or a voltage applied to the electronically conducting layers promotes a switch in the optical properties of the device via an electrochemical reaction**

![Schematic diagram](image)

**Fig. 1.42 - Transmittance variation as a function of the flow charge of a device where $W=WO_3$ $C=CeVO_3$ $E=LiClO_4$ in EC/DMC 1M**

![Transmittance graph](image)
Characterisation of transparent glazing for building applications

International and European standards for transparent glazing in building applications recommend that luminous and solar parameters be evaluated from (near) normal incidence transmittance and reflectance (T and R) spectral measurements. But, when the glazing is on the façade of a building, direct radiation from the sun is seldom perpendicular to the window and irradiation occurs at a variable incidence angle.

Knowledge of the luminous and solar parameters of fenestration at off-normal incidence leads to more accurate evaluation of daylighting and energy consumption for the rooms in a building. However, direct measurements of angular-dependent T and R spectra have proved difficult, expensive and time consuming, and experimental results from different laboratories often disagree. An alternative method is exhaustive optical characterisation of fenestration using normal-incidence measurements, which makes it possible to evaluate the luminous and solar parameters at each incidence angle. Unfortunately, this is very complex in the case of multilayer-coated glass, so complementary surface-analysis techniques (Rutherford backscattering, secondary ion mass spectrometry, x-ray or neutron reflectivity, etc.) are required in order to understand the multilayer structure.

Several simple algorithms to predict the fenestration parameters starting from normal-incidence measurements have recently been proposed. When using these algorithms, the coating composition has to be known in order to properly set some of the parameters according to a standard database classification.

A new and simpler method has been developed in collaboration with the Stazione Sperimentale del Vetro of Murano. To predict the off-normal fenestration parameters, the experimental normal-incidence measurements are processed by modelling the coated glass as an unrealistic equivalent uncoated material (EUM). Although EUM has no physical meaning (except in the case of really uncoated glass), its predictions are in very good agreement with those of more sophisticated models.

As an example, let us consider a commercial, coated glass sheet as the monolithic glazing of a room (square, 9 m per side and 3 m high) in a building in Rome, with a façade facing south over an unobstructed landscape. The coated glass sheet is the transparent component of two windows (1.5 m high and 2.5 m wide each), both positioned on the façade. A computer program named Heatlux is used to predict daylighting. Heatlux takes into account radiation from the sky and ground, direct radiation from the sun and multiple reflections due to the internal surfaces of the room. Table 1.IV reports simulation results for daylight illuminance on a horizontal working plane 0.8 m from the floor at midday in June (worst situation: maximum illuminance near the window) and December. Also reported is the reduction in internal illuminance obtained with glazing compared to illuminance for open windows. The table shows the good agreement between the results of the rigorous model (exhaustive coating characterisation) and those of the EUM.

In collaboration with the Stazione Sperimentale del Vetro of Murano, an innovative user-friendly computer program named Equivalent Substrate and based on the EUM algorithm is being developed (in the Microsoft Visual Basic 5.0 environment) to calculate the luminous and solar parameters of transparent glazing. A demonstrative version for PC-compatible platforms is already available and promotional distribution among interested users is foreseen. Equivalent Substrate permits calculation of the most significant luminous and solar parameters of transparent glazing at any incidence angle, according to the most important European and U.S. regulatory standards.

<table>
<thead>
<tr>
<th>Model</th>
<th>June at noon</th>
<th>December at noon</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>illum. (lux)</td>
<td>Reduct. (%)</td>
</tr>
<tr>
<td>Rigorous</td>
<td>252</td>
<td>25</td>
</tr>
<tr>
<td>EUM</td>
<td>251</td>
<td>24</td>
</tr>
<tr>
<td>Open window</td>
<td>1026</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 1.IV - Rigorous method and EUM model results for daylighting on the working plane
Optical characterisation of coloured LiF thin films

Electrons with energy of a few keV impinging on lithium fluoride (LiF) crystals and films produce different kinds of colour centres in a thin layer at the air/LiF interface. Coloured LiF exhibits several light-absorption bands in the visible and near UV because of the formation of different kinds of F-aggregate defects.

The formation of optically active defects, such as colour centres in LiF, induces an increase in the refractive index of the host material. This increase, in conjunction with the fact that the energy absorbed by the active centres in LiF is mainly released as fluorescence, makes coloured LiF a promising material both for guiding and for amplifying light. Promising results have been obtained at ENEA Frascati, with active channel waveguides emitting in the green and red spectral ranges being obtained for the first time in LiF crystals irradiated by 12-keV electrons.

Accurate optical characterisation of these coloured-LiF thin surface layers is essential for estimating their potential applications in the field of integrated optics. A crucial role in coloured-LiF-based active waveguides is played by the increase in the complex refractive-index after the electron-beam coloration process. Generally, determination of the complex refractive index of a single layer requires at least two independent measurements, e.g., spectral transmittance and reflectance, or spectral transmittance and ellipsometry. For the case of coloured-LiF channel waveguides, whose widths are typically of a few microns, only the spectral transmittance can be measured fairly easily.

A collaboration between ENEA Frascati and Casaccia has developed a new characterisation technique for coloured-LiF channel waveguides that requires just a single measurement of spectral transmittance by adopting a suitable model for electromagnetic radiation/colour centre interaction. The model considers a dipole-type interaction, as suggested by both classic and quantum theory. The accuracy of the characterisation technique was successfully checked by comparing the measured complex refractive index of a large-area coloured-LiF sample with that measured by standard optical characterisation, i.e., a combination of spectrophotometry and ellipsometry. The technique is being optimised for application to the case of actual channel waveguides. Further refinements are foreseen in order to include the possibility of measuring optically-pumped waveguides.

Characterisation technique: innovative ellipsometer

Ellipsometry is a polarimetric technique for characterising the optical properties of surfaces and thin films. The change in the state of polarisation induced by reflection is used as a probe to analyse different surface properties, such as optical constants, the presence of thin layers, their thickness and refractive index.

An innovative ellipsometer is being developed at ENEA Frascati in collaboration with the University of Rome Tor Vergata (Prof. E. Segre). It uses phase-sensitive detection to characterise the state of polarisation of the reflected optical radiation. Before reflecting from the sample surface, the incident polarisation of the optical beam is first linearly polarised and then modulated by a fixed retarder followed by a second retarder that rotates at a frequency \( \nu = \omega / 2\pi \). After reflection, the beam passes through a linear polariser, and the phases \( \phi_2 \) and \( \phi_4 \) of the respective second and fourth harmonics of the output signal are measured (fig. 1.43). This research work is partly supported by the European Community.

Commercial ellipsometers analyse the state of polarisation by measuring the intensity of the output signal; this value has to be very accurate to reduce the experimental errors. Since phase measurements are usually less affected by noise than amplitude measurements, this approach should be advantageous in the presence of low optical intensity and detector efficiency or when a noise source is present, as in industrial
environments. Moreover, the measurement of pure phases makes calibration very simple and stable. Once the azimuth values of the optical components are adjusted with respect to the incidence plane, no further calibration is required when the light source, beam size and intensity are changed. For the Frascati ellipsometer, the time resolution was limited to 25 ms by the rotation speed of the retarder.

To analyse noise rejection, the ellipsometer was tested for signal-to-noise (S/N) quality. Figure 1.44 shows two S/N levels; the average error was 0.05° (over 360°) in the best conditions (S/N=70). When the signal level was comparable with the noise (S/N=1.2), the error increased to 0.5°, which can be considered a successful result.

Fig. 1.44 - Output signal measured for two different values of S/N quality

After testing, the ellipsometer was used to monitor a real-time process. Worth noting is that with ellipsometry it is possible to detect surface modifications as small as a single monolayer without interfering with the process.

An electrochromic film made of WO$_3$ was coloured by electrochemical insertion of lithium ions. Figure 1.45 reports the results in terms of the ellipsometric angles. These data are used to calculate the change in the optical properties in terms of the refractive index and extinction coefficient of the film. The behaviour of the optical properties was also analysed as a function of time and found to be in agreement with what was expected from the diffusion coefficient value of lithium ions in the film.

The ellipsometer can also be used to monitor the optical properties of films under vacuum during the deposition process.

Fig. 1.45 - Ellipsometric measurements during electrochemical insertion of lithium ions in a WO$_3$ film

1.5.2 Digital holography and diffractive optics

Computer-generated holograms have diverse applications, e.g., in optical information processing, laser mode shaping and beam forming, 3-D displays, advanced seekers and sensors.

Phase and amplitude holograms have been designed, fabricated and tested at ENEA Frascati.
2.1 EXCIMER LASERS

The term excimer laser covers a family of laser systems that uses a gaseous mixture excited by electrical discharges as active medium. Excimer means excited-molecules bound only in the excited state and unbound (or weakly bound) in the ground state. This guarantees automatic lower-level depopulation, thereby allowing population inversion, as long as the excited molecules are present, and hence high laser output power. Among the excimer molecules, rare gas halides (RGHs) are the most efficient active media for emitting powerful ultraviolet (UV) laser light. One of the most effective RGH lasers is the XeCl, emitting laser photons at a wavelength $\lambda = 308$ nm. The wall-plug efficiency of commercial XeCl lasers ranges between 1% and 4%, one of the highest among UV lasers. This fact has promoted the widespread use of the XeCl and other excimer lasers in many applications requiring intense UV light, e.g., microelectronics, photochemistry, material processing, micromechanics, remote sensing and medicine. However, commercial excimer lasers are not suitable for important applications such as large-area material processing and propagation of high-energy and low-peak power laser pulses in optical fibres. This is due, respectively, to the limited ($<5$ cm$^2$) beam size (which in turn limits the output energy) and to the short ($< 30$ ns) laser pulsewidth typical of commercial laser systems. These problems were addressed at ENEA Frascati back in the late seventies, when work started on designing and constructing XeCl lasers with a large active medium, high output energy and long pulsewidth.

During 1998, the work at Frascati was mainly focused on developing and optimising the XeCl laser Ianus and on using the XeCl laser-facility Hercules to process materials and to develop a plasma x-ray source, in collaboration with universities and industries. In the framework of the European FOTO Project, the Frascati group designed the mechanical and electrical parts of an industrial XeCl laser called “Hercules L”, to be used for producing flat-panel displays with thin-film transistors by laser annealing of 10 cm x 10 cm a-Si. The laser will be assembled by the ELEN company and installed at the end of 1999 at ENEA Portici.

2.1.1 Ianus

The innovative feature of Ianus (fig. 2.1) is its double-discharge (three-electrode) structure, which makes it suitable for oscillator-amplifier configurations. The two laser discharges are geometrically in parallel so they can use the same gas-flow loop, and electrically in series so that they are simultaneously pumped. This guarantees their automatic synchronisation. The Ianus design is an ENEA patent.

Ianus was used to generate a laser beam with low-divergence, a requirement in many applications. The smallest of the two discharges (called “oscillator”) was equipped with a generalised self-filtering unstable resonator (GSFUR), a special kind of non-confocal negative-branch unstable resonator with magnification $M=8$, which enabled a laser output energy of 10 mJ with a full-width-at-half-maximum (FWHM) pulse duration of 90 ns. When injecting the oscillator beam in the amplifier, the energy of the amplified beam was nine times that of the oscillator.
To test the laser-beam optical quality, the experimental spatial energy distribution in the far field was compared with the diffraction-limited energy distribution, according to the most advanced definition of the "times diffraction limit" (TDL) number of highly diffracted laser beams. Figure 2.2 shows the interpolating function of the experimental far-field and diffraction-limited energy distributions calculated from the experimental near-field energy distribution. The oscillator laser beam was only 10% over its diffraction limit (TDL=1.1). This is an excellent result, considering the superradiant nature of high-gain excimer media and the small value of the diffraction-limited divergence due to the short wavelength emitted by excimer lasers.

The quality of the amplified beam, analysed with the same methods used for the oscillator beam, had a TDL=1.6. The discharge deterioration with time and the lack of suitable optical insulation between oscillator and amplifier account for the slight increment in the TDL. In any case, the most significant laser beam parameter, the beam radiance (defined as the laser peak-power/spot size/solid angle), increased from $5 \times 10^{13}$ W/cm$^2$/ster (oscillator) to $3 \times 10^{14}$ W/cm$^2$/ster (amplifier), one of the highest values reported in the literature for long-pulse UV lasers.

The foregoing measurements were repeated when operating the GSFlR in the burst mode up to a repetition rate of 50 Hz. A nearly diffraction-limited divergence was achieved from the beginning of the laser pulse and, most important, the values of the TDL, $M^2$ parameter and beam angular stability (BAS) were maintained, independently of the repetition rate. The BAS resulted in fluctuations smaller than one third of the beam divergence.

### 2.1.2 Hercules

Hercules, the oldest laser system operating at Frascati, was completed and characterised in the period 1987-1992. Since 1993, it has been available to users from universities as well as private and public companies interested in finding the optimum working point while irradiating and processing metals, semiconductors, glass, plastic and exotic materials and in driving soft-x-ray plasma sources.

Hercules is pumped by a discharge ignited by an x-ray pulse injected into the active medium when the desired voltage value across the electrodes is reached. This technique, called "phototriggered
discharge", allows reliable and almost jitter-free operation in the repetition rate mode. Regarding the discharge geometry, following a numerical study of the electric field distribution in the discharge chamber which takes into account the nearby current return parts, the electrodes were shaped adopting a "mixed" solution (Stappaerts cathode and Ernst anode). In this way, a uniform pumping discharge and a higher voltage breakdown level were achieved: no surface discharges on the insulator are detected even at the maximum repetition rate of 10 Hz.

Today Hercules is a XeCl laser system (fig. 2.3) operating in the repetition rate mode and emitting one of the highest energies per pulse in Europe, with long lifetime components and reliable performance (summarised in table 2.1).

When required, Hercules can also be used to amplify a 10-ns and 0.05-J XeCl laser pulse emitted by a commercial system; the amplified output laser pulse has a 2-J energy, 10-ns duration and \((0.1 \times 0.1)\) mrad\(^2\) divergence.

### 2.1.3 The EU FOTO project

The tasks of the excimer group at Frascati in the framework of the EU-funded FOTO Project are to develop the electromechanical design of a large-volume, high-output energy, industrial excimer laser called Hercules L and to use the actual Hercules to test the performance of a line-step beam homogeniser when annealing a-Si samples. Figure 2.4 shows the layout of the industrial prototype laser Hercules L.

Basically, Hercules L reproduces the scheme of Hercules, with some modifications to further enhance both laser performance and reliability (e.g., higher gas pressure, ceramic materials covering the insulator parts, state-of-the-art heat exchanger and easy access to optics and consumable parts). In particular, the preioniser is a new x-ray diode which uses commercial spark-plugs as the plasma cathode. Results show that this type of cathode is a low-cost, reliable, rugged and long-lifetime electron gun. After more than \(10^6\) shots, interrupted without any faults being found, the dose/shot was 7 mrd, the x-ray spatial distribution over a 100-cm length was uniform.
Fig. 2.5 - Intensity profiles of the Hercules laser beam in the overlap-plane of the line-step homogeniser along the horizontal a) and vertical b) directions. Note the different size of the beam along the two directions.

within 93% and the ionisation rate was greater than $10^{14}$ electrons/s/bar. These values guarantee an effective preionisation of XeCl excimer laser discharges. Due both to the long lifetime and to the substantial absence of maintenance, this x-ray diode seems suitable for preionising commercial gas lasers such as the excimer and the TEA CO$_2$.

The beam homogeniser was designed to transform the Hercules laser beam from 50 mm x 100 mm to 11 mm x 130 mm with a spatial uniformity better than 95%. The homogeniser consists of two arrays of cylindrical lenses, two cylindrical condensers, and a 45° mirror to bend the laser beam to a vertical direction (fig. 2.3). Figure 2.5 shows the intensity profiles of the laser beam in the overlap plane of the line-step homogeniser along the horizontal and vertical directions. Note that in the central 10-cm-wide region the homogeneity has a 3% root mean square (rms).

Preliminary annealing tests showed the formation of crystal grains with a size of about 1 µm, suitable for the production of high-mobility thin-film transistors. These results were obtained on a 500-Å a-Si film deposited on glass substrate, placed in a vacuum chamber and heated to 600°C. The homogenised laser energy density on the sample was 0.4 J/cm$^2$. Figure 2.6 shows a scanning electron microscopy (SEM) image of the grains in the irradiated Si.

Modelling of interactions at the interfaces

In the framework of the FOTO project, two different monodimensional models based on heat flow calculations were developed to simulate the laser irradiation process. In both cases the problem is solved numerically, using the following assumptions:

- the laser beam dimension is much larger than the absorption length;
- the surface is considered as isolated;
- the sample has infinite thickness.

Phase changes from amorphous to liquid and crystal states are included and the thermal and optical parameters correspondingly changed. In the first case, thermal profiles are obtained by simply assuming that if the system (a finite-difference cell) is undercooled to temperatures in the range from...
T_h to T_n (a-Si melting temperature ≈1420°K and nucleation temperature ≈1480°K, respectively) and remains there for a time t_n (nucleation time ≈4ns), a nucleation event is allowed to occur.

The model was first applied to the a-Si/glass system and then exploited to evaluate the effect of the high-power laser Hercules (E=10J, FWHM=128ns) developed in the project (fig. 2.7). As expected, due to its longer pulse duration a higher (+30%) energy is required to completely melt the amorphous silicon layer with respect to the commercial laser employed so far (FWHM=28ns).

The feasibility of several innovative configurations was evaluated; namely, a-SiC/glass, a-SiC/Si, a-SiC/SiC, a-InP, a-Si/poliestere, a-Si/polistirene and a-SiC/PVC. It was found that the high thermal conductivity of the substrate makes it necessary to have a film of SiO_2 in order to process the amorphous SiC film deposited on crystalline silicon or SiC. A thick film of SiO_2 is also required to prevent substrate modifications when the amorphous silicon is deposited onto plastic materials.

A second model was developed to answer the many questions arising from laser-induced recrystallisation of a-Si thin film. The use of nanosecond pulses in fact minimises both substrate heating and impurity diffusion but leads to phase transitions which take place very far from equilibrium. As a result, the average grain size is not always uniform through the recrystallised layer thickness and shows a non-monotonic dependence on pulse energy. The melt duration itself shows a strongly nonlinear dependence on the energy. Although some reasonable qualitative explanations of these phenomena have been offered, the available numerical models are as yet unable to explain these data.

The model is based on the standard nucleation and growth description of solidification from melt and includes a simplified set of equations that give a first-order description of microstructure evolution. The grain-concentration rate of change is described by classical nucleation theory, and their growth is governed by the same interface response function used for the movement of the planar solid-liquid interface. Unfortunately, the functional dependence of the interface response function and the absolute value of some parameters contained in the nucleation rates are not well known. Even the relevance of heterogeneous nucleation processes is not well established. Therefore, the first task is to choose a suitable set of input parameters.

Preliminary comparison of the results of the model with experimental data suggests the following:

- To match the melt duration data, the homogeneous nucleation rate has to be adjusted so as to become significant only at very large undercoolings (~500 K).
- As a consequence, to explain the explosive crystallisation phenomenon, heterogeneous nucleation at the amorphous-liquid interface has to be introduced.
- A sharp decrease in the interface response function for large undercoolings is necessary to obtain
2.1.4 Soft-x-ray generation

An interesting application of high-power excimer lasers is the generation of high-radiance soft-x-ray sources through creating a small-size, high-density plasma on the surface of a target. When the target is heated by a focussed pulsed laser beam with an energy per shot of 1–10 J, pulse duration of 1–100 ns and low divergence, this forms a plasma with a temperature of ~10^6 K which emits radiation in the soft-x-ray spectrum, say 10–100 Å. The shorter the laser wavelength, the deeper the penetration of the laser radiation inside the plasma and the higher the conversion efficiency from laser energy to soft-x-ray energy. As a result, excimer lasers are the best candidates for generating x-ray plasma sources. Hercules, when equipped with the positive-branch unstable resonator (PBUR) (see table 2.1), has the right energy, pulse width, divergence and wavelength for generating a high-radiance soft-x-ray source. Experiments based on focusing the Hercules laser beam into a 30-μm-diam circle, where the laser intensity reaches a value of 10^{13} W/cm^2, were carried out in the framework of a collaboration between ENEA, L'Aquila University, Milan University and the Italian Institute of Health (Rome). The measured sizes of the x-ray source and laser spot are comparable (30 μm) and the energy conversion efficiency from laser to x rays exceeds 20%. Hence, this x-ray source has a radiance value comparable to that of a synchrotron storage ring, especially in the spectral region below 1 keV.

The characteristics of this plasma source made it possible to work on the following experiments during 1998:

a) atmospheric pressure soft-x-ray microscopy;

b) propagation of x rays in capillary tubes;

c) reduction of particulates (debris) emitted by the plasma;

d) high-resolution x-ray spectroscopy;

e) construction of an extreme ultraviolet (XUV) laser.

a) A new x-ray microscopy technique based on the propagation of soft x-rays in He gas at atmospheric pressure was developed. In this way, the biological specimen can be quickly inserted into the laser-target interaction chamber; hence, even delicate and short-lifetime specimens can be imaged and the quality of the images is improved by the reduction in debris bombardment (He slows down the debris). Figure 2.9 shows x-ray microscopy images of ciano-bacteria and of an intracellular element (a mytocondrius). The resolution is better than 100 nm (fig. 2.9b), far beyond the resolution of a light microscope.

b) Preliminary results of propagation of soft x rays (at 70 and 1200 eV) in capillary tubes (see fig. 2.10) were obtained. These experiments are important as capillary tubes could be a powerful tool to transport the x-ray beam out of the laser-target interaction chamber and could potentially allow new applications such as near-field scanning microscopy: a transmission map of a biological specimen is obtained point by point with a spatial resolution better than 50 nm just by illuminating the sample with an x-ray microbeam coming out from a tapered glass microtube.

c) Reduction of particulate emission from the plasma is very important for specific applications like x-ray microlithography where fragile masks and optics must be placed close to the plasma source. Work was done on the characterisation and minimisation of both the amount and the speed of the debris emitted by the plasma for different laser parameters (pulse energy, spot diameter, etc.). A Faraday cup
and an electrostatic analyser were used to measure the charge state and the speed of ions emitted by tantalum, copper and aluminium targets (fig. 2.11).

A gated charge coupled device (CCD) camera allowed observation of hot debris emitted by a tantalum target (fig. 2.12). This experimental result is very interesting for projection microlithography applications: it was found that the laser parameters which optimise the emission at 70 eV (300-μm laser spot diameter and 120-ns pulse duration) significantly reduce both amount and speed of debris with respect to the laser parameters typically used in microlithography (less than 100-μm spot diameter and 10-ns pulse duration).

d) The interaction between the plasma and a cold gas (helium at atmospheric pressure) was studied, and the presence of hollow atoms (atoms with the first electron shell, n=1, empty) in the plasma obtained with a magnesium target was successfully investigated. These important results of basic plasma physics were obtained thanks to special high-resolution x-ray spectrometers manufactured by the Institute NPO “VNIIFTRI” of Moscow, in the framework of a bilateral co-operation between the governments of Italy and the Federal Republic of Russia.

e) In the framework of a collaboration between ENEA, L’Aquila University and Pecs University (Hungary), Frascati contributed to the design and construction of a laser system based on XUV emission from an argon gas pumped by a capillary electric discharge. The principle of operation is to discharge a 30-kA electric current through a capillary filled with 1-mbar argon; the magnetic pinch-effect squeezes the discharge into a narrow column (Φ< 0.5 mm), thus heating the argon at a temperature close to 10^6 K and creating a plasma with ions in the charge state Ar^8 (Ne-like). The construction of the laser was completed during 1998 at the Physics Department of L’Aquila University, and experiments are going on to achieve laser emission at λ=46.9 nm (26 eV).
2.2 SOLID-STATE LASERS AND SPECTROSCOPY

Crystal defects are very important in solid-state science mainly because many of the interesting properties of crystalline solids are dominated by effects due to tiny concentrations of imperfections in an otherwise perfect lattice. Among point defects in insulating materials, colour centres in alkali halides were the first to be studied systematically, at the beginning of this century. In the last two decades, basic investigations have added new critical information to the already vast knowledge of this model-case branch of solid-state physics; interesting applications have also been exploited, e.g., tunable laser sources operating in the visible and near-infrared, dosimetry, holography and optical information storage. Recent scientific and technological developments of innovative or advanced materials have further increased the primary role of point defects also in more complex materials characterised by peculiar microscopic structures, and their active optical properties are attracting renewed interest, especially in view of the development of innovative compact optoelectronic devices.

Up to a few years ago, activities at ENEA Frascati were limited to studying the optical properties of colour centres and their application to solid-state lasers operating at liquid nitrogen temperature (LNT). This class of defects allows tunable laser emissions in the range 0.5–4 μm. At Frascati, two lasers emitting around 2.7 and 1.5 μm were developed.

Recently, combining this long expertise in colour centres with thin-film-based technologies, the main activity was shifted to investigation and development of optical microsystems, whose applications are envisaged in many areas, ranging from optical communications to consumer optoelectronics and from sensors to displays.

However, some efforts have continued to be devoted to coloured bulk crystals, where a lot of phenomena await disentanglement. In particular, the luminescence in KF:Na has been studied in differently coloured samples and vs the temperature. Figure 2.13 shows anticorrelated emissions at 900 and 2150 nm as a function of temperature. These emissions were assigned to F_A centres of two different types. This has changed the well-known picture of F_A centres, which are no longer described by a consistent theory. Just as a reminder, note that the emission efficiency of this highly hygroscopic crystal is very close to unity. Moreover, one of the F_A emissions in KCl:Li was utilized in 1974 in the first colour centre laser.

In the much more manageable coloured KCl:Li
crystal it should also be possible to observe typical nonlinear effects. Analysis of the behaviour of $F_A$ reorienting colour centres has shown that, even if the reorientation of a single centre under resonant excitation with polarised light can be described in terms of linear optics, the macroscopic properties of the system are described in terms of nonlinear optics. Typical nonlinear effects can be induced at a low-excitation level in this case. As a result of the nonlinearity in the system under consideration, polarisation instabilities should be expected when the crystal is mounted inside a cavity. Polarisation bistability for the exciting light strongly modifies the luminescence gain, as shown in figure 2.14. Indeed, when the polarisation angle $\Psi_0$ of the pumping source is rotated, under certain experimental conditions the output intensity is highly unstable and undergoes macroscopic variations under small perturbations; this effect could be put to work in device development.

LiF and its colour centres merit a description apart. This crystal is relatively hard and resistant to moisture, possesses a wide optical gap and can be coloured only by irradiation with ionising radiations. Last but not least, its F centres, the simplest of all colour centres, do not show any emission under optical excitation, while many other more complex colour centres are stable and show intense luminescence, which has been utilized for room-temperature (RT) laser devices. In particular, $F_3^+$ and $F_2$ centres emit and lase in a pulsed regime in the green-red region of the spectrum. Figures 2.15 and 2.16 show the absorption and emission bands of such colour centres in LiF. The peculiar properties of the $F_3^+$ centre derive from its optical cycle (fig. 2.17). While
the four-level scheme explains the equilibrium absorption-emission measurements of figures 2.15 and 2.16, the new level $^3E_1$ introduces a perturbation element in the cycle, which produces an effective quenching of the emission in particular cases, as in figure 2.18. These quasi-nonlinear properties have been addressed at Frascati through accurate spectrally resolved stationary and dynamic investigations.

However, these highly efficient active colour centres have also been investigated in order to optimise them as laser media in conventional optical cavities. Encouraging results of laser action and/or superfluorescence were found in samples placed in Fabry-Perot cavities (fig. 2.19).

As far as thin films of LiF are concerned, attention is currently being focused on a) investigation of the optical properties of defects in relation to the material growth and preparation, b) the mechanisms of colour-centre creation by ionising radiation and c) studies of the radiative and nonradiative phenomena involved in their optical cycle. Regarding innovative miniaturised light sources, particular attention has been given to waveguide geometries, the integration of passive and active optical functions and their compatibility with integrated optics and electronics.

The exciting results obtained in 1998 for lithium fluoride treated with low-energy electron beams open interesting perspectives for the development of broadband miniaturised lasers and amplifiers tunable across the visible spectrum. The relative work was performed in the framework of the E.C. ESPRIT project N.24503 WAFFLE, coordinated by ENEA and involving CNR-IREO in Florence (Italy), CSIC in Madrid (Spain) and GeeO, a small company in Grenoble (France). For the first time, active waveguides with strong photoluminescence in the red and green spectral ranges were produced by irradiating LiF crystals and films with 12-keV electron beams. Low penetrating electrons create laser active defects at the same time as they induce a change in the refractive index. The resulting active waveguides emit and/or amplify visible light, and by a single-step lithographic process it is possible to
transfer a defined waveguide pattern onto the surface. Single-mode channel waveguides a few tens of microns wide and more than 10 mm long have been written onto LiF single crystals and polycrystalline films. Pumped with blue light from an argon laser, the samples emit green and red light visible to the naked eye.

Although the main spectroscopic features of these defects are similar to those in bulk crystals (figs. 2.15 and 2.16), the formation efficiency of F-aggregate centres is higher in polycrystalline films than in single crystals and depends on the peculiar nature of the films, whose structural and morphological properties are strongly influenced by the deposition conditions. The surface-to-volume ratio and the film compactness play the major role because they establish the density of the grain boundaries, which act as a source of vacancies during the colour-centre formation and stabilisation processes. Photoluminescence measurements provide a simple and powerful tool for the development of miniaturised components, particularly if they are performed on samples characterised by restricted geometries and/or non-transparent substrates (fig. 2.20).

Similar emissions have been observed in electron bombarded LiF films deposited on different kinds of substrates, including silicon (see fig. 2.21).

For the first time sizeable gain coefficients from 24 to 32 dB/cm were measured by the amplified spontaneous emission (ASE) technique on a coloured strip in a LiF film in the green-red spectral range. The experimental setup is shown in figure 2.22. Losses from 3 to 6 dB/cm were reached in LiF/NaF bilayer passive waveguides.
The spectroscopic properties of different kinds of insulating materials, such as diamond films, silicon nanoparticles and multilayered alkali halide films, were also investigated.

2.3 FREE ELECTRON LASERS

Due to their wide range of tunability and their high brightness, free electron lasers (FELs) are versatile sources of coherent radiation. The physical mechanism that produces coherent emission in a FEL is the interaction between a relativistic electron beam and a magnetostatic field with a spatially periodic configuration; in a conventional laser the stimulated emission from an atomic or a molecular system is exploited. Construction of these lasers is now worldwide and at present they cover the electromagnetic spectrum from millimeter waves up to vacuum ultraviolet. They can provide high peak power and short pulses or narrow linewidth in long-pulse operation, depending on the characteristics of the apparatus. Electronic efficiency as high as 30% has been demonstrated in systems employing tapered undulators, and a wide range of tunability has been achieved in many FELs, making them appealing for a variety of applications, from spectroscopy to solid-state physics, biology and medicine.

A FEL is basically composed of three parts: an electron accelerator, a magnetic undulator and an optical resonator. The electrons are forced by the magnetic field onto an oscillating trajectory, thus emitting synchrotron radiation. In the electron frame reference, the process can also be seen as a scattering between the electron beam and the virtual photons of the undulator. If an external field is present, the radiation is emitted in phase with this external field. The interaction between the laser field, the static magnetic field of the undulator and the electron beam has as a final effect the spatial bunching of the electrons on the scale of the radiation wavelength, and the transfer of energy from the electron beam to the laser field. The undulator can be considered as the equivalent of the "active medium" of a conventional laser system, while the electron beam is the equivalent of the "pumping system".

2.3.1 FEL experimental activity

The appealing features of FELs (e.g., tunability, high output power) are usually counterbalanced by a few drawbacks, such as large size, high cost and system complexity. Nevertheless, there is a wavelength range, not covered by conventional laser sources, where the FEL can meet the requirement of compactness: the far-infrared (FIR) and submillimeter (sub-mm) regions. The FEL experimental activity at ENEA Frascati is focused on this spectral range through the development both of a standard FIR/mm-wave waveguide compact FEL and of a machine based upon a new concept, the so-called "Phase Matching" FEL. In this spectral region low-energy accelerators can be employed, reducing cost and size of the system with less severe requirements on e-beam quality and radiation shielding. Electron transparent mirrors (ETMs) can be used in waveguide resonators, further reducing size and complexity of the system. The dispertion properties of the waveguide resonator provide additional control over the spectral characteristics of the emitted radiation.

The waveguide compact FEL experiment

For electron energies in the range between 2 and 5 MeV, significant gain is obtained for a small number of periods, thereby allowing FEL operation with a short undulator and resonator. An important requirement for a rf-driven FEL is the matching between the round trip time of the optical pulses in the cavity and the electron bunch spacing. Exploiting the dispersion properties of the waveguide, it is possible to slow down the wave velocity, allowing the superposition of the electron bunch and the light pulse all over the interaction region (zero slippage operation). In this situation, the gain curve has a broad bandwidth ($\Delta \lambda/\lambda = 1/N^{1/2}$), the FEL efficiency is doubled and the gain is less sensitive to the e-beam quality, when compared to the free-space case.

A mm-wave FEL facility was developed at ENEA Frascati. A compact waveguide undulator FEL was built and successfully provided 1.5 kW of output power in 4-μs pulses in the wavelength range between 2.1 and 3.6 mm. User experiments were performed in solid-state physics to test mm-wave detectors and materials.
This compact mm-wave FEL used a 2.3-MeV microtron as electron source. In order to extend the emission spectral region to the far infrared (FIR), the microtron energy was increased to 5 MeV and a new hybrid waveguide resonator was designed and built during 1998. The layout of the resonator is sketched in figure 2.23 and the experimental parameters are reported in table 2.II.

This resonator was tested using a FIR gas laser and is currently being installed on the e-beam line. The characteristics of the undulator spontaneous emission were investigated at 5-MeV electron energy, giving good agreement between theory and experimental data.

**Phase matching FEL experiment**

Coherent spontaneous emission (CSE) occurs in a FEL when the electron bunch length is comparable to the wavelength of the radiation generated in the undulator. Under such conditions all electrons in the bunch have a similar phase and emit coherently. The emission is proportional to $N^2$, where $N$ is the number of electrons in the single bunch ($\approx 10^8$), while the incoherent emission is proportional to $N$. Moreover, if the electron current is generated in a rf accelerator, it has modulation at the harmonics of the rf, $\omega_{RF}$, with a relative amplitude that depends on the electron bunch shape.

An interesting problem, which is currently the object of investigation, is the possibility of enhancing the CSE from a rf-modulated electron beam by proper manipulation of the electron distribution in the longitudinal phase space. Theoretical analysis and design development of a device were carried out to systematically investigate the CSE as a function of the longitudinal phase space distribution.

Utilising a simple physical model, it is possible to treat each electron bunch at the undulator entrance as an ensemble of $N_e$ particles distributed in the phase space $(\psi, \gamma)$, each having energy $\gamma_i$ and phase $\psi_i=\omega_{RF} t_i$ with respect to a reference charge injected at $t=0$ with velocity $\beta_{z0}$. The emitted power can be maximised when the single electron contributions interfere constructively with each other. This happens when the electrons are distributed in the longitudinal phase space as close as possible to the phase-matching curve:

$$\psi = -\frac{\pi L}{c T_{RF}} \left( \frac{1}{\beta_{z}(\gamma)} - \frac{1}{\beta_{z0}} \right)$$  \hspace{1cm} (1)

Theoretical analysis showed that, for a given temporal profile of the electron bunch, the emission from a “correlated” distribution of electrons in the $(\psi, \gamma)$ plane, satisfying the phase-matching condition (1), can be up to a factors of ten higher than that from an “uncorrelated” distribution. Further simulations
were performed, keeping the longitudinal emittance constant when manipulating the longitudinal phase space. Calculations on a bunch composed of 1250 macroparticles, each one with a 0.1 pC charge, are shown in figure 2.24 for two different distributions in the longitudinal phase space. The “horizontal” distribution is totally uncorrelated, while the other fulfils the phase matching condition. Also in this case a considerable increase in output power is calculated for the correlated distribution, as can be seen from the spectra in the figure.

A new device was designed to “manipulate” the electron bunches in the longitudinal phase space. The experimental setup consists of a linear accelerator composed of an electron gun, a short transport line and two accelerating sections followed by a permanent magnet undulator located at a distance of 30 cm (fig. 2.25).

A triplet of quadrupoles provides focusing at the undulator entrance. The undulator is 40 cm long, consists of 16 periods and operates with a magnetic field of 6000 Gauss corresponding to $K_W=1$. A rectangular waveguide, with cross section $axb=10.668 \times 4.318 \text{ mm}^2$, is located inside the undulator.

The electron beam (1 A – 13 kV) is produced by a pulsed triode gun equipped with a 7.7-mm-diam osmium-treated dispenser cathode. A suitable optical magnetic lens system matches the input admittance of the accelerator, which consists of the following two modules (fig. 2.26):

a) A $\beta$-graded on-axis S band (2998 MHz) linear accelerator (linac), with three full cells and two half end cells, operating in the $\pi/2$ mode. This section accelerates an electron macro bunch current of 0.40 A to an energy of 1.8 MeV; the coupling coefficient to the waveguide $\beta$ is 3.2.

b) A phase matching section (PMS) placed 4 cm downstream of the linac output. The drift space and the phase shift of the PMS are set to have the reference electron pass through the centre of the PMS with a phase close to zero. The coupling coefficient to the waveguide $\beta$ is 1.1. The PMS is composed of three on-axis coupled cavities (one and two halves) operating in the $\pi/2$ mode tuned at the same frequency as the linac. Two motorised plungers inserted in the end cavities adjust the frequency to the exact design
value. In addition, a cooling system keeps both linac and PMS at the fixed temperature of 30°C ±0.05°C.

The distribution of the bunched electrons in the phase space at the PMS output can be changed by varying the phase and amplitude of the rf field driving the PMS with respect to the linac. The total rf power required is about 2 MW. In order to control phase and amplitude independently, a suitable rf system has been designed. It uses a high-stability low-power cavity controlled oscillator, an amplifying chain and a 10-MW klystron equipped with a 3-dB power splitter: one arm feeds and controls the rf accelerating field amplitude to the linac, the other is equipped with a high-power variable attenuator and a variable high-power phase shifter (0-360°) enabling power and phase control of the PMS module.

Numerical simulations of the beam dynamics were performed using the PARMELA code. The calculation takes into account the space charge effects and uses 3000 particles leaving the gun with a charge per particle of 0.11 pC corresponding to a beam current of 1 A with an energy of 13 keV and an emittance of 17 π mm mrad.

A net increase in the CSE, from 2 kW to about 14 kW, is expected for a phase space distribution at the PMS output with optimum setting with respect to the distribution at the linac output (fig. 2.27). In the case shown in the figure, the electric field in the PMS is set to 50% of the electric field in the linac (E_{linac}= 25 MV/m), and the relative phase is adjusted in order to have proper correlation at the undulator input.

2.3.2 FEL theoretical activity

Analysis of FELs operating in the optical- klystron configuration

This activity was aimed at developing a theory of optical-klystron (OK) FEL devices including parametrization formulae capable of accounting for high gain, inhomogeneous broadening and saturation.

**High-gain effects.** It has been shown that the maximum OK small signal gain can be written as

\[
G_M = 0.85g_{ok} + 0.185g_{ok}^2 + 5.6 \times 10^{-5} g_{ok}^3 \\
g_{ok} = 8g_0 \left( 1 + 0.93 \frac{\delta}{1 + 0.037} \right), \quad \delta = \frac{N_d}{N_u}
\]  

(2)
where $g_0$ is the small signal gain coefficient, relative to one undulator, $N_d$ is the equivalent number of periods of the dispersive section and $N_u$ the number of periods of one undulator (see fig. 2.28).

**Inhomogeneous effects.** The inclusion of the e- beam relative energy spread $\sigma_e$ has been shown to induce a gain depression, which can be evaluated by exploiting the simple relation

$$G_{M,0} = G_M \exp\left(-1.228\mu_e^2\right),$$

$$\mu_{ok} = 2(1+\delta)\mu_e, \mu_e = 4N_u\sigma_e \quad (3)$$

The relevance of the inhomogeneous broadening effects is shown in figure 2.29.

**Saturation effects.** The OK saturation intensity has been introduced and is defined as

$$I_{s,0} = \frac{I_s}{[4f(\delta)]^2}$$

$$f(\delta) = 1 + \frac{0.995\delta}{1 + 0.172/\delta} \quad (4)$$

where $I_s$ is the saturation intensity of a conventional FEL operating with one undulator section only. It has also been shown that the OK FEL gain depends on the intensity according to the formula

$$G_M(x) = \frac{1}{2}G_M \left[1 + (1 - \chi)e^{-x(a+b\delta^{1/3})}\right],$$

$$\chi = \frac{I}{I_{s,0}} \quad (5)$$

where $I$ is the intracavity intensity, if the device is operating as an oscillator. The limits of validity of the above formula were carefully discussed and its comparison with the results of a numerical simulation is shown in figure 2.30.

**Analysis of electron beam energy phase correlations in FELs**

The theory of FELs operating with a prebunched e-beam and self-induced coherent harmonic generation has played a role of paramount importance in the design of FELs operating at short wavelengths in the mirrorless self-field amplified configuration. The work described in this section complemented that activity and was aimed at verifying that the radiation emitted by an energy-phase
correlated e-beam consists of two contributions: spontaneous coherent and stimulated emission.

Spontaneous coherent emission has been shown to be linked to the e-beam longitudinal distribution parameters by

$$a_c(\tau) = -2\pi g_0 \int_0^\tau \exp \left[ -\frac{1}{2} \left( \frac{\sigma_T^2}{1 + \alpha_v^2} \right) - \frac{1}{2} \left( \tau' + \frac{\alpha_v}{\gamma_v} \sigma_v^2 \right) \right] \mathrm{d}\tau'$$

(6)

where \(\sigma_T\) represents the initial rms microscopic bunching and \(\alpha_v\) the Twiss parameter of the initial e-beam longitudinal distribution defined as

$$f(v, \xi) = \frac{1}{2\pi \Sigma_v} \exp \left[ -\frac{1}{2 \Sigma_v} \left[ \beta_v (v - \bar{v})^2 + 2\alpha_v (v - \bar{v}) \xi + \gamma_v \xi^2 \right] \right]$$

(7)

with \(v\) denoting the electron energy in the FEL canonical variable domain and \(\Sigma_v\) representing the longitudinal phase-space emittance. The degree of beam energy phase correlation is just measured by \(\sigma_v\). An idea of the dependence of \(a(\tau)\) on the beam distribution parameters is given in figure 2.31.

Stimulated emission has been shown to split in two more terms:

$$a_G(\tau) = i\pi g_0 \int_0^\tau \int_0^{\tau_1} \int_0^{\tau_2} \exp \left[ -i\bar{v}_2 - \frac{1}{2} \tau_2^2 \sigma_v^2 \right] a_c(\tau_1 - \tau_2)$$

$$a_{B_2}(\tau) = i\pi g_0 \exp \left[ -\frac{2 \Sigma_v}{\gamma_v} \right] \int_0^{\tau_1} \int_0^{\tau_2} \int_0^{\tau_3} \exp \left[ -i\bar{v}_3 - \frac{1}{2} \left( 2\tau_1 - \tau_2 - 2\alpha_v \right) / \gamma_v \right] a_c(\tau_1 - \tau_2)$$

(8)

The first term leads to the usual gain contribution, \(\sigma_v\) is the e-beam energy spread in the \(v\)-space. The second term represents the contribution of the prebunching stimulated emission. The total radiated field is therefore

$$a_T = a_G + a_{B_2} + a_c$$

(9)

![Fig. 2.31](image-url)
The importance of this additional contribution is shown in figures 2.32, 2.33 where $|a_T|^2$, $|a_G|^2$, $|a_{B_4}|^2$ is plotted vs $\alpha$ using the hypothesis of constant bunching. Emission is always dominated by the coherent contribution, while that of the other terms becomes appreciable for $g_0 > 1$.

For $g_0 > 4$ at $v = 2.6$, the $G$ and $B_4$ contributions amount to about 35% of the total. Note (see fig. 2.32b) the constructive interference between the various contributions in (9), which can be inferred from the fact that

$$|a_T|^2 > |a_G|^2 + |a_{B_4}|^2 + |a_c|^2$$

This analysis also shows that one of the most efficient means to create an e-beam phase correlation is the FEL interaction itself. It has also proved that energy-phase correlation is only one aspect of the mechanisms associated with e-beam bunching.

**Analysis of FELs operating with variably polarising undulators**

The theory of FELs operating with variably polarising undulators (VPUs) has been developed because this type of device may provide elliptically polarised radiation and because storage ring OK FEL devices exploiting undulators with opposite circular polarisation may offer the possibility of getting linear on-axis polarisation without the contribution of higher on-axis harmonic emission, thereby reducing the problems associated with mirror damage.

It has been shown that the gain of a FEL operating with a VPU, i.e., an undulator with field components (see figs. 2.34, 2.35)

$$B_x = -B_0 \sin(\phi) \cos(k_u z + \phi)$$

$$B_y = B \cos(\phi) \sin(k_u z + \phi)$$

$$B_z = 0, \quad K_U = 2\pi/\lambda_U, \quad \phi = \pi d/\lambda_U, \quad B_0 = \sqrt{2} B_{a,b}^0$$

is specified by the small signal gain coefficient

$$g_0(\phi) = \frac{16}{\gamma} \lambda_I [m] L_U [m] N^2 \frac{J(A / m^2)}{1.7 \times 10^4 \cos(2\phi)} f(\Theta, \phi)$$

$$f(\Theta, \phi) = J_0(\Theta)^2 + J_1(\Theta)^2 - 2 \cos(2\phi) J_0(\Theta) J_1(\Theta)$$

where

$$\Theta = \frac{k^2 \cos(2\phi)}{4 \left(1 + \frac{k^2}{2}\right)}, \quad K = \frac{eB_0 \lambda_{U}}{2\pi n_0 c^2}$$

and by the saturation intensity

52
where $I_s$ refers to the saturation intensity of a FEL operating with a linearly polarised undulator.

Apart from the Bessel factor, the description of a FEL operating with a VPU does not present any significant difference with respect to the ordinary case. It is evident that for $\phi=\pi/4$ the above relations reduce to the usual expressions relative to the helical case. Figure 2.36 reports the small signal gain coefficient and saturation intensity vs $\phi$. It is evident that linearly polarised undulators ($\phi=0, \pi/2, \pi, ...$) exhibit the smallest value of $g_0$ and the largest value of saturation intensity.

As already mentioned, the possibility of operating a FEL in the OK configuration by exploiting two VPUs with opposite polarisations ($\phi_1=-\phi_2$) is attractive for a number of reasons. If the two undulators have equal number of periods $N_u$ and dispersive section $L_d=5L_u$, the polarisation angle with respect to the x-axis reads as

$$\Psi = \tan^{-1} \frac{\sin(\phi)[J_1(\Theta)+J_0(\Theta)]}{\cos(\phi)[J_1(\Theta)-J_0(\Theta)]} \left[ \frac{(1-\cos (v(1+\delta)+2\phi))}{(1+\cos (v(1+\delta)+2\phi))} \right]^{1/2}$$

(15)

Note that in such an OK FEL configuration the positive interference effect leading to enhancement of the small signal gain is balanced by the negative contributions due to the opposite polarisation.

The OK FEL gain for opposite polarisation writes as

$$G(v,\phi,\delta) = -2\pi g_0 \frac{\partial}{\partial \nu} \left[ \left( \frac{\sin(v/2)}{v/2} \right)^2 \left[ 1 + M(\phi) \cos (v(1+\delta) + 2\phi) \right] \right]$$

$$M(\phi) = \frac{\cos(2\phi)(J_1(\Theta)^2+J_0(\Theta)^2)-2J_1(\Theta)J_0(\Theta)}{J_1(\Theta)^2+J_0(\Theta)^2-2\cos(2\phi)J_1(\Theta)J_0(\Theta)}$$

(16)
This last formula was derived by applying Madey's theorem. An idea of the behaviour of the interference factor $M(\phi)$ is given in figure 2.37.

Examples of spontaneous spectrum profiles for different parameters are reported in figures 2.38, 2.39.

It is evident that the effect of dispersive section modulation is always smaller than it would be for an undulator with equal polarisation and, furthermore, that it is clearly absent in the case of $\phi=\pi/4$, which on the other hand does not appear very sensitive to inhomogeneous broadening effects.

**Analysis of storage ring FELs with the inclusion of longitudinal and transverse instabilities**

Activities on storage ring (SR) FELs were aimed at clarifying the interplay between laser dynamics and transverse and longitudinal e-beam instabilities and at serving as support to the ELETTRA FEL project.

The theory of SR FELs operating with an e-beam affected by some kind of instability (microwave, sawtooth, head-tail, etc.) has attracted a lot of interest because several experimental results seem to suggest that under appropriate conditions the onset of the FEL counteracts the growth of the instability and could even switch it off.

The strategy exploited to deal with this kind of problem proceeded by gradual steps. Initially treated were the problems relative to microwave and sawtooth instability.

Regarding the first case, the starting point was the Boussard criterion, which fixes a threshold current above which this instability grows and manifests itself through an anomalous increase in the energy spread and bunch lengthening. Since the FEL induces an increase in the energy spread, it was argued that the FEL may provide a shift of the microwave instability threshold. By combining FEL and Boussard equations, it was possible to set a laser power density threshold for instability switch-off and, indeed, the following was obtained:

$$ I^* = 1.673 \frac{d^2 - 1}{\xi_0 \Sigma} \mu_e^2 \left( \frac{1}{4N_u P_s} \right), \quad d = \frac{\hat{I}}{I_{th}} $$

where $\hat{I}$ and $I_{th}$ are the e-beam peak and Boussard peak threshold currents, respectively; $\Sigma$ the laser...
cross section and $P_s$ the power lost by synchrotron radiation. Comparison of this prediction with numerical analysis results is reported in figure 2.40, where the existence of a threshold that switches off the instability without creating additional effects is evident. The problems associated with sawtooth instability (STI) were tackled by developing a model for the instability itself: by means of a couple of nonlinear equations of the Volterra type and by combing these equations with the SR FEL rate equations; namely,

$$\frac{d\alpha}{dt} = \frac{A}{(1+\sigma^2)^{1/4} - B(1+\sigma^2)^{1/2}} \alpha$$

$$\frac{d\sigma^2}{dt} = \alpha\sigma - \frac{2}{\tau_s} (\sigma^2 - x_0)$$

$$\frac{dx_0}{dt} = E x_0 \left( \frac{1}{\sqrt{1+\sigma^2}} - \frac{1}{1+1.7\mu_s^2(1+\sigma^2)^2} \right)$$

were $\alpha$ is the instability growth rate, $\sigma$ the ratio between the e-beam energy spread and the natural energy spread and $x_0$ is linked to the intracavity power density. The constants $A,B,E$ depend on the machine and FEL parameters while $r$ is linked to the cavity losses.

Examples of FEL-instability evolution are given in figures 2.41, 2.42. In this case, too, the FEL may counteract the instability growth, but the dynamics is strongly dependent on the machine parameters.
3.1 INTRODUCTION

At present, particle-accelerator activities at ENEA Frascati are mainly focussed on developing these devices for medical, industrial and research applications. The theoretical/technological experience and know-how acquired in the particle-accelerator field has also been transferred to Italian industry and government institutes.

An S-band electron linear accelerator (linac) for intra-operative radiation therapy (IORT) of cancer was designed and constructed in a collaboration between ENEA and HITESYS, an ENEA associate company. Some machines are in operation at public hospitals.

Under an official agreement (signed in November 1997) with the Italian Institute of Health (Istituto Superiore di Sanità [ISS]), ENEA has provided ongoing expertise in the design and construction of a highly innovative proton linac for cancer proton therapy (TOP linac). The ISS program also includes using a proton beam at the energy needed to produce radioisotopes for positron-emission topography (PET), radiobiology studies and applications.

The accelerator scenario includes design and development of low-energy electron linacs with special radiofrequency (rf) systems and e-beam manipulation techniques, for free-electron lasers (FELs) and electromagnetic (em) radiation generators in the millimetre, sub-millimetre and far infrared wavelength range, and the implementation of a 20-MeV microtron at ENEA Casaccia.

Laboratory applications of accelerators include:

- a 5-MeV circular microtron used as a driver for the millimetre compact waveguide FEL;
- a 3-MeV S-band electron linac currently in operation for e-beam irradiation tests of materials, dangerous substance degradation, sterilisation of waste water, cross-linking of polymers and colour-centre creation in alkali halide crystals;
- a racetrack microtron for γ-n reaction studies, applications in activation analyses and short-lived radioisotope production, which is fully assembled and almost ready to become operative.

The most important results obtained during 1998 in the field of particle accelerator development and application are reported in the following. Table 3.1 summarises the accelerator scenario at the laboratory.

Table 3.1 - Particle accelerator scenario at ENEA Frascati

<table>
<thead>
<tr>
<th>Accelerator</th>
<th>Energy (MeV)</th>
<th>Current (mA)</th>
<th>Pulse dur. (μs)</th>
<th>Status</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Circular microtron</td>
<td>5</td>
<td>200</td>
<td>4</td>
<td>running</td>
<td>waveguide FEL</td>
</tr>
<tr>
<td>Racetrack microtron</td>
<td>15-85</td>
<td>140-25</td>
<td>4</td>
<td>fully assembled</td>
<td>γ-n reactions</td>
</tr>
<tr>
<td>Proton linac (TOP)</td>
<td>65-200</td>
<td>10-3</td>
<td>5</td>
<td>under design</td>
<td>cancer therapy</td>
</tr>
<tr>
<td>S-band linac</td>
<td>3</td>
<td>180</td>
<td>4</td>
<td>running</td>
<td>irradiation tests</td>
</tr>
<tr>
<td>S-band linac</td>
<td>3</td>
<td>400</td>
<td>4</td>
<td>in construction</td>
<td>FEL driver</td>
</tr>
</tbody>
</table>
3.2 ACCELERATORS FOR FELs

3.2.1 5-MeV circular microtron

This machine has been successfully used and has shown good reliability as a driver for a compact FEL in the millimetre wavelength range of the spectrum. Facility in changing the output beam energy has allowed a wide range of FEL-radiation emission to be explored. A view inside the microtron is shown in figure 3.1. The overall machine performance was improved by adopting the new technology used in constructing the pressosinterised LaB$_6$ cathode and by applying a special welding procedure between emitter and rhenium holder.

3.2.2 S-band linac

A linear accelerating structure in the S-band was designed (table 3.1 and fig. 3.2) to test the efficiency of coherent-radiation generators in the mm-wave and far-infrared regions (see also sect. 2.3.1, for further details).

The machine is composed of two modules:

- a 3+1/2 cell beta graded self-focusing rf linac operating at 2998 MHz to accelerate electrons to 2 MeV of kinetic energy;
- a special particle-matching section (PMS) made of two on-axis coupled cavities operating at the same linac frequency to manipulate the phase-space distribution of the particles by imposing an energy-phase correlation in the bunched beam, thereby providing an extremely powerful tool for controlling the efficiency of the radiation generator.

The distribution of the bunched electrons in the phase space at the PMS output can be changed by varying the phase and amplitude of the rf field driving the PMS with respect to the linac rf exciting field. The PMS employs appropriate rf equipment, including a high-power remotely controlled phase shifter, attenuator and hybrid 3-dB divider (fig. 3.3). The linac is to be constructed by HITESYS; the PMS by ENEA Frascati.

3.2.3 High-brightness electron sources

Simulation of high-intensity electron beams with the TREDI code

Recent progress in the field of rf injectors with photocathodes has made it possible to improve the attainable beam brightness by several orders of magnitude compared to that achievable with conventional methods. High-brightness beams are essential for the operation of short-wavelength FELs; an example is the Tesla Test Facility FEL, Hamburg that requires 2.5 kA of peak current with \( \approx 2\times 10^{-4}\text{mm}\times\text{mm}\text{rad} \) of normalised transverse emittance. To achieve this performance, emittance compensation schemes have to be used to neutralise part of the space-charge emittance growth at low energy, and multiple stages of bunch compression at higher energies to increase the final peak current. At low energy, calculations concerning the beam dynamics rely on the assumption that the system has axial symmetry. This assumption naturally arises from the "nearly" axial symmetry.
symmetry of both the accelerating cavities and the accelerated beam. On the other hand, there are generally sources of "three-dimensional perturbations", e.g., multipole rf components induced by coupling apertures, slight misalignments of the laser spot on the photocathode, or inhomogeneities of the photocathode quantum efficiency itself. When the beam dynamics is governed both by rf fields and by nonlinear forces due to self-fields (i.e., when space-charge forces cannot be considered as a small perturbation), the consequences of those distortions cannot be easily predicted and computer simulation is required. Although the TREDI code was originally developed to simulate rf injectors in non-axisymmetric conditions, it can provide interesting information whenever the wavelength associated with the self-consistent fields is comparable with the beam size. Indeed, it can be used in the simulation of emittance dilution in beam compressors, long-wavelength ultrashort optical pulse production, coherent harmonic emission and superradiance in FELs. A lot of effort has been devoted to obtaining experimental evidence of the self-amplified spontaneous emission (SASE) process. The possibility of numerically investigating the conditions for radiation amplification to occur was an opportunity worth exploiting.

A schematic layout of the simulated device is shown in figure 3.4. A laser pulse of 0.8-ps duration
extracts 1 nC of charge in a 1.625-cell S-band photoinjector with a peak field of 120 MV/m. A solenoid is used for emittance compensation and transverse matching of the beam in the undulator. The energy at the injector exit is 4.6 MeV. A 6-cell S-band linac is then used to boost the beam up to 18 MeV. With an undulator of 5 cm of period and \( k = 1.64 \) at 18 MeV of beam energy, the resonant wavelength is 46 \( \mu \)m.

Figure 3.5 showing the phase space at the beginning, in the middle and at the end of the undulator provides clear evidence of both energy modulation (in the middle) and bunching (at the end), as expected according to SASE instability.

Study of photoemission from ferroelectric ceramic materials

A better understanding of the mechanisms governing the photoemission process in these materials and the possibility of exploiting such cathodes in rf accelerators are the aims of a collaboration with the INFN laboratories of Frascati and the Physics Department of Milan University.

The photoemission characteristics of ceramic disks of lanthanum-doped lead zirconate titanate (PLZT) have been investigated. The reasonably good emissivity at wavelengths varying from green to UV, coupled with robustness, make PLZT ceramic a worthwhile subject of research as an efficient and robust photocathode for switched power linacs, next-generation accelerators, FELs and ultrashort x-ray sources. A schematic of the experimental setup is shown in figure 3.6.

A frequency doubled Nd-YAG laser provides light at 532 nm with a pulse length of 25 ps. The cathode is illuminated over an area of about 10 mm\(^2\). The incidence angle is around 60°. The cathode is set in front of a flat anode, at a distance of about 3 mm. A coaxial copper anode (Faraday cup) matched with a 50-\( \Omega \) cable collects the photocurrent.
charge. The Faraday cup is directly connected to a 200-MHz-bandwidth oscilloscope. Experiments were carried out with a PLZT composition 8/65/35 and 4/95/5 (lanthanum [in relation to lead], zirconium and titanium relative atom percentages). The emitted charge was measured as a function of laser energy and accelerating voltage. For each pulse, the laser intensity and the relative emitted current were recorded and integrated (see fig. 3.7).

The main experimental findings are:

- electron emission from these materials has photon energy of 2.3 eV;
- quantum efficiencies in the range $10^{-6}$ to $10^{-7}$ were observed;
- specimens without a front electrode compared to those with have a larger yield and different behaviour;
- ferroelectric 8/65/35 specimens showed higher yield and higher nonlinearity vs laser power density ($Q=I^4$) than the antiferroelectric 4/95/5 ($Q=I^{2.5}$);
- evident hysteresis was observed for the 4/95/5 specimens.

3.3 ACCELERATORS FOR MEDICINE, INDUSTRY AND SCIENCE

3.3.1 Racetrack microtron

Studies on the orbits and the final design were completed. The machine was installed in its bunker (table 3.1 and fig. 3.8) and the experimental area and control room were finished.

The main application of this accelerator is to demonstrate that it is competitive, both economically and quality-wise, in producing radioisotopes through the $(\gamma, n)$ nuclear reaction compared to the $(p, n)$ reaction with the use of cyclotrons. The proposed reaction utilises 25-MeV $\gamma$ rays produced by 50-MeV electrons impinging on a bremsstrahlung Ta target. The $\gamma$ radiation on a $^{124}$Xe isotope (3% enriched) compressed at 200 atm produces a $^{123}$I isotope with high spectral purity, following the reaction:
Another possible application is the production of other short-lived radioisotopes such as \( \text{^{15}O}, \text{^{11}C}, \text{^{13}N}, \text{^{18}F} \), which are useful in positron emission tomography (PET).

### 3.3.2 AMERICA microtron

The Acceleratore per la Metrologia delle Radiazioni Ionizzanti (AMERICA) at ENEA Casaccia is a singular particle accelerator. It was designed at Frascati according to the specifications of the Istituto Nazionale di Metrologia delle Radiazioni Ionizzanti (INMRI) at Casaccia, built by the Officine Galileo in Florence, mounted and installed in a special laboratory at Casaccia and implemented and tested with the substantial contribution of Frascati. The accelerator (fig. 3.9) is a microtron with a variable gap and an internal diameter of ~1 m, which delivers a pulsed beam of electrons with energy ranging from 4 to 20 MeV, pulse duration 0.2 to 3 μs, repetition pulse ~100 Hz maximum, peak current ~20 mA. The beam on the target, 6 m away from the accelerator, has diameter ~5 mm² and divergence 10⁻³ and will be used as a radiation reference for radiotherapy and dosimetry measurements in Italy.

### 3.3.3 Linac for intra-operative radiation therapy

The experience accumulated in the accelerator field has been utilised to promote industry in this expanding field as well as to collaborate with other ENEA units.

Through a general agreement, transfer of knowledge between ENEA and HITESYS has been used in the development of advanced linear accelerators. ENEA is contributing with the modelling and design of the accelerating structure and the brazing and vacuum technology involved in the machine construction. The latest most important application is in the field of tumour irradiation during surgery. This technique, which is called intra-operative radiation therapy (IORT), has several advantages over the standard methods of patient irradiation before or after removal of the cancer mass. The final objective of the work is to design and construct an innovative 7-MeV electron linac (NOVAC 7), with autofocusing properties, low diffused x radiation and light enough to be mounted on a motorised arm with 6° of freedom for direct use in operating theatres. The Ministry for Universities and Scientific and Technological Research (MURST) approved the overall design at the end of 1998.

### 3.3.4 Proton linac for the TOP project

Proton and ion therapy is rapidly expanding all over the world. By the end of 1998, 26000 patients had been successfully treated in centres in Europe, the U.S.A., Russia and Japan. The big advantage of this type of therapy is that protons and ions deliver the highest dose at the end of their path, thereby sparing internal organs as well as superficial and surrounding tissues. Tumours of the prostate, liver, gastro-enteric apparatus, at the base of the skull, in the back of the eye and paediatric neoplasms are the most responsive to hadrontherapy.

The Italian Institute of Health (ISS) launched the Terapia Oncologica con Protoni (TOP) project calling for construction of a proton accelerator. In 1995 the ISS accepted ENEA's proposal to build a linear accelerator (linac), and at the end of 1997 the two parties signed an agreement to start constructing the accelerator according to ENEA's design.

\[
\text{^{124}Xe(\gamma, n)} \rightarrow \text{^{123}Xe} \rightarrow \text{^{123}I}.
\]
The proton linac was chosen because a) it is modular, so its construction can proceed according to the flow of funds and, also, a working instrument is obtained at practically each construction phase; b) it has fairly similar technological aspects to the electron linacs used in conventional radiotherapy, so its development should result in technology transfer to industry.

The TOP linac will be a pulsed (5 μs, 300 Hz) accelerator composed of a sequence of three linear accelerators (fig. 3.10):

- A 7-MeV injector: a 425-MHz rf linac, to be purchased commercially. It will also operate in a special high-current mode to produce the beta-emitter radionuclide $^{18}$F for PET analyses.
- A 7- to 65-MeV 3-GHz linac: the most innovative section of the whole accelerator. A new type of 3-GHz accelerating structure (side-coupled-drift tube linac - SCDTL) has been patented. The 1- to 10-nA average current beam will be used for proton treatment (of eye melanoma in particular) and radiobiology studies in a radiobiology room.
- A 65- to 20-MeV variable energy 3-GHz linac: a 1- to 10-nA average current beam, dedicated to proton treatment of deep-seated tumours. The maximum range will be 25 cm in water. The irradiation fields will be as large as 20 × 20 cm$^2$ and a dose rate of 2 Gy/min will be available.

After completing the general design, work in 1998 was devoted to preparing the tender to buy the injector and to beginning the SCDTL construction. For the first task, the machine specifications were defined and a tender committee was set up. The second task in particular is very challenging as this is the first time 3-GHz structures have been applied to accelerate protons. The SCDTL (fig. 3.11) consists of two typical accelerator structures (side-coupled and drift-tube linac) combined so that adjacent drift tube tanks are coupled together by side-coupling cavities.

Each tank is a 6-cm internal-diam Alvarez cavity with five small drifts, each one held at the opposite sides by a stem containing a cooling channel. A 3-cm-long permanent magnet quadrupole for focusing is placed on axis in each inter-tank space. Construction of the SCDTL requires high precision machining, tuning and brazing. Several models have been built and successfully tested at low power.
Figure 3.12 shows a "triplet" formed of two tanks and a coupling cavity. For a thorough understanding of the rf behaviour of the cavities, several 2-D and 3-D simulations as well as a lot of theoretical studies have been performed. The first linac module (fig. 3.13) under construction is 1.3 m long and consists of 11 tanks and 10 coupling cavities. It will be tested with a 7-MeV proton beam to accelerate it up to 13.4 MeV.

3.3.5 Services

The 3-MeV S-band on-axis coupled linac is used to provide services to the scientific community and to industry in the field of e-beam and x-ray processing of materials (table 3.1 and fig. 3.14). In 1998 it was used by:

- ENEA Frascati solid-state laboratory for creating colour centres in LiF crystals at room temperature;
- the firm of LABEN (Milan) for laboratory simulation of the electron and x-ray irradiation conditions existing in the space environment in order to test the electronic equipment of artificial satellites and the screening properties of some materials.
4.1 POSITRON SPECTROSCOPY

4.1.1 Development of new experimental equipment

1-D momentum density

A new positron annihilation spectroscopy (PAS) experiment for measuring 1-D electron-positron momentum density \( \rho(p) \) was completed. The experimental setup includes two Ge detectors in coincidence and a multiparametric acquisition-representation system. The 2-D spectrum of pure copper obtained with this device is shown in figure 4.1, where \( E_{n1} \) is the energy measured by the first detector and \( E_{n2} \) the energy measured by the second. The elongation of the central peak along the \( E_{n1} + E_{n2} = 511 \) keV diagonal line is due to the Doppler-broadened \( \gamma \) rays. The spectra yielded have a signal-to-noise ratio \( (10^5) \) 50 times higher and a resolution factor 1.41 better than a similar experiment already in use (measuring the same quantity with one Ge detector in coincidence with a NaI detector). Thanks to its much higher sensitivity, the experiment is promising for characterising the chemical environment near open-space defects, traditionally well monitored by PAS.

Data analysis routines were implemented, some of which with innovative methods.

2-D momentum density

The apparatus for measuring 2-D angular correlation of electron-positron annihilation photons (2D-ACAR) is nearing completion. The data of figure 4.2 were taken with the ENEA 2D-ACAR spectrometer when based in Bristol, U.K. The integration direction is along the c-axis of

![Fig. 4.1 - 2-D spectrum of pure copper obtained with the two-detector Doppler broadening coincidence system](image-url)
the hexagonal single crystal. The narrow central peak is ascribed to the momentum distribution of parapositronium, the electron-positron singlet bound state. The first and second series of satellite peaks are images at high momenta of the parapositronium peak, due to the effect of the periodic crystal potential. The broad distribution beneath is ascribed to annihilation of free positrons with valence electrons.

At present the following apparatus is operative:

- γ-ray spectrometer (2-D position-sensitive detectors, coincidence and representation system and mechanical support with several degrees of freedom);
- sample-holder chamber with vacuum and cryogenic facilities;
- water-cooled 2-T magnet for magnetic focusing of the positrons onto the sample.

The support of the magnet-sample holder system will soon be ready. It was designed and built (at ENEA Brasimone) to allow precise horizontal and vertical displacements of the whole system for alignment and calibration purposes.

The $^{22}$Na radioactive source (1.9 GigaBq) has been purchased.

In addition, several routines were implemented for 3-D reconstruction of electron-positron momentum density from 2-D projections and for data analysis of experimental spectra. Figure 4.3 reports: a) Reconstruction operated with an artificial neural network algorithm. This innovative procedure simultaneously performs reconstruction and deconvolution from the smearing of the experimental resolution. b) Reconstruction operated with the standard filtered back projection technique commonly used in medical imaging. In c) and d) the original 2-D matrix is shown; the full 3-D matrix is then reconstructed by piling up the reconstructed planes.

4.1.2 Defect studies

A collaboration was set up with ENEA Portici to study porous silicon, which is attracting a lot of attention because of its photoluminescence properties. PAS measurements should be useful to characterise the pore structure.

In co-operation with Turin University, a campaign of measurements was started on Al (95% Wt) Cu Mg alloys to study the kinetics of precipitation phenomena. Indeed, it is well known that the age
hardening process, of metallurgical interest, is strictly related to the sequence of precipitation. In particular, the measurements should provide information on "clustering"—a precursor of the precipitation sequence—thanks to their sensitivity to the early stages of precipitation.

4.2 SMALL-ANGLE NEUTRON SCATTERING FOR STUDIES OF MICROSTRUCTURAL INHOMOGENEITIES IN SOLID SYSTEMS

A typical application of small-angle neutron scattering (SANS) in material science is the investigation of inhomogeneities in a uniform matrix, ranging in size from 2 to 200 nm. More specifically, their size distribution can be reliably determined by transformation of the SANS data. SANS spectra can be measured over a limited Q-range, in a number of experimental points, while their transform, giving the autocorrelation function of the investigated system, is defined over the real space of inter-particle distances. While for a liquid or an amorphous homogeneous system the autocorrelation function has a direct physical meaning, this is not so for systems with inhomogeneities having sizes much larger than interatomic distances. Obtaining significant information (typically the size distribution of precipitates or microvoids) is no longer a typical Fourier transform problem and a model for the inhomogeneities of the sample is necessary. An example is the "two-phase model", which already in the most general case allows average size information to be obtained from the scattering profile at very large and very low Q-values (Porod and Guinier approximations). Making use of further assumptions, "shape-analysis" computer codes were developed in order to exploit information contained in the whole spectrum. During 1998 the codes were used to analyse complex materials employed in different technological applications:

- Martensitic steels developed for experimental fusion reactors (MANET steel) were studied in order to understand the effect of different thermo-mechanical treatments on the micro- and magnetic structure of the alloy. The measurements were performed at the Laboratoire Leon Brillouin (LLB) France and Forschungszentrum Geesthacht (GKSS) Germany in the framework of a collaboration with Ancona University and Forschungszentrum Karlsruhe (FZK), Germany. Figure 4.4 shows the 2-D SANS cross section of MANET steel quenched from 1075°C, measured with a 0.6-nm wavelength at a distance of 5.6 m. Figure 4.5 reports the volume distribution of the same steel as obtained from a measurement at GKSS and compared with the results of the same measurement at LLB (upper right corner).
- Helium-bubble growth in irradiated steels was studied to simulate radiation effects in experimental fusion reactors. Measurements were performed at the high-flux reactor of the Institute Laue Langevin (ILL) France, in cooperation with FZK; the dependence of bubble size on temperature was investigated by shape analysis of the scattering profile of different samples (fig. 4.6).
- Microcrystalline laser-synthesised powders of Si...
and SiC (see sect. 1.3.1) were analysed with SANS measurements and it was demonstrated how this technique can give useful information on their microstructure. The different "sizes" characterising microcrystals in the two different samples were clearly pointed out by shape analysis of the measured scattering profiles. The size distributions obtained for the two different samples were in agreement with the average sizes (3 nm and 6.5 nm) obtained by the Brunauer-Emmett-Teller (BET) technique (fig. 4.7).

- The stress field in different kinds of brazes was analysed as a function of temperature for the divertor of a fusion reactor for NET/ITER and the CEA/EURATOM Underlying Technology Programme. Neutron diffraction measurements were performed at LLB and ILL.

### 4.3 LOW-BACKGROUND RADIOMETRY

The main idea behind selecting a research program for the group working in this field is that the skills and techniques developed for basic research could be the source of useful new applications that would not otherwise obtain sufficient support and know-how transfer from commercial laboratories. The 1998 activities were directed along three main lines, particularly stimulating both for basic research and for potential applications: environmental sciences, cultural heritage and development of new laboratories and techniques.

#### 4.3.1 Environmental sciences

In collaboration with the Geological Survey of the Emilia Romagna Region, $^{14}$C activity in stratigraphic soil series is being determined in order to date the soil horizons. The objective is to reveal past geomorphologic phenomena that have modified the stratigraphy and then use this information to elaborate an accurate geological map of the region. A first series of measurements has been completed.

Preliminary, high-precision measurements of fossil CO$_2$ dissolved in the groundwater of the Gran Sasso were carried out in order to date major aquifer recharges and to determine the present recharge rate. The work comes under a collaboration between ENEA Bologna, Rome University 3 and the Gran Sasso National Laboratories.

Figure 4.8 shows part of the chemical section in the radiocarbon laboratory, where the carbon of the sample is initially transformed into carbon dioxide (CO$_2$) and then after a sequence of chemical reactions and purification steps into benzene.

Under a collaboration with the University of Bologna (Geology Department) and the Centre de Fiables Radioactivités, Paris, France, both radiocarbon and uranium thorium methods are being used to date coralline formations in the Adriatic Sea.
A preliminary evaluation on using $^{137}$Cs as a tracer in studies of soil erosion through gamma spectrometry calibration is in progress; a first sample collection was carried out in the Brasimone area.

During 1998, the contribution of the group to paleoclimatic studies continued, with precise measurements of atmospheric $^{14}$C in samples of ancient dendrodated wood. The cellulose-extraction method for $^{13}$C/$^{12}$C isotope fractionation measurements was also evaluated.

### 4.3.2 Cultural heritage and archaeology

The main activities in this field concerned:

- Radiocarbon dating of samples of wood from ancient Ferrara buildings, in collaboration with the Soprintendenza Archeologica Emilia Romagna.
- Dating of archaeological samples from excavations in the Bilancino area (Florence) before flooding by the new artificial lake, in collaboration with Soprintendenza Archeologica Toscana and the firm of SNAM.
- Dating of samples from Misa (Marzabotto, Bologna), Oman, Turkmenistan and South America, in collaboration with the Archaeological Department of Bologna University.
- Analysis of ancient manuscripts in the Biblioteca Malatestiana (Cesena) by x-ray fluorescence, in collaboration with ENEA/INN/ART and Bologna University.

### 4.3.3 Development of new laboratories and techniques

The tandetron accelerator of the CNR Institute for Material Technology and Electronic Components (LAMEL) Bologna was equipped with a new channel for particle-induced x- and γ-ray emission (PIXE-PIGE) studies to be carried out in collaboration with CNR-LAMEL and the AGLAE laboratory of the Louvre Museum. This type of measurement will be used to identify the origin of inks of ancient manuscripts or in general to determine the atomic-isotopic composition of artistic and historic objects. The measurements will also be funded by the “Bologna, European Capital of Culture” programme.

Good progress was also made in setting up the following facilities:

- A sample treatment laboratory for radiocarbon dating with accelerator mass spectrometry. The activity is supported by CNR in collaboration with University of Lecce and PASTIS of Brindisi.
- A computer-assisted digital imagining system for dendrochronologic dating and morphologic analysis of tree rings, in collaboration with the Physics Department of Bologna University.
- A laboratory for uranium thorium dating in collaboration with Bologna University (Engineering) and the Centre de Fiables Radioactivités, Paris, France.
- A liquid scintillation counter installed in the underground laboratory of Gran Sasso to extend the age span of radiocarbon dating and to improve the precision of the method. This facility was calibrated and is now operative.
5.1 MATHEMATICAL AND STATISTICAL METHODS OF DATA ANALYSIS

5.1.1 Neural network image reconstruction

Medical computerised tomography, e.g., positron emission tomography (PET) and single-photon emission tomography (SPECT), requires image reconstruction. A radioactive tracer injected in the patient emits photons that are detected by a set of counters placed around the body; a computer is then used to reconstruct the density distribution from the detector counts. The classical reconstruction method, used in commercial apparatus, is "filtered backprojection" (FBP). It is fast but produces "dirty" images, which are not suitable for new-generation high-resolution tomographs.

Different reconstruction methods for analysing data produced by high-resolution tomographs were tested. Iterative methods are able to produce good images but their heavy computation needs massive parallel computers, so they cannot be used routinely in a hospital.

Porting of an iterative code to the T3D at the Interuniversity Computation Centre of North-East Italy (CINECA) gave good results. Methods based on artificial neural networks (ANNs) allow the analysis to be split in two parts: a learning part (computationally heavy) and a reconstruction part (computationally fast). Learning can be performed on a massive parallel computer, the reconstruction can be implemented on a low-cost workstation, available at the hospital diagnostic centre. A prototype reconstruction system with good-quality images was developed. Figures 5.1 and 5.2 show how the different methods work. In fig. 5.1 the reconstruction of an ideal noiseless image is reported; in fig. 5.2, the reconstruction of a noisy image. The neural reconstruction method is clearly superior to the FBP. This work was done in collaboration with the Istituto Nazionale di Fisica Nucleare (INFN) (Bologna) and Bologna University.

A similar problem arises in solid-state physics studies. The technique based on 2D measurements of the angular correlation of positron annihilation radiation (2D-ACAR) thanks to its direct access to the electron momentum wave function is a unique tool for investigating the electronic structure of intermetallic compounds. The 2D-ACAR experimenters considered several reconstruction methods. Some of these methods (such as Fourier transform and FBP) are borrowed from medical imaging.

The idea was to find the coefficients of a polynomial expansion of the momentum density on the basis of the

![Fig. 5.1 - Reconstruction of ideal image: a) original; b) FBP; c) ANN](image)
projected data. With this technique, the crystal symmetry is explicitly inserted into the reconstruction in order to reduce the degrees of freedom of the problem. The problem of deconvoluting experimental data from the smearing due to the experimental resolution is a recurring issue in data analysis. Several recipes including iterative, filtering and maximum entropy algorithms were attempted, with the same drawback (too heavy computation) as explained previously in the case of PET medical imaging. Results are reported in section 4.1 (Positron Spectroscopy) of this report.

5.1.2 Weighted regularisation in data analysis for Compton scattering tomography

Medical applications of Compton scattering tomography imply the use of highly-efficient, low-resolution NaI(Tl) detectors. Hence, unfolding for the response function becomes a crucial point for 3-D density evaluation because the ill-conditioned nature of the problem leads to critical amplification of experimental errors and this usually makes it impossible to reach a meaningful solution in real cases.

Monte Carlo simulated spectra with realistic response functions and statistical experimental errors were used with deconvolution methods to test different regularisation procedures. Figure 5.3 shows folded and unfolded Compton spectrum (including the multiple scattering contribution) obtained by Monte Carlo simulation of right-angle scattering of a 59.54-keV beam in a water-filled cylinder.

If a non-parametric unfolding procedure is applied to a spectrum with simulated Poisson noise, strong long-range fluctuations appear in the solution. Employing the well-known Tikhonov regularisation is not sufficient to obtain satisfactory results, as shown in figure 5.4 (order-two regularisation). In fact, by increasing the regularising parameter the fluctuations decrease, but the peak shape is too wide. More specific information (not a simple standard regularisation) has to be introduced in the deconvolution procedure using the more general framework of the Bayesian approach, which is in principle able to include information about the particular shape of the scattering profile.

To improve the results, a weighted regularisation procedure was used, where the regularisation constant is multiplied by an energy function (as a weight) depending on the statistical errors in the different energy channels in which the spectrum is measured.
Another constraint of positive solution was added which made it possible to greatly improve the quality of the solution, as shown by figure 5.5 where the simulated unfolded spectrum is compared with that obtained by the simulated experiment with weighted regularisation.

Parametrisation with cubic B-spline functions as an additional smoothing constraint and further improvements in regularisation techniques are in progress.

5.1.3 Multidimensional statistical data analysis in marketing research

A strong link exists between superior service quality and positive business performance for firms operating in the service sector. For managers, the challenge is being able to identify those strategies that focus on the critical service quality dimensions from the customer's viewpoint. However, measurement problems have hindered this achievement.

Service quality is an abstract and elusive concept because many of its aspects are intangible and consist of a number of dimensions that vary in importance depending on the context. In statistical terms, service quality is a multidimensional variable with correlated dimensions, and analyses of quality data need multidimensional statistical methods.

A promising approach to measuring consumer perceptions of service quality that is strongly based on the new multidimensional methods of data analysis is the new Quality Targeting System (QTS). The premise is that service quality is the difference between consumer expectations and perceptions. Expectations are the desires or needs of consumers: what they feel a service provider should offer. Perceptions are how well the service provider performs that service.

To measure service quality, a two-part survey questionnaire consisting of 15–30 Likert-type items has been formulated. It requires respondents to rate their expectations on each item and then rate their perceptions of a known service provider of the same items. To collect the expectation/perception data, a seven-point scale ranging from "Strongly Disagree" (1) to "Strongly Agree" (7) is used. The expectation questions ask respondents to rate the extent to which the ideal service company should have the feature. The perception questions ask respondents to rate the extent to which the specific service organisation has the feature.

The QTS model of quality is based on the idea that gaps between expectations and perceptions for items cannot be directly cancelled because the items are to some extent correlated. Instead, gaps have to be expressed through a set of a few uncorrelated quality factors, extracted from the expectation data. Expected and perceived quality can be displayed on maps, so that the gaps can be clearly understood by the management. Once the management has decided which gap is worth cancelling, QTS is able to convert these gaps from quality factors to original items, the true "leverages" which the management can act on in order to raise the perceived quality to the same level as the expected quality.

5.2 POSITION-SENSITIVE DETECTORS

X- and γ-ray position-sensitive detectors are essential in numerous fields, such as astronomy, crystallography, material diagnostics and medical analysis. The common interest of the Applied Physics Division of ENEA Bologna and the CNR Institute for Extraterrestrial Radiation (TESRE) in this kind of detector led to the Pixellated Imaging CsI Telescope (PICsIT) project. The European Space Agency (ESA) selected the PICsIT for the International Gamma Ray Astrophysics Laboratory (INTEGRAL) satellite, a medium-size
scientific mission to be launched in 2001. An international consortium of research institutes from nine European countries (and co-operation from the American [NASA] and Russian [IKI] space agencies) was formed and committed to develop, build and fly this instrument (fig. 5.6) with the collaboration of some hi-tech industries.

The goal is to provide an unprecedented combination of spectroscopy and imaging in a wide x- and γ-radiation energy range, including the optical band, with the angular resolution necessary to disentangle the spectra of neighbouring sources in crowded regions such as the Galactic Centre. The imager on-board integral satellite (IBIS), one of the two core instruments, will be composed of two layers, one of which the PICsIT.

The 1998 activities resulted in the following:
- A thermal structural model (fig. 5.7), delivered to ESA.
- Final design, implementation and testing of the component pixels (first lot of CsITls), analog and digital front-end electronics (AFEE and DFEE) board, auxiliary electronics box for the engineering model to be delivered in 1999.
- Software to determine the light output (an important qualification parameter) of the CsITl detector.

New pixellated gamma-cameras for medical applications were studied in the framework of the collaboration with the TESRE Institute and in co-operation with Bologna University. In particular, the use of avalanche photodiodes (APDs) coupled to fast inorganic scintillators was evaluated. Several tests were done on different configurations built by coupling commercially available APDs with scintillators such as yttrium aluminium perovskite (YAP) and gadolinium silicate ortho (GSO). Their performance, e.g., energy range, energy and time resolution, was experimentally evaluated.

Starting from these results, Monte Carlo simulations were carried out to model a multi-element detector designed for possible PET applications.

Some quality factors were defined to compare the characteristics of the different detectors tested. The Monte Carlo results will also be used in a feedback process in order to optimise the use of a single element of the arrays.

5.2.1 Determination of light output of a CsI(Tl) sample coupled to a photodiode

A procedure was developed to determine the light emitted from a scintillator for each energy unit released by an impinging γ-ray. The light output measurements are indirect as related to the number of electrons emitted from
the photodiode coupled to the CsI(Tl) sample after illumination with two γ-ray sources. In this way, a complete evaluation of the investigated sample is obtained, accounting for all significant quantities (physical and geometrical characteristics of the scintillating crystal, optical coupling with the photodiode, quantum efficiency of the photodiode, etc.).

The system is tuned by illuminating the detector with an Am$^{241}$ source, whose output spectrum has three peaks (Fig. 5.8), the first at 60 keV, the second at ~30 keV and the third at ~17 keV. In this way it is possible to obtain a linear relation between the number of electrons emitted from the photodiode and the corresponding channel of the spectrum (Fig. 5.8). As a by-product, the noise of the electronic system can be determined from the width of the clean 60-keV line.

The 661-keV peak of a Cs$^{137}$ source is used for intensity calibration. Note that the energy resolution and lower energy threshold of a pixel unit are both dependent on light output and electronic noise.

As the PICsIT imager will have the best 4096 CsI mini-detectors (pixels) chosen from about 6000 samples, to speed up the calibration procedure a specific peak analysis program with the capability to find the peaks in the Am$^{241}$ and Cs$^{137}$ spectra and choose the best fit interval has been developed.

Manual intervention is foreseen when automatic analysis is unsatisfactory.

### 5.2.2 AFEE electronic board

The AFEE board directly interfaces the detectors by means of an array of application-specific integrated circuits (ASICs) named ICARUS. ICARUS was designed to interface CsI(Tl) + PD gamma detectors operating from 100–5000 keV.

Each channel, constituting a complete spectroscopic chain, consists of a charge pre-amp, shaper-amp and stretcher, an energy-threshold and timing discriminator and an analog MUX and readout logic.

The most challenging requirements of the device are time accuracy, radiation tolerance and the capability to operate
in the presence of a heavy noise level, typical of a space environment.

ICARUS was built using MIETEC 0.6-mm technology on a multiproject wafer (MPW). Figure 5.9 shows the first prototype (MPW1) die. During 1998, the complete functional tests and preliminary performance evaluations carried out on ICARUS MPW1 allowed the final MPW2 prototype to be designed.

Results of a test campaign on ICARUS radiation immunity done at the European Space Technology Centre (ESTEC-ESA showed that it can successfully survive the space environment.

Construction of the ASIC was one of the critical points of the PICsIT project so the positive results achieved can be considered a major step forward in the program development.

5.2.3 Gamma-ray detection with fast scintillators coupled to an APD in PET application

Inorganic scintillators, such as the GSO or YAP, with good efficiency for gamma rays and with fast time response could be candidates for applications in fast pixellated gamma-cameras where the size of a single crystal determines the spatial resolution.

Miniaturised front-end electronics in which each scintillator is viewed by a photodiode (PD) can be developed using very large scale integration (VLSI) technology. This solution has many advantages:

- a crystal-PD element-based array can be replicated up to the desired final dimensions with the small dead area uniformly distributed over the whole detector;
- the detector is robust and insensitive to magnetic field;
- the detection efficiency of a system can be increased by stacking similar arrays.

The most widely used material for PDs is silicon. Compatibility between the scintillator emitted light and the silicon spectral response determines the signal level at the PD output; both device speed and noise level depend on the PD technology. Detector parameters such as minimum detectable energy, energy resolution and timing resolution are given by the signal-to-noise ratio.

Comparison of the noise level achievable with the three PDs (positive intrinsic negative [PIN], silicon drift chamber [SDC] and avalanche photodiode [APD]) mainly used in nuclear applications is reported in figure 5.10. Silicon drift chambers have low noise, but as they are slow they are not the best candidates.

Fast scintillators generally have relatively poor photon generation and their emitted spectra do not match the Si spectral response. As these problems can be overcome by using an APD detector, comparison of different APDs was carried out. Experimental results were compared with Monte Carlo simulations and a way to optimise the overall performance of a PET detector was found.
5.3 DIAGNOSTIC ENGINEERING OF COMPLEX MECHANICAL SYSTEMS

5.3.1 Misfire detection

The increasing attention focused on problems regarding engine emission reduction has obliged the automotive industry to design on-line procedures for diagnosing the occurrence of cylinder misfire. A collaboration between ENEA Bologna, the Department of Mechanical Engineering of Bologna University, Magneti Marelli and Lamborghini Automobili industries was set up to develop on-line procedures to be implemented on the electronic control unit of a vehicle.

An original procedure based on analysis of the time between consecutive combustion cycles was developed to detect misfire in a high-performance 12-cylinder engine. The methodology was then tested under the worst-case condition of a random misfire, with the car driven on a circular speedway at low and high load, in different gears, under acceleration and during a normal urban cycle.

Some results are reported in figure 5.11. A misfire while starting the vehicle was correctly diagnosed. Figure 5.12 shows the diagnosis of fifteen consecutive misfires during a test with the car running at 190 km/h.

5.3.2 Engine torque estimation

Electronic throttle control is increasingly considered a viable alternative to conventional air management systems in modern spark-ignition engines. In such a scheme, driver throttle commands, together with many other inputs, are interpreted by a power-train control module rather than directly commanding the throttle position; the driver now simply requests torque—which has to be appropriately interpreted by the control module.

Engine control under these conditions needs optimal control of the engine torque required by the vehicle subsystems, ranging from heat-ventilation air conditioning (HVAC), to the electrical and hydraulic accessories and the vehicle itself. Hence, real-time estimation of engine and load torque can play a very important role, especially if it can be performed using the same signals already available to the power-train control module.

In a collaboration between the Department of Mechanical Engineering of Bologna University, the Department of Mechanical Engineering of Ohio State University (U.S.A.) and Magneti Marelli, a method was developed
5.3.3 Film fluid dynamics

To control engine dynamics and consequently engine emissions, the actual air and fuel that enter the cylinder have to be estimated. To do this it is necessary to follow the behaviour of the fuel leaving the injector (see figs. 5.16, 5.17).

In a collaboration with the Department of Mechanical Engineering of Bologna University, the Department of Mechanical Engineering of Ohio State University (U.S.A.) and Magneti Marelli, the intake manifold dynamics, including the internal exhaust gas recirculation (EGR) and the fuel film effects, were studied using a sophisticated engine model. Comparison between experimental and estimated data of the air mass flow rate is shown in figure 5.18.
5.3.4 Acoustic emission analysis

Racing-car builders not only gain publicity from competing in a Formula I automobile race but also acquire technological knowledge that can be used to improve their products. This explains the huge research effort each racing team devotes to the development and construction of a Formula I car. It is also important that each team be able to check on another's progress and then minimise any technological differences as soon as possible: the more the information obtainable, the more selective the modifications to the vehicle.

A fairly simple way to obtain general information about engine performance is related to the availability of a large amount of acoustic-emission data directly measured aboard the vehicle by the microphone of the in-car camera. By comparing analysis of the acoustic emission with data acquired by means of the telemetry system on one of its cars, the team can regulate the engine speed recovery methodology.

The collaboration between ENEA Bologna, the Department of Mechanical Engineering of Bologna University and the Department of Mechanical Engineering of Ohio State University (U.S.A.) developed a signal-processing procedure for extracting important engine parameters from acoustic emissions during a car race.

Figures 5.19-5.21 show results of an analysis of car performance using only publicly available information. The data were acquired on a Ferrari during the 1998 Grand Prix of San Marino (Imola) (fig. 5.19). Figures 5.20 and 5.21 show the behaviour of the crankshaft speed while the car is racing in the straightaway (rettilineo) and in the Rivazza curve, respectively. In figure 5.20 the presence of the different subharmonics of the acoustic signal is clear, as also are the gear shifts; the actual crankshaft speed is represented by the upper curve. Analysing figure 5.21, the decrease in the crankshaft angular speed during the curve and the gear shifts before and after it are evident, as is the presence of some subharmonics.
5.4 DIAGNOSTICS, IMAGING AND SIGNAL/IMAGE PROCESSING FOR APPLICATIONS IN MEDICINE, INDUSTRY AND CULTURAL HERITAGE

Algorithms and numerical methods were developed to reconstruct 1- and 2-D images from physical diagnostic observations and microscopy of works of art. A suitable deconvolution procedure, previously used for problems in basic and applied sciences—from geophysical and electrodynamic prospecting to astrophysical observations, from computer tomography to the restoration of smeared and defocused images—was developed for processing images obtained in nondestructive analyses of historical objects and works of art. An integral-equation formulation is first used, where the kernel accounts for image degradation due either to chromatic aberration generated by inelastically scattered electrons in scanning electron microscopy (SEM) or to defocusing and smearing, and then filtered approximations to the "real" unperturbed image are built by means of constrained regularisation methods. As a result, the quality of the degraded image is greatly improved.

Computing codes were developed and different statistic and deterministic methods were compared in order to choose the regularisation parameter.

5.4.1 Compton scattering tomography

Compton scattering is a suitable nondestructive technique for density evaluation in large or fixed objects. However, when sizeable samples have to be examined with a relatively high spatial resolution, the large number of detected photons required to obtain a statistically accurate density evaluation for each sensitive volume (SV) is a severe limit on its application. The aim of this work is to show that principal component analysis (PCA) of the spectra recorded from $n$ SVs of the same sample layer can result in a statistically significant evaluation of the density variation even for a low number of detected photons.

In Compton scattering techniques, density measurements are obtained by evaluating the spectral distribution of the photons arriving at the detector. The detected photons may have a different spatial origin: i) photons undergoing at least one collision inside the SV, which provide information on its density; and ii) photons coming from outside the SV. In terms of PCA, this implies that the multivariate structure of spectra recorded from a single layer might be described with two PCs at most. The first describes the fraction of spectrum made by photons coming from both the regions; the second refers to the photons from outside the SV only. In other words, the density variation inside the layer may be described by a simple linear model $z = \sum_i I_i u_i^1 + \sum_j I_j u_j^2$. Here the $I_i$ values are the significant eigenvalues of the covariance matrix describing the variation of the spectral structure and the $u_i$ are the eigenvectors outlining the density distribution for each sensitive volume.

In order to validate this PCA approach, a Monte Carlo simulation of Compton scattering density measurements was performed by means of the EGS-4 code on a water slab of $5 \times 5 \times 3$ volume elements (in $x$-$y$-$z$ directions, respectively and where each element is $1 \text{ cm}^3$), with incoming photon energy $E_i = 59.54 \text{ keV}$ and the detector positioned at a $90^\circ$ scattering angle.

A collimator diameter of 0.6 cm for both the source and detector completely circumscribed the SV in the tested volume element; the mean number of photons for each spectrum was $100 \pm 8$ (s.e.m).

Figure 5.22 shows the variance explained by

![Figure 5.22 - Analysis of the main components of the Compton measurements](image_url)
eigenvalues $l_1$ and $l_2$, calculated for the central layer in the $x$-$y$ plane when all ($\circ$) the SVs have the same density and, respectively, three ( ) and six (A) out of the twenty-five SVs are substituted by void elements. Clearly, when the number of void SVs increases, the fraction of total variance corresponding to $l_1$ decreases, while that to $l_2$ increases. This confirms the two different spatial origins of the photons arriving at the detector, as previously explained, and supports the PCA approach evaluating the layer density by a two-component linear model.

5.4.2 A computing laboratory for digital image processing

A picture is worth a thousand words as the saying goes. A good picture is better than a defocused one. A major task in any scientific investigation is to obtain clear and univocal results from data analysis. Large amounts of data require cumbersome calculations in order to improve the experimental resolution and to correct the observed signal or image for noise and statistical as well as systematic errors, etc.

The desk-top personal computer is now as powerful as mainframe computers were ten years ago and advances in technology mean that its performance is increasing and the barrier between PC and workstation is less and less defined, while prices should continue to decrease. Networked PCs and workstations represent the simplest and most accessible form of parallel computation with high performance in many interesting applications, such as image analysis and scientific visualisation. Modern software can run on the most appropriate point (or points) on the network and communicate results to the user through the local window (PC or workstation, or simply some kind of terminal). It is, therefore, quite feasible for the commonly available computing facilities to embark upon high-quality image reconstruction and enhancement.

Moreover, image databases and archives give the microscopist rapid and convenient computerised access to digital images, including the latest optical microscopes and SEMs, as well as to a wide range of imaging sources. The specific SEM operating conditions for the specimen under consideration can be saved for future reference. In the past, microscopists may have occasionally rejected the idea of using a computer-based image storage system because of the ease with which the original slide could be re-examined, only seeing the computer as introducing additional work and complexity. However, information, such as the current objective, illumination settings, focus and position of the motorised stage, can be linked to the relative digital image and stored in the archives for query and successive utilisation.

Whereas digital imaging for SEM has been the standard for years, more and more laboratories are now equipping their scanning and transmission electron microscopes (TEMs) for digital image capture. Developments in both hardware and software have thus opened the way to new possibilities for data acquisition and display. As a result, it is possible to easily acquire images from optical and electron microscopes, photographs, negatives, films, slides and radiographs as well as share them with other laboratories around the world in real time, due to the computing network facilities (Internet, etc.). Furthermore, presentation of results to workshops, seminars and conferences can be directly projected from a desktop PC.

However, the resolution and readability of images can be greatly improved by means of suitable algorithms that can be implemented on a large number of computing systems, from PCs to massively parallel architectures. An imaging computing system, developed by the computing centre of the Applied Physics Division of ENEA Bologna and studied in collaboration with the recently established computer-science laboratory of the Faculty of Conservation of the Cultural Heritage (Bologna University) at Ravenna, is being implemented for acquisition, storage, processing and automatic retrieval of multimedia data referring to works of art, mainly paintings on canvas and frescoes.

Methods and criteria are included in highly structured databases containing chemical and physical analysis results, diagnoses and information about materials, past restorations, etc., to provide a significant number of pictures, textual descriptions and comments on the state of conservation, and the
means to prevent deterioration and create the best conditions for safeguarding the cultural heritage. Since a huge amount of pictorial data is involved, suitable solutions are being developed for efficient storage and processing of the data in the framework of the whole database.

The whole system is organised on the basis of four main components:

- a hypertext with picture description components;
- picture and text automated indexing and filing;
- a picture and text retrieval component;
- an image processing and analysis component.

The high-resolution acquisition procedure is essentially based on commercial hardware and its performance is comparable with that of existing facilities. Parts of the computer system and the relative multimedia database are also available on the network through a vision-enhanced user interface, thereby allowing long-range and multiuser interaction.

Some numerical methods were developed for reconstructing 1- and 2-D images, as described in the previous sections. The software will be included in the management tool of the multimedia database in order to provide suitable on-line facilities allowing the user to perform his/her own image processing and virtual reconstruction operations on the high-resolution digital reproduction of the original document or painting. This work originates from a scientific collaboration between the ENEA Bologna Applied Physics Division, the Faculty of Conservation of the Cultural Heritage (Bologna University) at Ravenna, and the Scientific Laboratory of the National Gallery in London where the Visual Arts System for Archiving and Retrieval of Images (VASARI) project was partly carried out in the framework of ESPRIT II.
6.1 INTRODUCTION

Activities in applied mathematics have manifold motivations. However, the main reason for interest in this field is still as support to theoretical physics research on quantum and classical optics, synchrotron radiation, free electron lasers (FELs) and charged beam transport.

One of the topics in applied mathematics that has had a significant impact on theoretical physics is the development of methods to allow, e.g., faster and more reliable analysis of dynamic systems. The notion of a dynamic system is fairly general and may be relevant to the propagation of electron beams in a magnetic channel or storage ring, or to the solution of the Schrödinger equations ruling the evolution of quantum systems.

In the past, the notion of dynamic group was associated with that of an evolution system. The use of dynamic groups, along with that of rigorous ordering methods, allows a dynamic system to be characterised in terms of an appropriate evolution operator written as a product of the exponential of the Lie group generators. This procedure numerically implemented has provided the basis for dealing with various problems and, recently, an appropriate extension of the methods has allowed the inclusion of dissipative effects.

It is well known that special functions can also be viewed as matrix elements of irreducible Lie group representations. This fact and the previous considerations justify the interest in further developments in this field. Furthermore, a deeper interest in the theory of special functions is motivated by the need to introduce new types of special functions to deal with otherwise unsolvable problems in analysis of radiation emission by relativistic electrons in undulators and in the theory of quantum states with reduced quantum fluctuations.

At present, the problems considered in the framework of applied mathematics range from those concerning group theoretical methods to those related to the theory of generalised difference operators, as the field of physical applications is extremely wide.

6.2 SPECIAL FUNCTIONS

The work described here was conducted in collaboration with the Department of Mathematics and Statistics of the University of Victoria (Canada) to support activities relevant to quantum and classical optics, free electron lasers and charged-beam transport.

During 1998, the properties of generalized Hermite and Laguerre polynomials were explored within the context of the quasi-monomiality principle.

A polynomial \( f_n(x) \) (\( n \in \mathbb{N}, x \in \mathbb{R} \)) is said to be quasi-monomial, under the action of the operators \( \hat{M} \) and \( \hat{P} \), if

\[
\hat{M} f_n(x) = f_{n+1}(x), \quad \hat{P} f_n(x) = n f_{n-1}(x).
\] (1)
It is clear that $\hat{\mathcal{M}}$ and $\hat{\mathcal{P}}$ play the roles of multiplication and derivative operators. Furthermore if $f_0(x) = 1$, the quasi-monomial can be constructed as

$$f_n(x) = \hat{\mathcal{M}}^n$$

(2)

In the case of Hermite polynomials, in the Kampé de Feriét (KdF) form, namely,

$$H_n(x, y) = \sum_{s=0}^{[n/2]} \frac{(n-s)!}{s!(n-2s)!} y^s x^{n-2s}$$

(3)

the multiplication and derivative operators are specified by

$$\hat{\mathcal{M}} = x + 2y \frac{\partial}{\partial x}, \quad \hat{\mathcal{P}} = \frac{\partial}{\partial x}$$

(4)

Therefore, by just exploiting the rules associated with the above two operators, all the properties of this family of polynomials can be derived. Two properties of particular importance are given below:

$$\left(x + 2y \frac{\partial}{\partial x}\right)^n = \sum_{s=0}^{n} \binom{n}{s} H_{n-s}(x,y) \frac{\partial^s}{\partial x^s}, \quad H_n\left(x - 2y \frac{\partial}{\partial x}, y\right) = \sum_{s=0}^{n} \binom{n}{s} (-2y)^s x^{n-s} \frac{\partial^s}{\partial x^s}$$

(5)

Another important property associated with this family of polynomials is the proof that they can be defined through the operational identity

$$H_n(x, y) = e^{2x^2 / y^2} x^n$$

(6)

This relation is of particular importance because it states that $H_n(x, y)$ are the Gauss transform of the ordinary monomials (the importance of the Gauss transform and associated concepts will be discussed below) and allows the conclusion that the general solution of the heat equation

$$\frac{\partial F(x, y)}{\partial y} = \frac{\partial^2 F(x, y)}{\partial x^2}$$

(7)

can be cast in the form

$$F(x, y) = H g(x, y)$$

(8)

where $H g(x, y)$ is the function $g(x)$ defined on the basis of the KdF polynomials, i.e., by replacing the ordinary polynomials with $H_n(x, y)$ in the Taylor series expansion of $g(x)$.

The concept associated with $H$-based functions has allowed the development of the theory of Hermite-Bessel functions defined as

$$H_{J_n}(x, y) = \sum_{r=0}^{\infty} \frac{(-1)^r H_{n+2r}(x, y)}{2^{n+2r}(n+r)!}$$

(9)

with the generating function
This class of functions has been thoroughly investigated because of their central role in the derivation of the properties of the radiation emitted by electrons in magnetic undulators and their link with multivariable Bessel functions. Examples of Hermite-Bessel functions are given in figures 6.1-6.3.

The two variable Laguerre polynomials

\[ L_n(x,y) = n! \sum_{s=0}^{n} \frac{(-1)^s y^{n-s} x^s}{s! (n-s)!} \]  

have been proved to be quasi monomials under the action of the operators

\[ \hat{M} = y - D_x^{-1}, \quad \hat{P} = -\frac{\partial}{\partial x} x \frac{\partial}{\partial x} \]  

where \( D_x^{-1} \) is the inverse of the derivative operator. Use of the multiplicative and derivative operators allows a deeper study of the properties of the polynomial family defined by (12) and the derivation of previously unknown generating functions, as e.g.,

\[ \sum_{n=0}^{\infty} \frac{t^n}{n!} L_{n+1}(x,y) = e^{yt} \sum_{s=0}^{1} \left( \frac{1}{s} \right) C_s(xt) \]  

Fig. 6.1 - a) Contour plot of \( _1J_0^{(2)}(x,y) \); b) 3-D view of \( _1J_0^{(2)}(x,y) \)

Fig. 6.2 - Same as fig. 6.1 for \( _1J_1^{(2)}(x,y) \)

Fig. 6.3 - Continuous line: \( _1J_4^{(2)}(x,-1) \). Dotted line: \( J_4(x) \)
Another significant result is the fact that $L_n(x,y)$ satisfy the partial differential equation

$$\frac{\partial}{\partial y} L_n(x,y) = - \frac{\partial}{\partial x} \frac{x}{y} L_n(x,y)$$  \hspace{1cm} (15)

which is particularly important in the theory of wave paraxial propagation.

The concept of quasi monomiality associated with Laguerre polynomials has been exploited to introduce the Laguerre-Bessel function, defined by the series expansion

$$L J_n(x,y) = \frac{\sum_{r=0}^{\infty} (-1)^r L_{n+2r}(x,y)}{2^{n+2r} r!(n+r)!}$$  \hspace{1cm} (16)

with the Jacobi-Anger expansion

$$\sum_{n=-\infty}^{\infty} e^{i n \theta} L J_n(x,y) = e^{ix \sin(\theta)} C_0(ix \sin(\theta))$$  \hspace{1cm} (17)

Examples of Laguerre-Bessel functions are given in figures 6.4–6.6.
6.3 EVOLUTION OPERATORS

This line of research was developed to support work on charged beam transport, optical propagation
and stochastic processes. The central point is the theory of generalised exponential operators and
associated rules with particular reference to the concept of a generalised shift operator and generalised
Gauss transform.

The exponential operator

\[ \hat{E} = e^{\lambda q(s) \frac{d}{dx}} \]  

is defined as a generalised shift operator and its action on a generic function \( f(x) \) is specified by

\[ \hat{E} f(x) = f \left( F^{-1}(\lambda + F(x)) \right) \]  

where \( F \), called the similarity factor (sf), reads as

\[ F(x) = \int_0^x \frac{d\xi}{q(\xi)} \]  

and \( F^{-1}(\sigma) \) is its inverse. An example of application of (19) is provided by the so-called dilatation
operator

\[ e^{\lambda x \frac{d}{dx}} f(x) = f(e^{\lambda x}) \]  

with sf

\[ F(x) = \ln(x) \]  

The generalised Gauss transform has been associated with the solution of partial differential equations
of the type

\[ \frac{\partial}{\partial \lambda} Q(x, \lambda) = \left( q(x) \frac{\partial}{\partial x} \right)^2 Q(x, \lambda), \quad Q(x, 0) = g(x) \]  

and is defined as

\[ Q(x, \lambda) = e^{\lambda \left( q(x) \frac{d}{dx} \right)^2} g(x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-\xi^2} g \left( F^{-1}(2\xi \sqrt{\lambda} + F(x)) \right) d\xi . \]  

The generalised shift operator has been exploited to get the solutions of difference equations of the type

\[ \sum_{\alpha=0}^{N} a_{\alpha} g \left( F^{-1}(\alpha + F(x)) \right) = 0 \]  

in the form

\[ f(x) = \sum_{\alpha=1}^{N} c_{\alpha} R_{\alpha}^{F(x)} \]
while the generalised Gauss transform has been exploited to solve a wide class of Fokker-Plank equations often encountered in storage-ring physics. In particular, the equation

\[ \frac{\partial}{\partial t} f(x,v,t) = \left[ \frac{v}{\partial x} - p(x) \frac{\partial}{\partial x} \right] f(v,t) + 2 \frac{\partial}{\partial v} f(v,t) \]

(28)

\[ f(x,v,0) = g(x,v) \]

which models the longitudinal dynamics of a storage ring FEL amplifier is considered. Without going into the physical meaning of the equation, the problem can be dealt with by introducing the operators

\[ \hat{L} = v \frac{\partial}{\partial x} - p(x) \frac{\partial}{\partial x} \]

\[ \hat{D} = 2 \frac{\partial}{\partial v} (v + F(v) \frac{\partial}{\partial v}) \]

(29)

Then the evolution operator associated with the Fokker-Plank equation (28) is

\[ \hat{U}(t) = e^{(\hat{L} + \hat{D})t} \]

(30)

Exact solutions have been found for (28) for a few specific cases of the function F(v). The search for the numerical solution has been greatly simplified by using the symmetric-split approximation

\[ \hat{U}(\delta^i) \equiv e^{\frac{1}{2} \delta^i \hat{L}} e^{\delta^i \hat{D}} e^{\frac{1}{2} \delta^i \hat{L}} + o(\delta^i) \]

(31)

where \( \delta^i \) is a suitably chosen time step. The extension to a finite time interval can be obtained by repeated applications, namely

\[ \hat{U}(t) \equiv \prod_{i=1}^{N} \hat{U}(\delta^i), \quad \delta^i = \frac{t}{N} \]

(32)

Examples of distribution evolution are presented in figures 6.7 and 6.8.

6.3.1 Development of recursive decomposition methods for disentangling evolution operators

Symplectic integrators are numerical schemes for Hamiltonian systems conserving the phase space structure exactly. Symplecticity is connected with the fundamental properties of the evolution of mechanical systems in the classical realm (Liouville Theorem) as well as in the quantum domain (unitarity of evolution operator). Interest in these methods stems from the fact that they are free from a number of problems affecting other time-proven algorithms. It has been proved that the symmetric split-
operator technique (SSOT) can be exploited to obtain naturally symplectic integrators of arbitrarily high order for autonomous Hamiltonian systems, with very little programming effort. Finite-difference methods have also been developed for systems driven by explicitly time-dependent forces (e.g., non-autonomous Hamiltonian systems). Integration of evolution-like equations can be implemented by including time-ordering effects. This goal can be achieved either by modifying conservative schemes in order to account for the energy variation or—conversely—by exploiting a time-ordered expansion to provide an evolution operator symplectic at any order in time. Here, only the latter is presented in some detail in the context of Liouville-type equations. The solution of an evolution-like equation of the type

$$\frac{\partial \rho}{\partial t} = \hat{L}(t)\rho$$

(33)

can be cast in the form

$$\rho(t) = \hat{U}(t)\rho(0)$$

(34)

where \(\hat{U}(t)\) plays the role of the time-displacement operator and \(\rho(0)\) specifies the initial conditions. According to the Magnus-Fer time-ordering procedure, \(\hat{U}(t)\) can be factorised as an infinite product of operators:

$$\hat{U}(t) = \prod_{j=1}^{\infty} \delta_S^{(t)}$$

(35)

where the \(\delta_S^{(t)}\)’s can be expressed as time-ordered integrals of the type

$$\delta_S^{(t)} = \int_{0}^{t} \hat{L}(\tau)d\tau$$

$$\delta_S^{(t)} = \int_{0}^{t} d\tau_1 \int_{0}^{\tau_1} d\tau_2 [\hat{L}(\tau_2), \hat{L}(\tau_1)]$$

(36)

etc. An approximant of the evolution operator can be derived from (35) by truncating the product at some order. The problem of specifying the action of the operators \(e^{\delta_S^{(t)}}\), \(e^{\delta_S^{(t)}}\) can then be solved by exploiting standard recursive decomposition techniques. The proposed integration procedure has been applied to the Liouville equation associated with a time-dependent harmonic oscillator (which can be used to model the electron transverse motion through quadrupole magnets):

![Fig. 6.8 - As in fig. 6.7 for p(x)=-\frac{1}{6}x^3, \sigma_x=0.5, \sigma_y=0.3](image)
An extension of the decomposition techniques mentioned above has been developed and will be described briefly. It has been proved that, given an exponential operator $e^{i\Omega t}$ and a $m^{th}$-order approximant $\hat{Q}(m)$ ($\tau\Omega$), a $(m+1)^{th}$-order approximant can be cast as

\[ \hat{Q}^{(m+1)}(\tau\Omega) = \prod_{j=1}^{r} \hat{Q}^{(m)}(\xi_{m,j}\tau\Omega) \]  

for $r>2$, provided the set of weights $\{\xi_{m,j}\}$ fulfils the following conditions:

\[ \sum_{j=1}^{r} \xi_{m,j} = 1 \quad \sum_{j=1}^{r} \xi_{m+1,j} = 0 \]  

It can be proved that the method can be extended to yield at least a $(m+3)^{th}$-order approximant $\hat{Q}^{(m+3)}(\tau\Omega)$ provided the set of weights $\{\xi_{m,j}\}$ fulfils the most natural generalisation of (39):

\[ \sum_{j=1}^{r} \xi_{m,j} = 1 \quad \sum_{j=1}^{r} \xi_{m+1,j} = 0 \quad \sum_{j=1}^{r} \xi_{m+3,j} = 0 \]  

The decouplings associated with (40) made it possible to dramatically shrink the amount of factors involved in disentangling a given exponential operator. In numerical codes, this results in significant speedup as well as reduction in the memory required to solve practical problems. The technique has been applied to solve the difference-differential equations of the "harmonic" Raman-Nath type:

\[ i \frac{dC_1}{dt} = \epsilon l^2 C_1(t) + \Omega \left( \sqrt{1+iC_1(t)} + \sqrt{1-iC_{1-1}(t)} \right) \quad C_1(0) = \delta_{n_0,1} \]  

\[ (l=0,\ldots,\infty, \text{usually } n_0=0) \]. Figure 6.10 shows the residual of the equation for $C_{n_0}(t)$ (giving an estimate of the accuracy) as a function of time for $n=200$ and $n=200$ steps.

\[ H(q,p) = \frac{1}{2} \left( p^2 + \alpha(t) \frac{k}{2} q^2 \right) \]  

where $\alpha(t)$ is a piecewise linear function of time. In this case the Hamilton equations can be solved exactly and the results compared with the same problem integrated numerically.

Figure 6.9 shows the error on the coordinate ($\hat{q}$) obtained integrating the Liouville equation associated with the Hamiltonian (37). The numerical scheme is $4^{th}$-order accurate and fully symplectic.
7.1 INTRODUCTION

Computational science has added new dimensions to traditional experimental and theoretical approaches to scientific research and technology development, becoming vital to many fields of science and engineering. It promotes interdisciplinary collaboration between theorists and application experts and enables them to deal with complicated problems in a wide range of areas.

The work performed in 1998 is an example of computational technologies and approaches applied to problems encountered in materials science, engineering, environmental science, ecology and medicine, in the context of national and international projects.

7.2 COMPUTATIONAL METHODS FOR ENGINEERING

This research activity has been present for quite some time in the fields of advanced technology, material developments, environmental safeguards and energy saving. A better understanding of the physical phenomena involved in many industrial processes plus the constant search for new and advanced materials have made it increasingly important to improve product quality and save on materials and man-hours.

7.2.1 Thermo-structural analysis: industrial process simulation

The study and research activities developed for numerical simulation of metal forming processes (started in 1988 and ongoing) have been extended to other interesting engineering fields, such as hot bending and metal-sheet welding processes (especially laser and tungsten inert gas [TIG]). These processes constitute a sample of the most interesting and complex problems found in nonlinear engineering, as all the possible types of nonlinearities (geometrical, material and boundary nonlinearities) are present. Welding (and also hot bending) processes in particular present the problem of having to accurately represent the moving heating source and, in TIG welding, introduction of the filler material. Moreover, because the physical phenomena or the processes are complex, it is important to simplify and approximate them.

The aim of the present activity is mainly to build up a knowledge basis to allow systematic use of computer codes in industrial design and production phases.

NOSA code development

The algorithm for treating material plastic anisotropy and the code development for resolving the problem in 3-D geometry were included in an advanced version of the NOSA code developed by CNR CNUCE and were recontrolled and revalidated with regard to the numerical resolution techniques for the algebraic system to which each problem is reduced. (NOSA is intended for simulating drawing and rolling processes of industrial interest.)
Simulation of laser welding processes

Following numerical tests and comparisons with the models applied in previous activities, an algorithm to be used in the ABAQUS/S code was developed to evaluate metallic material elastoviscoplastic behaviour at high temperatures. The work was carried out in collaboration with the Engineering Institute of Ferrara University.

As is known, correct simulation of welding processes (particularly by laser) should consider viscosity effects at high temperatures.

TIG-type industrial welding processes

The work to define and implement calculations for validation of and support to the welding activities at Belleli Energia S.p.A. was started in March 1998 and completed in July 1998. Belleli had been contracted by NET to construct reduced-dimension test models of the first toroidal-field coil case for ITER.

Preliminary studies and research on the feasibility of using ABAQUS/S to simulate a welding technique with filler material, such as TIG, were carried out. In fact, the filler material required for welding very thick sheets poses the problem of how to simulate the introduction of the filler material during each welding pass. For this reason, models with reduced and simple geometry were studied in order to single out the most suitable methodology to be used.

The heat source distribution, as energy power distribution, on the material during welding was then experimentally studied with the collaboration of ENEA Faenza.

A thorough bibliographic investigation was made to find out as much as possible about all the physical and mechanical properties of the AISI-316LN steel adopted for ITER that could be of calculation interest.

Calculations were first performed for some experimental models with reduced dimensions (compared to the Belleli models), considering a limited number of welding passes with filler material. The results obtained were encouraging and sufficiently satisfactory as regards both temperature distribution and mechanical response; in particular, it was shown that ABAQUS/S is able to simulate a TIG welding process. The next step is to improve the methodology adopted in order to simulate complete welds for geometrically more complex models.

Figure 7.1 shows the temperature distribution during the TIG welding simulation performed for a model consisting of two AISI-316LN steel sheets, each one 150×100×20 mm³; nine passes (eight with and one without filler material) were made for a welding length of 100 mm. For the same simulation, figure 7.2 shows the temperature history in the central point of the lower surface of the model, at mid point along the welding direction; figure 7.3 shows the angular displacement of the sheets and the equivalent plastic strain distribution after the nine passes.

![Fig. 7.1 - TIG welding simulation: temperature distribution](image-url)
7.2.2 Finite-element methods and stress analysis

Stress analysis is necessary in a wide range of problems connected with the use of materials both for industrial products and for research devices. The experience acquired in this area has been used for ENEA projects as well as in national/international collaborations.

Ceramic materials: biomedical prostheses

Activities in biomedical engineering began in 1994 as a collaboration between ENEA and the Orthopaedic Departments of Rome Catholic University and Ancona University in the framework of the STRIDE-CETMA project. The study concerned ceramic components for orthopaedic prostheses and had to determine the possible reasons for failure of the alumina ceramic head of an implanted hip-joint prosthesis (fig. 7.4). Two parameters were found to be mainly responsible for head breaking, i.e., cracks in the heads and errors in the conical mating between head and stem.

The goals (partially reached) of the work are:

- to work out a criterion, based on finite-element analysis (FEA) codes, for evaluating the influence of the two critical parameters on the head mechanical strength;
- to determine some specifications about the maximum allowable crack dimensions and tolerances in the stem–head taper fit.

The importance of this work lies in the fact that the implanted ceramic heads are insufficiently characterised, so it is necessary to impose limiting specifications to improve their reliability.

The head geometrical dimensions are reported in the schematic cross-section in figure 7.5. A 2-D model was considered because of the axial symmetry of the geometry.

During 1998, the investigation addressed the effect of errors in the conical mating between head and stem on the head.

Fig. 7.2 - TIG welding simulation: temperature history

Fig. 7.3 - TIG welding simulation: final angular displacement of sheets after nine welding passes. a) Numerical simulation; b) result of the corresponding experimental test

Fig. 7.4 - Schematic of the human pelvis: comparison between natural (left) and artificial (right) articulation. 1) Alumina ceramic hemispherical cotyloid cavity; 2) titanium ring externally threaded to block the cotyloid cavity; 3) ceramic ball head of the hip joint prosthesis; 4) stem; 5) ceramic layer covering the stem; 6) pelvis; 7) femur
mechanical strength, i.e., a so-called second-type conical error, to which corresponds a stem summit angle smaller than the one in the head hole (see fig. 7.6). This conical error changes the head stress considerably, so this study can be considered decisive for a later correct assessment of its resistance to breaking.

Mechanical analysis of the structure was performed using the CASTEM 2000 code, which made it possible to determine the head stress field ($\sigma_R$, $\sigma_T$, $\sigma_s$, Von Mises $\sigma_{VM}$ and Tresca $\sigma_T$ stresses) for a certain set of applied loads and errors in conical mating. To limit the number of cases to analyse, parametric analysis was carried out by considering:

* errors in the conical mating between $1^\circ$ and $10'$ with a $10'$ angle step and later errors between $10'$ and $1'$ with a $1'$ step; as a borderline case, a zero error in conical mating (nominal case) was also considered;
* compressive loads between 70 kg (nominal body weight) and 490 kg (the highest supposed load) applied to the stem, with a 70-kg load step.

The stress distribution was done only for the hole edge, where the highest stresses are located. These stresses decrease rapidly with increasing radius.

Two zones of the hole edge were studied in particular:

* The zone corresponding to the final mating between stem and head, where the highest Von Mises and Tresca stresses are reached. Here, also compressive radial stresses $\sigma_R$ and axial compressive stresses $\sigma_z$ are very close to their maximum values.

The $\sigma_R$, $\sigma_z$ and $sJ$ stresses along the head edge are shown in figure 7.7. The figure gives a good idea of the behaviour of stress distribution as a function of error in conical mating for a 490-kg load and a conical mating error of $1^\circ$, $30'$ and zero (nominal case).

**Design verification of a handling system**

The compact muon solenoid (CMS) is one of the particle detectors planned for the Large Hadron Collider (LHC) under construction at CERN in Geneva. The 100,000 crystals of the electromagnetic calorimeter (ECAL) of the CMS will be assembled in submodules and "baskets" in one of the worldwide regional centres of CMS-ECAL. In the framework of the ENEA-INFN collaboration, one of these centres is located at ENEA Casaccia.

Hundreds of crystals have to be tested and assembled in each basket and, at the end of the process, the basket will be delivered to CERN Geneva for installation. The handling system must assure the integrity of the crystals and avoid giving rise to any shocks or vibrations that could cause relative motion between crystals and submodules during the process. A dedicated handling system has to be
specifically designed for this purpose; its performance can then be verified by finite-element simulations.

The design goal is to maximise the isolation of the basket. This can be achieved by shifting down, by means of mechanical isolators, the natural frequency of the system as far from the exciting frequency as possible. Air springs have been chosen for the suspension system because they produce the lowest natural frequency of all the existing vibration isolators.

A preliminary design of the type shown in figure 7.8 is currently being investigated by FEA and by means of:
- natural-frequency extraction, to evaluate the mechanical isolation coefficient;
- random response analysis, for the response to continuous excitation (acceleration) expressed in a statistical sense by means of an input power spectral density;
- modal dynamics, to find the time response to a given input acceleration.

Fracture mechanics of thin plates: 3-D finite-element analysis

The problem of aircraft structural integrity recently led to renewed fundamental engineering research on the fracture mechanics of cracked thin plates. Cracks in the skin of aircraft fuselages (or other shell structures) can be subjected to very complex stress states, resulting in mixed-mode fracture conditions. For practical applications the basic point is characterisation of the fracture behaviour through correlation of experimental data by means of “stress intensity factors”. Central to this problem and the object of a research activity carried out in collaboration with Cornell University (Ithaca NY, U.S.A.) is the nature of the stress field near the crack tip in thin plates.

![Fig. 7.8 - Handling system of the baskets for CMS-ECAL: lateral view](image)
The validity of the Kirchhoff stress fields as far-field boundary condition and the 3-D nature of the stress field near the crack tip were examined by performing 3-D FEA of a linearly elastic cracked plate under pure bending, shearing and twisting moments. Figure 7.9 shows the out-of-plane shear stress for a thin cracked plate under uniform shear. Away from the crack tip the distribution is approximately parabolic as predicted by plate theory, but very close to the crack tip the stress is nearly constant through the thickness.

The 3-D FEA results were compared with asymptotic solutions for stress fields of Kirchhoff plate theory and Reissner theory. The FEA results confirm that the Kirchhoff near-tip field (for the case of bending and shear) provides a good approximation to the in-plane stresses in the region $r > h$ ($h =$ plate thickness). As expected, in the region $r < h$, the Kirchhoff theory differs significantly from the 3-D theory, while the Reissner theory seems to provide reasonable agreement at distances very close to the crack tip ($r < 0.02h$). A universal linear relation between the Kirchhoff and the 3-D stress intensity factors was also found (fig. 7.10).

### Parallel finite-element analysis method

In FEA, most of the computing time is spent on the solution of a linear (or linearised) equation system, whose coefficient matrix is usually large, sparse and scarcely populated. Direct solvers are very precise, reliable and flexible, but they can be very time consuming in large 3-D problems and are not very well suited to parallel computers, particularly those with single-instruction multiple-data (SIMD) architectures. Therefore, in this research activity dedicated to numerical methods for SIMD computers, it was decided to investigate the performance of iterative solvers in FEA, and specifically of the well-known preconditioned conjugate gradient method (PCGM).

Previous research work had led to the development of a "distributed" PCGM, a parallel algorithm, which was implemented and tested on an 8-node Quadrics. Quadrics is a family of SIMD massive parallel computers with a 3-D architecture based on a cubic lattice of processing nodes, developed in a collaboration between ENEA and INFN. The method showed very good scalability but the performance was not quite satisfactory in terms of convergence rate and computing time.

A new approach based on multigrid techniques was attempted: the domain is discretized in a "coarse" mesh and in a nested "fine" mesh, and the unknown displacement field is interpolated by means of nodal values of both grids. The FE method combined with this multigrid technique leads to a stiffness matrix, which has the coarse and fine stiffness matrices as diagonal blocks. The FE equation system is then solved with the "distributed" PCGM, and at each step a coarse mesh solution can be used as main
preconditioner for the iteration on the fine grid. This preconditioning proved very powerful and the method was implemented both in a sequential program on an IBM-RISC590 and in a parallel program on a 128-node Quadrics-QH1, with very good results (fig. 7.11).

7.3 MATHEMATICAL AND COMPUTATIONAL PHYSICS

The several years of experience gained in mathematical and physical modelling and in numerical simulation have made it possible to tackle a wide range of problems and applications.

7.3.1 Radiation transport and matter interaction

Computer simulations of radiation and particle transport are requested for resolving problems in very different research fields. The following sections describe activities concerning the environment, fusion machines and medical issues.

Radiation transport in the atmosphere

Joint activities between ENEA Brasimone and Bologna concerning the use of innovative optical technologies and numerical simulation for observing and interpreting climatic phenomena have been in course since 1994. In 1998, the following projects were undertaken:

- radiative forcing due to volcanic aerosols;
- measurement of columnar ozone by a radiometric technique;
- transport of polarised radiation.

Measurement activities were carried out by means of the Brasimone and Sodankyla lidars and a multispectral radiometer, while numerical simulations were performed with the Monte Carlo PREMAR-2 code developed by ENEA Bologna.

Radiative forcing. On the basis of the lidar measurements done in 1996, a study was carried out to determine the mean spatial distribution of volcanic aerosols and the consequent radiative forcing during that year. The measurements were performed knowing precisely the atmospheric molecular profile, thanks to the radio-soundings (two a day) at the Agenzia Regionale Protezione dell' Ambiente (ARPA) station of S. Pietro Capofiume (Bologna). The "lidar ratio", i.e., the ratio between the backscattering and extinction coefficients of electromagnetic radiation, was then derived from the measurements. On the basis of the empirical considerations of Wandinger and coworkers, which were derived from field measurements, it was possible to obtain information about aerosol microphysics using the hypothesis of spherical particles.

Methods proposed in the literature were used to calculate the dimensional and mass distribution of volcanic aerosols in the Brasimone stratosphere and to reconstruct the atmospheric configuration generating the real conditions for optical interaction and multiple-scattering radiation exchange.

A Monte Carlo simulation was then performed for all the wavelengths of the spectrum between 0.3 and 2 μm (fig. 7.12), and from the result of the numerical calculations it was possible to evaluate the radiative forcing produced by volcanic aerosols in the geographic area of central-northern Italy. A negative contribution of -0.76 W/m² was found, hence with a cooling effect.
**Columnar ozone.** Spectral measurements of solar irradiance in the UVB range are routinely performed at ENEA Brasimone, and numerical analysis is carried out to determine the ozone columnar content. Measurements of UVB solar radiation are performed by means of an interferential-filter radiometer working on four wavelengths (300, 306, 312 and 318 nm) and using a rotating shadowband. This device is guided by a microprocessor, programmed according to the local ephemris so as to perform measurements when the solar disc is shadowed and thereby distinguish the different components of irradiance.

Besides the direct irradiance method of determining the columnar ozone, a new method that uses global irradiance was developed. Using this method with Monte Carlo simulations it was possible to obtain a series of parametric curves (fig. 7.13) of the irradiance ratio between radiation intensities at 317.7 nm and 305.5 nm at ground level as a function of ozone concentration. The curves were then used to quickly determine the columnar content of atmospheric ozone. The curves are particularly useful when direct irradiance cannot be measured because of poor atmospheric conditions.

**Polarised radiation transport.** In the framework of a EU contract, SAONAS, a study of the simulation of polarised radiation transport was carried out in order to interpret the backscattered lidar signal in the presence of polar stratospheric clouds (PSCs).

The Monte Carlo method is capable of simulating multiple-scattering processes, such as those controlling radiative exchange in the atmosphere, particularly within the clouds; in fact, it is possible to numerically process a large number of photonic “stories” governed by phenomena caused by radiation/atmospheric-component interaction.

In 1998, polarised radiation transport studies were performed (also in collaboration with the University of Bologna), aiming at a future implementation of the Stokes polarisation matrix in the PREMAR-2 code.

The studies showed that the Stokes parameters are suitable for interpreting the optical properties of clouds and that they can be used to adjust lidar data by taking into account multiple collisions.

**Radiation transport and activation calculation**

**EU ITER breeding blanket decay heat evaluation.** To qualify the EU ITER breeding blanket design from a safety point of view, accident transients due to decay heat were assessed.

The neutron multiplier is beryllium and the breeder material is lithium metazirconate in the form of a binary pebble bed (fig. 7.14). A set of neutronic and activation calculations was performed to evaluate the breeding blanket decay heat after plant shutdown. Figure 7.15 shows the decay heat at plasma shutdown for the breeder (pure metazirconate: 9.07% Li, 31.35% O, 59.58% Zr) and the cladding (AISI...
316 LN (IG) of three breeder rods: radial ring 1 (distance d from first wall (FW) = 1.5 cm); radial ring 5 (d = 10 cm); radial ring 8 (d = 19.5 cm). Also reported is the decay heat of the Be neutron multiplier at different distances from the FW.

The after-heat vs time after plasma shutdown (up to 1 min) was calculated for Be and lithium metazirconate and then analysed to study its sharp decrease.

**Waste characterisation of the ITER toroidal field coil casing.** As support to waste characterisation of the toroidal field coil casing (AISI 316LN), a set of activation calculations was carried out, mainly to evaluate Nb94 production and which fraction of Nb94 (at 100 years after shutdown) comes from activation of Mo and which from Nb.

The ANITA-4/M codes were used to obtain i) specific activity and contact dose rate of dominant nuclides; ii) nuclide contribution to total activity and total contact dose rate; iii) fraction of Nb94 production from Mo/Nb activation, for the M6 pulsed scenario at 100 years after shutdown (table 7.I).

**Activated corrosion product evaluation.** The European Home Team performed activation corrosion product source terms evaluation as a contribution to the ITER Non-site Specific Safety Report. To support the "Corrosion Product Modelling and Inventories" task, a set of Sn neutron transport and activation calculations was done for the various in-vessel zones of the first wall, shield blanket, baffle limiter, vacuum vessel and divertor regions of ITER. Table 7.II reports the first-wall steel cooling-pipe activation characteristics in various poloidal regions at plasma shutdown and after one day's cooling time.

Activation of the poloidal first wall/inboard baffle (PFW/IBB), limiter/outboard baffle (LIM/OBB) and vacuum vessel (VV) primary cooling loops of ITER was assessed to provide input data to the PACTOL code. The VV structural material is AISI 316 LN-IG (Mn 1.8%, Co 0.1%). Five poloidal configurations (PCI to PC5) differing in radial geometry and material composition were defined to account for shape and neutron power load variations. Two irradiation scenarios (SA1 and M5a) were considered for the ITER Basic Performance Phase and two (SA2 and M6) for the Enhanced Performance Phase.

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Activity (Bq/cm³)</th>
<th>Nuclide</th>
<th>Dose rate (Sv/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni63</td>
<td>4.98 x 10²</td>
<td>Nb94</td>
<td>5.31 x 10⁻⁹</td>
</tr>
<tr>
<td>Ni59</td>
<td>9.12 x 10⁰</td>
<td>Co60</td>
<td>2.02 x 10⁻⁹</td>
</tr>
<tr>
<td>Mo93</td>
<td>4.65 x 10⁰</td>
<td>Nb91</td>
<td>1.15 x 10⁻¹</td>
</tr>
<tr>
<td>Nb94</td>
<td>1.06 x 10⁻¹</td>
<td>Al26</td>
<td>1.49 x 10⁻¹⁺</td>
</tr>
<tr>
<td>Total</td>
<td>5.22 x 10²</td>
<td>Total</td>
<td>7.45 x 10⁻⁹</td>
</tr>
</tbody>
</table>

Table 7.1 - Nuclide contribution to activation of AISI 316 LN coil casing (Mo=3.0% Nb=0.01% Ti=0.05% Co=0.05%) 100 years after shutdown.
Table 7.11 – AISI 316 LN cooling-pipe activation characteristics (activity, decay heat, dose rate) in various poloidal regions at plasma shutdown (values in italics refer to one day’s cooling time)

<table>
<thead>
<tr>
<th>Poloidal region</th>
<th>0.3 MW-y/m²</th>
<th>1 MW-y/m²</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SA1</td>
<td>M5a</td>
</tr>
<tr>
<td></td>
<td>a    b    c</td>
<td>a    b    c</td>
</tr>
<tr>
<td>PC1</td>
<td>728  0.175 25979</td>
<td>697  0.173 25625</td>
</tr>
<tr>
<td></td>
<td>231  0.012 2047</td>
<td>200  0.010 1678</td>
</tr>
<tr>
<td>PC2</td>
<td>798  0.192 28497</td>
<td>757  0.189 28054</td>
</tr>
<tr>
<td></td>
<td>253  0.013 2226</td>
<td>211  0.010 1767</td>
</tr>
<tr>
<td>PC3</td>
<td>1213 0.293 43344</td>
<td>1112 0.288 42419</td>
</tr>
<tr>
<td></td>
<td>380  0.019 3229</td>
<td>279  0.014 2277</td>
</tr>
<tr>
<td>PC4</td>
<td>1035 0.244 36094</td>
<td>943  0.239 35207</td>
</tr>
<tr>
<td></td>
<td>351  0.018 3054</td>
<td>259  0.013 2150</td>
</tr>
<tr>
<td>PC5</td>
<td>589  0.140 20772</td>
<td>572  0.139 20512</td>
</tr>
<tr>
<td></td>
<td>195  0.010 1777</td>
<td>177  0.009 1506</td>
</tr>
</tbody>
</table>

AISI 316 LN activity at plasma shutdown (PC3-zone 3, scenario SA1). To validate the codes, data and calculation procedures used in decay heat prediction, the ITER Joint Central Team launched an international benchmark. Decay-heat results for two of the most relevant fusion-related materials, AISI 316 and copper, obtained using the ENEA activation code ANITA-4/M, were compared with decay-heat measurements made on specimens of ITER-relevant materials irradiated by the 14-MeV neutron flux of the JAERI Fusion Neutronics Source. Total decay heat vs cooling time of Cu and AISI 316 specimens irradiated for 7 h is shown in figure 7.16.

Two neutron activation libraries, EAF-4.1 and FENDL/A-2, and two radioactive decay data libraries, JEF-2.2 and FENDL/D-2, were used by the ANITA-4 code for the decay heat calculation. Two series of irradiations were performed, one lasting 5 min and one 7 h, with decay energy calculated at cooling time up to about one hour and one week for the AISI 316 and the copper specimens, respectively.

Comparisons of calculation with experiment for the total decay heat vs cooling time of AISI 316 are shown in figures 7.17 and 7.18.

The discrepancies between ANITA-4 experimental results are lower than 10% for both the copper and
the steel specimens and for both the irradiation scenarios.

Radiation transport for hadrontherapy

The collaboration in the ISS TOP project on proton therapy of cancer (see sect. 3.2.4) continued with dosimetric research activities for the proton calorimeter.

Proton mass stopping powers and mean energies were calculated by means of Monte Carlo simulations at depths corresponding to the spread-out Bragg peak (SOBP) for various beam maximum energies and SOBP widths. The simulations were performed with and without considering nuclear interactions in water and tissue. The data obtained show that mass stopping powers and mean energies vary appreciably in the SOBP, so this effect has to be properly accounted for in dosimetry. The values obtained for the same residual range depended only slightly on the maximum energy of the modulated beam, the sole exception being depths near the end of the proton range. Switching off nuclear interactions leads to a mass stopping power maximum decrease of 5% and to a corresponding mean energy maximum increase of 2.6%. Comparison of a 250-MeV non-modulated beam with a modulated beam (fig. 7.19) of the same maximum energy showed that the mass stopping power values at the same depths were up to 21% lower for the first case.

Water-air stopping power ratios at the SOBP depths were calculated according to Spencer-Attix cavity integral theory. The values of the ratios appear to increase slightly with depth in the medium and, near the end of the proton range, with diminishing incident proton energy. The above values are almost completely independent of the various parameters studied. For instance, they are not affected by inclusion or not of nuclear interactions. Even a non-modulated beam has the same values (within 0.1%)
as a modulated beam of the same maximum energy. The water-air stopping power values for modulated beams were also calculated by means of the Bragg-Gray cavity integral. They were up to 0.5% lower than the values calculated with the Spencer-Attix cavity integral.

7.3.2 Fluidodynamics and magnetohydrodynamics

In 1998, activities continued in the framework of long-standing collaborations on environmental problems concerning hydrodynamic processes in closed and semiclosed basins and on national and international fusion projects. Numerical simulations of combustion processes were also carried out.

Closed and semiclosed basin dynamics

Thermohydrodynamics and dispersion processes in marine basins. Thermohaline circulation and mixing processes induced by the presence of a polynya in Terranova Bay (Ross Sea, Antarctica) were studied in the framework of the Italian Program for Antarctic Research. Analysis was carried out by means of oceanographic observations and numerical simulations.

In this “latent heat” polynya, the ice formed is continually swept away by strong katabatic winds, leading to a huge loss of fresh water. The formation rate of dense water at the surface gives rise to thermohaline circulation with mixing of the water column down to great depths.

A time-dependent model for numerical simulation of thermohaline circulation in a vertical section was used to investigate the contribution of thermohaline-forcing to the circulation pattern; ice production, which is consistent with the observed salinity distribution, was also estimated.

Dispersion processes in semi-enclosed basins with stationary flows were studied by means of an Eulerian advection-diffusion model. Special attention was given to the quantities that characterise the macroscopic state of the system: the normalised total quantity \( C(t) \) \((C(0)=1)\) of a tracer inside the basin, and its residence time \( T \).

The sensitivity of the results to a number of parameters, including flow structure, Peclet number, initial and boundary conditions, were studied; in particular, the difference between unidirectional flows and flows with recirculation was investigated.

It was found that despite the fact that the details of dispersive processes depend strongly on various parameters, \( C(t) \) and \( T \) could be characterised in a general way. A priori estimates of the value of \( T \) were provided, valid for a wide range of parameters. For unidirectional flows, \( T = T_{\text{out}} + T_0 \), where \( T_{\text{out}} \) is the time the tracer takes to reach the outflow and \( T_0 \) is the principal eigenvalue of the advection-diffusion problem. Both parameters \( T_{\text{out}} \) and \( T_0 \) can be computed knowing the flow structure and Peclet number and are representative, respectively, of the initial and asymptotic phases of dispersion. For flows with recirculation it was found that \( T = T_0 \) over the whole parameter space considered. Conceptually, the difference is due to the tendency of the recirculation to trap the tracer, which enhances the importance of the asymptotic phase. For these flows, the values of \( T \) do not change significantly in the range of realistic Peclet numbers considered, suggesting that macroscopic dispersion properties depend only weakly on the eddy diffusion coefficient.

Oxygen dynamics in a highly trophic aquatic environment. Oxygen dynamics in a highly trophic environment was studied through analysis of in situ field data and through mathematical modelling. The case investigated was the Orbetello coastal lagoon (central Italy), monitored by ENEA during 1993-94.

From analysis of the time series of meteorological and hydrological data collected in the lagoon, it followed that the oxygen time evolution can be described in terms of a first-order autoregression process with periodical forcing. This process is the discrete analog of an oxygen global mass balance in water and allows estimation, from experimental data, of the production, consumption and transfer rate of oxygen.

A representation of the main processes, in terms of the chemical species \( O_2 \) and \( H_2S \), affecting the oxygen dynamics in a horizontal homogeneous environment, and for time periods no longer than a few
weeks, was presented. As these processes depend on depth, in particular on the compartment sediments and water, the vertical dimension was considered in modelling the oxygen dynamics.

**Simulation of advection-diffusion processes in closed or semi-enclosed marine basins.** The objective of this task is the development of a numerical Monte Carlo code (MABAR) for calculating the evolution of a passive constituent released at a given point of a basin and subsequently dispersed by sea motion. The dispersion process is described by an advection-diffusion model and the hydrodynamics is supposed known.

So far, a discrete form of the 3-D unsteady advection-diffusion equation has been derived by a finite-volume method, subjected to boundary conditions of three different types (Dirichlet, Neumann and Robin). The time-dependent behaviour of the contaminant was investigated following two different viewpoints: The first, Eulerian, provides the evolution with time of the tracer concentration at some fixed points of the physical domain. The second, Lagrangian, allows the observer to follow the spatial evolution, in time, of the tracer, starting from an initial spatial configuration. Preliminary numerical tests were performed with both models. A typical result is shown in figure 7.20.

**Fusion plasmas**

**Support to the design of IGNITOR.** The significant numerical support to the IGNITOR design followed the evolution of the reference parameters of the machine. The changes in the poloidal field system involved a new assessment of all the computational work, based on a set of developed codes. The main activities (requested by ANSALDO, ABB and the ENEA Fusion Department) concerned:

**A) Optimisation of operating scenarios**

The scientific objectives of the experiment can be achieved because of the high magnetic field and plasma current. In a collaboration with the CNR Fusion Association and the Plasma Physics Institute of Milan to support the physics predictions, numerous analyses of plasma evolution during current ramp and flat-top were carried out using the 1+1/2 JETTO code.

The most advanced scenario, 12 MA, was considered and discussed first. Figure 7.21 shows a typical evolution of the plasma poloidal cross section.

It was found that Ohmic ignition could be attained even...
assuming energy confinement times close to the ITER89-P scaling, provided that the ramp-up phase is carefully programmed. It turned out that density is always the main parameter in following the path to ignition, but other items, such as plasma shape and dimensions, current density profile and impurity content, require attention. To avoid instabilities and to optimise the parameters involved (such as power and peak temperatures), ignition must be reached immediately after the current ramp. The 11-MA scenario was further optimised by an extensive series of simulations.

With confinement times closely matching the more recent ITER96 scaling law for the L-mode, ignition can still be achieved. To attain ignition conditions while maintaining the safety factor profile marginally near unity, the density increase was analysed by varying the particle influx rate. A higher initial density increase allows improvement in plasma performance, while avoiding the Greenwald density limit (figs. 7.22 and 7.23). To different increases in density correspond different approaches for ignition conditions (fig. 7.24).

B) Design of the poloidal field magnets and equilibrium studies

The poloidal field magnets provide and control the plasma equilibrium throughout the plasma operation cycle. Their function is fundamental to IGNITOR operation. The design of this system requires evaluation of several interrelated parameters, such as the current to the poloidal windings, the magnetic flux requirement and the electromagnetic forces acting on the coils. The availability of all these data primarily involves
computation of magnetohydrodynamic (MHD) equilibrium configurations, with all the parameters connected with the magnetic topology, such as poloidal plasma current, poloidal beta, etc. The new geometries considered for the transformer coils and the radial electromagnetic press necessitated carrying out a set of such computations.

The MHD equilibrium configurations relative to the 11- and 12-MA scenarios were optimised imposing ideal MHD stability through minimising the $q=1$ surface.

Finally, the equilibrium configurations required as "key" data for simulations of the plasma evolution were optimised for the different situations analysed.

C) Evaluation of force and temperature distribution in the toroidal magnet

Evaluation of stress distribution in the toroidal field magnet requires computation of temperatures and loads as a preliminary step. This is done by a finite-element code, FORTE, which solves the system of coupled temperature and magnetic field diffusion equations. FORTE was applied to evaluate the maximum pulse length allowable in the toroidal magnet in a scenario with a 9-T toroidal field. The maximum flat-top duration was found to be 14 s.

Interpretative models for the electron cyclotron resonance heating (ECRH) experiment on the Frascati Tokamak Upgrade (FTU). Experimental results of electron cyclotron heating (500 kW for 100 ms) on FTU ($R=0.53m$, $a=0.30m$, $B_t$ up to 8T) confirmed its significant influence on sawtooth dynamics, as already observed in several machines. In low-current (360 kA) discharges, proper localisation (just across the $q=1$ surface) of the injected waves allows temporary suppression of sawtooth oscillations with an injected power of 0.7 MW. These experimental data were reproduced by extensive simulations based on a consistent numerical code. The "profile consistent" electron diffusivity coefficient given by the Coppi-Mazzucato-Gruber expression produces a satisfactory representation of the plasma behaviour. The work was done in collaboration with the CNR Fusion Association and the Plasma Physics Institute of Milan.

Upgrading of the equilibrium code ESCO. A simplified version (V6ESCO) of the equilibrium module of the equilibrium-transport code JETTO is available for the case of a fixed plasma boundary. This feature is useful when one starts from experimental equilibrium configurations. Data relative to the poloidal flux are required in the form of bicubic spline coefficients.

An auxiliary code (SPLESCO) was developed to generate these coefficients starting from the usual bidimensional map of the poloidal flux. SPLESCO was tested on experimental data from FTU and the U.S. DIII-D tokamak. In both cases, the initial equilibrium configuration was carefully reproduced by V6ESCO. This code also has been revised.

Combustion and heat conduction processes

In the framework of a joint activity with ENEA Casaccia, work was started on developing and
implementing computer codes aimed at predicting turbulent combustion for industrial burners and combustors (e.g., gas turbines).

Tests were performed to improve the predictive capabilities of the GTTURBO code developed at the Centro Ricerca Sviluppo e Studi Superiori in Sardegna (CRS4 Cagliari) and check the code against experimental data. This activity required an in-depth study of several subjects related to turbulence and hydrocarbon-chemistry modelling. A synthesis of the work was presented at a seminar held in Bologna in March 1998.

7.3.3 Ecosystem and population dynamics: biological control

Numerical-mathematical models to simulate interaction processes between organisms and with their environment are increasingly requested by ecological and biological research programs on protected crops and breeding. Some models and applications developed in collaboration with the Maths Department of Parma University are described in the following.

A deterministic model for studying the local dynamics of trophic interactions in acarine predator-prey systems was developed starting from experimental data concerning individual properties relative to population dynamics. As a second step, a stage-structured population model was used to simulate reproduction, development and elimination processes of a single population dynamics, under the assumption of unlimited food. This model allows a stable stage structure of both predator and prey population to be developed. Then, by means of demographic analysis, lumped parameters of a single population (maximum specific growth rates, predator elimination) are estimated. These parameters are then introduced in a lumped model that describes the trophic interactions between predator and prey in terms of population biomass (biomass is a better currency of trophic interaction than numbers). The trophic interaction is described by a functional response of the predator on the prey biomass, and depends on a parameter representing the efficiency of the predation process. In this analysis, the functional response is assumed to satisfy only some basic properties. The mathematical properties of the lumped model are studied in order to explore its dynamic behaviour, depending on the efficiency of the predation process. This model was developed to improve biological control techniques, particularly in greenhouses.

A deterministic model for the study of the local dynamics of a three-level trophic chain (in terms of biomass) was developed. The non-negative and positive steady states are determined as functions of the efficiencies of the predation processes, as well their local stability characteristics. This model is the basis for studying the dynamics of gypsy moth populations in a homogeneous stand. The three levels of the trophic chain are:

- foliage biomass density, food source for gypsy moth;
- gypsy moth biomass density;
- natural enemy biomass density.

The model can be altered to make it more realistic. Spatial and seasonal dynamics should be taken into account.

7.4 PHYSICS OF COMPLEX SYSTEMS

The complexity of the world contrasts with the simplicity of the basic laws of physics. In recent years, considerable study has been devoted the world over to systems that exhibit complex outcomes. The interplay between simplicity (the so-called reductionist approach) and complexity, which implies both highly organised (the case of biological systems or coherent structures in fluids—a tornado for instance—or particles and radiation—lasers, etc.) and chaotic behaviour, can then produce very beautiful, rich and patterned outputs and lead to better knowledge of nature. Last but not least, understanding the peculiar behaviour underlying a physical, chemical or biological process can be used
to control a specific situation and develop technological applications. A striking example is provided by protein folding, a very complicated and structured process whose understanding and prediction is essential, particularly in planning new drugs and generally in many biotechnological applications.

In order to extract significant knowledge from a complex system, it is necessary to focus on the right level of description: experimental, computational and theoretical. In particular, the computational aspects, based on numerical simulations, can be used to check understanding of a particular process or phenomenon, leading to the so-called experimental mathematics. A particular dynamics can be followed over many different scales (this is the case of protein folding and lots of other molecular dynamics simulations) and suitable models built when a purely theoretical approach is not feasible and experiments are difficult or even impossible at the present technological level.

Theoretical models, numerical simulations and the relative computing codes have been developed to deal with some problems of particular interest and applied technological importance in the field of complex systems. The available computing facilities were used, especially the parallel computing hardware (IBM SP2, cluster of PC and workstations) in LoadLeveler and message-passing interface (MPI) environments. A dedicated computing laboratory mainly devoted to image techniques and processing was implemented. Many studies were carried out in collaboration with universities and laboratories both in Italy and abroad, especially when measurements were needed for checking the model predictions obtained at ENEA Bologna.

7.4.1 Quantum many-body systems and order-to-chaos transitions

The regular and chaotic dynamics of medium-mass even-even nuclei was investigated in the framework of the Interacting Boson Model-2 (IBM-2), which is a realistic model of nuclear structure where the isospin degree of freedom is explicitly introduced.

To perform this investigation, the fluctuation properties (departures of the energy level distribution from uniformity) of nuclear levels were studied by using the Random Matrix Theory (RMT). The Gaussian Orthogonal Ensemble (GOE) in particular was used, as chaotic many-body systems with time-reversal symmetry (such as nuclei) are associated with it.

Spectral functions were studied as a function of the IBM-2 Hamiltonian parameters in the shape-transitional regions intermediate between the dynamic symmetry limits of the model (U(5) vibrational nucleus, SU(3) rotational nucleus, O(6) γ-unstable nucleus, SU(3) triaxial nucleus). Contrary to expectations, the results showed a persistence of regular motion patterns even far from the dynamic symmetry limits.

A first explanation of the persistence of regular rather than chaotic features even when strong violations of the usual dynamic symmetries have occurred can be connected with the recently investigated existence of the so-called partial dynamic symmetries.

Indeed, partial dynamic symmetry arises when the dynamic symmetry of the model is broken in such a way that some (but not all) of the eigenstates of the Hamiltonian still exhibit the properties of that dynamic symmetry. Therefore, even if a dynamic symmetry is broken (as happens in shape-transitional regions), it is still possible to observe a regular feature of the nuclear dynamics.

As for the dynamic behaviour of relativistic quantum systems, a generalised quantum relativistic kinetic equation (RKE) of the Kadanoff-Baym type was obtained on the basis of the Heisenberg equations of motion where time evolution and space translation are separated from each other by means of the covariant method. The same approach is used for a covariant modification of the real-time Green's function method based on the Wigner representation. The suggested approach does not contain arbitrariness elements and uncertainties, which often arise from derivation of RKE on the basis of the motion equations of the Kadanoff-Baym type for the correlation functions in the case of systems with inner degrees of freedom.

Possibilities of the proposed method, developed in collaboration with Los Alamos, JINR Dubna and Saratov State University (Russia) laboratories, are demonstrated by examples of Vlasov-type RKE derivation and Boltzmann-Uehling-Uhlenbeck (BUU)-type collision integrals in the framework of the
σω-version of quantum hadrodynamics, for the simplest case of spin saturated nuclear matter without
an antinuclear component. Here, the quasiparticle approximation in a covariant performance is used. A
generalisation of the method for a description of strong non-equilibrium states based on the non-
equilibrium statistical operator is presently under investigation.

7.4.2 Complex systems in condensed matter and biophysics

Functional-analysis techniques for macromolecular dynamics

A functional method to derive exact solutions for a wide class of Volterra integro-differential equations
in terms of Bessel-Clifford functions of half-integer order has been developed. These equations are
applied to describe chemical reactions and to model protein dynamics in non-Markovian cases, thus
generalising the usual Kramer approach in an easily computable way.

Functional-analysis techniques may be introduced as a useful complement to molecular-dynamics
methodologies for proteins in order to investigate local and collective motions of macromolecules. An
example is the time evolution of atomic fluctuations in bovine pancreatic trypsin inhibitor studied by
examining time-series correlations of the atoms' mean-square displacements with respect to their
average positions; the local principal axis system for mean-square displacements corresponding to the
thermal ellipsoid was employed. In addition to analysis of correlation functions, the simple harmonic-
oscillator Langevin equation was used to obtain insight into the nature of the motions. In spite of the
relatively rough model, very meaningful information about the structural-biochemical mechanism of
action of this inhibitor was obtained. It was shown that the atomic fluctuations that contribute to the
temperature factor can be separated into local oscillations superimposed on motions with a more
collective character. The former have a subpicosecond length, while the latter involve a few
neighbouring atoms on the tenths-of-a-picosecond time scale. As for the distributed modes, they are
likely to be very sensitive to the external medium and to other environmental perturbations. For this
reason, it is believed that refinement of the coupling model, including interactions on a larger time
scale, could provide a structural tool for simulating the biochemical behaviour of this protein inhibitor
with better accuracy. Work is in progress to derive a microscopic master equation including "inside"
protein condensed-phase features and find its solution with the functional techniques so far developed.

Algebraic methods for the structure of atoms, nuclei and macromolecules

In collaboration with the Sloane Center for Theoretical Physics of Yale University, an algebraic
approach based on the introduction of suitable Lie algebras and Bose-Fermi (super)symmetries has
been developed to treat weak interactions in the nuclear environment and to investigate the structural
properties of atoms, nuclei and macromolecules of interest in biotechnological applications (such as
polymers and proteins). The method is based on the assumption that microscopic degrees of freedom
can be approximated by bosons with suitable quantum numbers, for the case of coherent collective
excitations, and by fermions for single-particle patterns. Hence, the computational complexity of the
full quantum-mechanical problem can be greatly reduced and reliable computing codes have been
written in order to solve the complete eigenvalue problem in realistic cases.

Analogies with many-body problems in nuclei and atoms (superconductivity, metal clusters and
resonances, etc.) have also been investigated and theoretical results and experimental information have
been compared.

Protein folding and prediction of secondary and tertiary structures. The highly accurate prediction
of secondary structures of proteins starting from aminoacid residues is a major goal in protein science.
This would greatly simplify a possible ab initio search of the folded structure and help in solving the
folding problem. Traditional secondary-structure prediction methods based on neural networks or
statistical methods score as high as 65% for the secondary structural state per residue, when correctly
tested on the basis of statistic indexes. This predictive efficiency was increased up to 67–68% only
when extensive input information was used, such as the evolutionary information contained in the
multiple alignments of the predicted protein with the homologous sequences of the database. Recently, the database of non-homologous crystallised proteins used to train neural networks was extended to include some 660 samples of high-quality crystals containing non-redundant information about folding motifs.

In a collaboration with the Biocomputing Group of the Centro Interdipartimentale per le Ricerche in Biotecnologie (CIRB) of Bologna University, extensive studies were made to verify whether a neural network architecture can reliably process all the available information and to determine the accuracy of the predictive method as compared to performances previously obtained on smaller databases. The analysis led to the conclusion that the 75% value for predictive accuracy is the maximum score obtained when three structural motifs (alpha-helices, beta strands and random coil) are discriminated according to the single sequence of the protein. Introduction of the sequence profile, however, contributes to a slight increase in the predictive efficiency of the method.

7.4.3 Biophysical and biochemical processes for soil remediation

In the eighties, following public awareness of the state of health of the environment, scientists and technologists became interested in the use of microorganisms as a possible solution to the world-wide problem of contaminated sites. Widespread releases of contaminants into soil systems, ranging from surface soils to deep aquifers, represent a major challenge for biotechnological applications. Bioremediation has been proved a potentially valuable tool in solving this problem. However, for a detailed description of the processes set up by introducing different micro-organisms into the soils for bioremediation of surface and subsurface contamination, numerous physical, chemical and biological mechanisms and mutual interactions have to be known, in addition to the inherent difficulties in obtaining reliable experimental information. Suitable biophysical and biochemical models can describe these processes and provide the necessary insight for optimising the whole procedure in each particular case.

Modelling processes underlying bacterial degradation of organic compounds and soil bioremediation thus belong to the typical class of complex systems with nonlinear many-body dynamics of the mesoscopic and microscopic components. In the past, the relevant system was described by means of phenomenological kinetic equations. A recently proposed modelling approach that is promising is based on the random Boolean network of genetic networks, where the biomass is represented by a network of interacting genes.

With respect to conventional simulations of diffusive systems based on molecular dynamics or Monte Carlo methods, this random-walk cellular automaton technique has inherent computational efficiency and is very suitable for running on high-speed massively parallel computers.

There are two main improvements on the previous simulations:

- The random-walk cellular automaton code in C language is adapted to a simple yet low-cost and efficient parallel architecture consisting of a network of biprocessor PCs with a Linux operating system and a MPI procedure.
- The biophysical model takes into account a more refined bacterial growth model than the conventional one (often used in simplified approximated forms). It includes memory effects by means of algebraic and functional-analysis techniques, which provide a convenient yet computationally simple framework for describing the dynamic behaviour of macromolecules.

As widely discussed in the literature, the total biomass can be considered as a set of interacting genes, due to the large genetic exchange between different bacterial cells, as well as to the genetic similarity between different species. The interaction between genes is simply parametrized, while a distinction is introduced between different species and the effects of intracellular reactions within the cell membranes, whose edge effect is explicitly taken into account. The dynamics of chemical processes induced by existing contaminants in the soil or added nutrients and intermediate metabolites is explicitly considered in the biochemical model.

Parallel implementation of the model—resulting in fast simulations—makes it possible to deal with
such long time intervals as to include genetic evolution and possible modifications (crossover, stochastic mutations, etc.) in the gene ecology.

It is worth recalling that in the standard Kauffman model a single cell is considered, as the main interest is in genetic intracellular dynamics. Generalisation of this model introduces a number of different cells, so intercellular dynamic interactions can be considered. However, it needs another parameter—called the activity of a given gene—which is closely related to the number of genes of that type present in the biophysical system at each given time.

The interactions among different genes are then approximated by Boolean functions, according to Kauffman's original idea. The resulting random Boolean network can describe the genetic evolution through a suitable input matrix, defining how each gene influences all the others. Randomness is widely used in choosing, for instance, the input genes from the whole population. The relative networks thus evolve according to synchronous dynamics at each time step, at which the state function of each gene is computed by applying the Boolean function to the state of its input nodes (interacting genes).

The significant quantity in the simulation process is the gene activity, which is proportional to the number of genes of a given type existing at each time step and which is obtained by suitably averaging on the statistical ensemble.

Memory effects have been introduced: The activation values at a given time depend on each activation value of each input node as well as on higher-order terms, which take into account the previous history of the system. The approach is essentially based on suitable analytical expressions. In addition, interaction between different genes and the chemicals introduced in the system can be described by means of appropriate discretisation of the diffusion and chemical reaction equations.

Parallel implementation of the theoretical model is mainly based on a simple domain decomposition of the ensemble of genetic network simulations. The statistical ensemble which allows determination of "macroscopic" quantities, such as gene activity and the time evolution of the relevant population, is then partitioned into a number of subdomains, each assigned to different processors. This reduces data exchange among different blocks to a minimum, with a significant improvement in the computing performance. At each time iteration, only a communication step is needed in order to update the ensemble statistics and perform the relevant averages.

The parallel algorithm was developed on a homogeneous cluster of eight PCs. Each node of the hardware structure consists of a dual Pentium II processor (300 MHz) with 128 Mbytes DIMM RAM and 4.5 Gbytes HD SCSI UW. A fast Ethernet connection at 100 Mbit/sec links the nodes together and a typical peak performance of 187 MFlops per cycle and single processor has been observed on sample calculations.

The operating system is a Linux RedHat 5.0 and the cellular automaton code has been written in standard C language. A MPI environment has been adopted for parallel simulation of the statistical ensemble. The whole procedure can be immediately extended to a larger number of processors or applied to a heterogeneous cluster of workstations with the same software characteristics.

To evaluate the parallel performance of the proposed computational strategy, with respect to sequential calculations, the classical speed-up and efficiency parameters were considered.

Theoretical improvements of the model—in addition to those previously described—are currently in progress. In particular, the macroscopic description of physical diffusive processes will be introduced with a suitable 3-D spatial mesh. Parallel implementation will then allow extensive calculations and it will be possible to check different forms of both intracellular and intercellular interactions in the gene population.

Such a realistic model of gene dynamics and ecology will allow comparison between the bacterial population dynamics resulting from the statistical average of gene activities and the usual models of bacteria evolution in laboratory and real environments. This will provide a useful insight into the microscopic foundations of phenomenological models of bacterial dynamics.
Technical and administrative support for the research and development activities of the Applied Physics Division is provided by the Unità di Supporto Tecnico-Funzionale (INN-FIS-FUN Unit).

This unit assists and supports the division in focussing on research opportunities at home and abroad and deals with administrative, legal and protocol matters related to national and international research contracts, co-operative programs and collaborations. It is responsible for co-ordinating the activities related to nuclear and environmental safety of personnel and plants assigned to the division and works in close co-operation with the Safety Authorities. The unit handles all purchasing orders and also organises (as Scientific Secretariat) seminars and conferences of interest to the division.

Personnel from the Applied Physics Division Directorate are responsible for financial management and for administrative matters related to personnel training and to guest hospitality at the division’s laboratories. They also keep the division informed on forthcoming conferences and workshops.
9.1 REPORTS

OPTICAL SYSTEMS

Laser Remote Sensing


Molecular Spectroscopy


Optical Components

A. COLUCCI and E. NICHELATTI: A reflectivity profilometer for the optical characterisation of graded reflectivity mirrors in the 250 nm–1100 nm spectral region. RTI/INN/98/5.


LASER SOURCES

Solid-state lasers


G. BALDACCHINI, R.M. MONTEREALI, M. GIORGI, F. MENCHINI and S. BOYKO: Laser action of \( F^2_3 \) and \( F_2 \) centers in LiF at room and low temperature. RT/INN/98/14.

Free Electron Lasers


PARTICLE ACCELERATORS

Accelerator for Medicine, Industry and Science


DATA AND SIGNAL ANALYSIS

Position Spectroscopy


APPLIED THEORY AND MODELLING

Computational Methods for Engineering

E. RAVAGLI: Individuazione dello stato tensionale in una testina di materiale ceramico per protesi d'anca con un errore di comicità del secondo tipo nel suo accoppiamento con lo stelo. RT/INN/98/4.


Mathematical and Computational Physics


S. MIGLIOLO, G. CENACCHI: On the stability of Ignitor against internal \( n=1 \) pressure driven modes. MIT/RLE/PTP/98/1.

Physics of Complex Systems

9.2 PUBLICATIONS

OPTICAL SYSTEMS

Laser Remote Sensing


Molecular Spectroscopy


Laser processing and Diagnostics


Optical Components


LASER SOURCES

Excimer Lasers


Solid State Lasers


Free Electron Lasers


PARTICLE ACCELERATORS

FEL Dedicated Accelerators


Accelerator for Medicine, Industry and Science


DIAGNOSTICS SYSTEMS

Positron Spectroscopy


Small Angle Neutron Scattering for the Study of Microstructural Inhomogeneities in Solid Systems


Low-Background Radiometry Application Laboratory


DATA AND SIGNAL ANALYSIS

Mathematical and Statistical Methods of Data Analysis

S. BEVILACQUA, D. BOLLINI, R. CAMPANINI, M. GALLI, N. LANCONELLI: A new approach to

APPLIED MATHEMATICS

Special Functions


Evolution Operators


APPLIED THEORY AND MODELLING

Mathematical and Computational Physics


Physics of Complex Systems


9.3 CONFERENCES

**OPTICAL SYSTEMS**

Laser Remote Sensing


R. BARBINI, F. COLAO, R. FANTONI, A. PALUCCI, S. RIBEZZO: *Local and remote fluorescence techniques for phytoplankton and sea water quality monitoring used during the XIII Italian Antarctic Oceanographic Campaign*. Proc. of the 5th Int. Conf. on Remote Sensing for Marine and Coastal Environments. Published by ERIM Int. 1509-1516.


Molecular Spectroscopy


R. FANTONI, L. DE DOMINICIS, M. GIORGI, P. CAVALIERE: OH DFWM $A^2\Sigma^+ \rightarrow X^2\Pi$ transitions in flames: saturation effects in the (0,0) and (1,0) bands. Presented at ECW'98 (Besançon 1998).


Laser processing and Diagnostics


P. DE PADOVA, R. LARCIPRETE, C. OTTAVIANI, S. PRIORI, C. QUARESIMA, A. REGINELLI, B. RESSEL, and P. PERFETTI: Ge/Bi/Si(001)-4x2 interface studied by high resolution core level spectroscopy. 10th Int. Conf. on Solid Surfaces (ICSS-10) (Birmingham 1998).

P. PERFETTI, P. DE PADOVA, R. LARCIPRETE, C. OTTAVIANI, B. RESSEL, C. QUARESIMA: Strained Ge/Si(111) interfaces in presence of Sb and Bi surfactants. 12th Int. Conf. on Vacuum Ultraviolet Radiation Physics (VUV-XII) (San Francisco 1998).


Laser Metrology and Artificial Vision


Optical Components


C. BATTAGLIN, F. CACCAVALE, A. MENELLE, M. MONTECCHI, P. POLATO: Characterisation of coating on glass by neutron reflectometry supported by already established techniques. Proc. of XVII Int. Conf on Glass (ICG XVII) (San Francisco 1998).


LASER SOURCES

Excimer Lasers

Solid State Lasers

Free Electron Lasers
PARTICLE ACCELERATORS

FEL Dedicated Accelerators


G. DATTOLI: Saw-tooth instability and storage ring free electron laser. Workshop on Non Linear Problems in Charged Beam Transport in Linear and Recirculated Accelerators, Analysis of Transverse and Longitudinal Instabilities (Frascati 1998).

L. GIANNESI: 3D simulation of space charge dominated beam dynamics Workshop on Non Linear Problems in Charged Beam Transport in Linear and Recirculated Accelerators, Analysis of Transverse and Longitudinal Instabilities (Frascati 1998).

L. MEZI: Storage ring FEL amplifiers and microwave instability. Workshop on Non Linear Problems in Charged Beam Transport in Linear and Recirculated Accelerators, Analysis of Transverse and Longitudinal Instabilities (Frascati 1998).

M. QUATTROMINI: Symmetric split techniques and time ordering problems. Workshop on Non Linear Problems in Charged Beam Transport in Linear and Recirculated Accelerators, Analysis of Transverse and Longitudinal Instabilities (Frascati 1998).

A. TORRE: A unified point of view on transport problems in optics and charged beam propagation. Workshop on Non Linear Problems in Charged Beam Transport in Linear and Recirculated Accelerators, Analysis of Transverse and Longitudinal Instabilities (Frascati 1998).


Accelerator for Medicine, Industry and Science


DIAGNOSTICS SYSTEMS

Positron Spectroscopy


Small Angle Neutron Scattering for the Study of Microstructural Inhomogeneities in Solid Systems

Low-Background Radiometry Application Laboratory


DATA AND SIGNAL ANALYSIS

Mathematical and Statistical Methods of Data Analysis


Position Sensitive Detectors Activity


Diagnostics Engineering of Complex mechanical Systems


Diagnostics, imaging and signal/image processing for applications to medicine, industry and cultural heritage


G. MAINO: *Gli strumenti della memoria: informatica e diagnostica fisica per i beni culturali*. Conferenza su invito per l'Associazione per la promozione del restauro (Ferrara 1998).


G. MAINO: *I laboratori di diagnostica e di informatica per i beni culturali*, Invited paper at the Int. Conf. on Studi su Storia della Scienza e Beni culturali, Istituto Italiano per l'Africa e l'Oriente - ISIAO, (Ravenna 1998).

**APPLIED MATHEMATICS**

Evolution Operators

APPLIED THEORY AND MODELLING

Computational Methods for Engineering


Mathematical and Computational Physics


D.G. CEPRAGA, G. CAMBI: Contribution to validation of activation data ENEA decay heat ANITA 4M code evaluation. EU-SEA5 Validation of Computer Codes and Models Meeting (Garching 1998).

D.G. CEPRAGA, G. CAMBI, M. FRISONI: ENEA contribution to "activation" calculations: The ANITA-4M code validation and its applications. EU-SEA5 Validation of Computer Codes and Models Planning Meeting (Garching 1998).


Physics of Complex Systems

G. MAINO: Attività di ricerca della Divisione Fisica Applicata dell’ENEA sui sistemi complessi, relazione su invitato al Planning Board dello IASG (Firenze 1998).


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G. MAINO: *Dynamical symmetries in nuclear weak interactions*. Int. Conf. on Nuclear structure at the extremes (Lewes 1998).


### 9.4 SEMINARS AND MEETINGS

#### SEMINARS

**12 05 98** H. SRIVASTAVA - University of Victoria (Canada)
The Generating function method and special functions

**15 05 98** E. CUPINI - ENEA - Bologna (Italy)
Il codice PREMAR-2 per la simulazione monte Carlo del trasporto radiativo in ambienti atmosferici

**04 06 98** A. KERMAN - MIT - Massachussets Institute of Technology (USA)
Laser acceleration

**12 06 98** ASHOK KUMAR - Dept. of Electrical Engineering -University of South Alabama (USA)
Pulsed laser deposition of advanced materials

**18 06 98** A. DMITRII SIDOROV BIRYUKOV - Moscow State University and International Laser Center - Moscow (Russia)
Laser spectroscopy techniques for monitoring gases and plasma in hostile environments

**10 07 98** A. PALUCCI - ENEA - Frascati (Italy)
XIII Campagna oceanografica antartica: laboratorio integrato di telerilevamento laser delle acque marine

**08 09 98** C. DAN DUMITRAS - National Institute for Laser, Plasma and Radiation Physics - Dept. of Laser - Bucharest (Romania)
Increasing sensitivity of a CO₂ laser photoacoustic system

**06 11 98** GIUSEPPE DATTOLI - ENEA - Frascati (Italy)
Conceptual design of short wavelengths free electron lasers

**11 11 98** PIERO MARIO AZZONI - ENEA - Bologna (Italy)
Analisi tempo frequenza dell' emissione acustica di un veicolo di formula uno per la stima delle prestazioni del motore

**01 12 98** GIUSEPPE BALDACCHINI - ENEA - Frascati (Italy)
Porous silicon or else?
MEETINGS

26 03 98 Giornata di Studio su “Energy Phase Correlation and Bunch Tailoring” idee e spunti di riflessione
G. Gallerano

13-15 05 98 Non Linear Problems in charged beam transport in linear and recirculated accelerators, analysis of
transverse and longitudinal instabilities
G. Dattoli

19 06 98 Colloquio - Diffusione Neutronica: Applicazioni in chimica-fisica, biofisica e scienze della terra
R. Coppola

3-4 12 98 Meeting Progetto BRITE
E. Giovenale
In the Divisione Fisica Applicata there are four scientific advisers: P.M. Azzoni, R. Barbini, E. Cupini, E. Menapace, and two Division Assistant: G. Maino, A. Vignati.
The following list of Applied Physics Division personnel (as of 31 December 1998) is ordered according to the divisions and units shown in the Organization Chart.

DIVISIONE FISICA APPLICATA
DIREZIONE FRASCATI
Renieri Alberto (Director)
Azzoni Piero Mario
Barbini Roberto
Bartolini Luciano
Batisti Emilia
Buffoni Giuseppe
Chiappini Paola
Cupini Enrico
Fubini Alessandro
Izzo Amelia
Maino Giuseppe
Menapace Enzo
Muciaccia Donatella
Pagliardini Anna
Piergentili Cinzia
Saruis Anna Maria
Vignati Angelo
Villalba Adolfo

UNITÀ DI SUPPORTO
TECNICO-FUNZIONALE
Simeoni Alfredo
Bartolomei Giulia
Coccoluto Giovanni
Rispoli Gianluca
Rossi Tiziana
Vari Tiziana

METODOLOGIE DIAGNOSTICHE E FISICA DI BASE
Stefanoni Mario
Bartolomei Paolo
Biasini Maurizio
Cantoni Gianfranco
Cini Stefano
Coppola Roberto
Ferro Gianclaudio
Galli Marcello
Garagnani Alberto
Giampieri Roberto
Magnani Marco
Mauri Alessandro
Mengoni Alberto
Petrella Carlo
Porceddu Cilione Carlo
Valli Monica
List of Personnel

LASER E ACCELERATORI
Baldacchini Giuseppe
Battaglia Marco
Bollanti Sarah
Bortoli Mario
Campana Ezio
Coleschi Salvatore
Di Lazzaro Paolo
Doria Andrea
Falchi Sandro
Fascetti Mario
Fastelli Antonio
Flora Francesco
Gallerano Gian Piero
Giabbai Italo
Giovanale Emilio
Giraldo Mario
Giubileo Gianfranco
Grossi Roberto
Mattogno Giovanni
Messina Giovanni
Mola Alessandro
Montevecchi Rosa Maria
Murra Daniele
Pace Angelo
Picardi Luigi
Rivelli Piergiorgio
Ronci Giuseppe
Ronisvalle Concetta
Schina Giovanni

VISPArelli Daniele
Zucchini Alberto

DISPOSITIVI OTTICI
PiegaAngela
Canave Luisa
Colucci Alessandro
Fiori Daniele
Gentili Angelo
Grasso Giuseppe
Masotti Enrico
Mercante Germana
Montecchi Marco
Moschetta Vincenzo
Nichelati Enrico
Sarto Francesca
Seaglione Salvatore

SPETTROSCOPIA APPLICAZIONI
LASER E MATERIALI SPECIALI
Renieri Alberto (acting)
Bacchi Enzo
Bordone Andrea
Borsella Elisabetta
Botti Sabina
Caponero Michele
Ciardi Roberto
Colao Francesco
D'Amato Francesco
Del Bugaro Dino
Di Fino Mario
DiImperio Roberto
Fantoni Roberta
Ferri De Collibus Mario
Fiasconaro Vincenzo
Fornarini Lucilla
Fornetti Giorgio
Garosi Franco
Giorigi Mariano
Giovagnoli Roberto
Lai Antonio
Laricciro Rosanna
Marcelli Stefano
Morici Luigi
Nagni Claudio
Nardelli Marco
Palucci Antonio
Poggi Claudio
Ribecco Sergio
Todino Stefano

MATHEMATICA APPLICATA E
METODOLOGIE COMPUTAZIONALI
PER L'INGEGNERIA
Ottaviani Pier Luigi
Balchini Elia Maria
Barbaro Mario
Cannigna Bruno
Cenacchi Giovanna
Cepraga Dan Gabriel
Cinti Paolo
Ferriani Stefano
Lorenzutta Silveria
Musumeci Alfio
Orru' Giuseppe
Pagnuti Simonetta
Ravagli Ermengildo
Rosetti Maurizio
Simonini Rolando
Taroni Adolfo
Toselli Gabriella
Vacari Marco
List of Personnel

UNITÀ FISICA TEORICA

Dattoli Giuseppe
Ciocci Franco
Giannessi Luca

Mezi Luca
Quattromini Marcello
Torre Amalia
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>AFEE</td>
<td>analog front-end electronics</td>
</tr>
<tr>
<td>AM</td>
<td>amplitude-modulated</td>
</tr>
<tr>
<td>AMERICA</td>
<td>Acceleratore per la Metrologia delle Radiazioni Ionizzanti</td>
</tr>
<tr>
<td>ANN</td>
<td>artificial neural network</td>
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<tr>
<td>AOM</td>
<td>active optics module</td>
</tr>
<tr>
<td>APD</td>
<td>avalanche photodiode</td>
</tr>
<tr>
<td>ARPA</td>
<td>Agenzia Regionale Protezione dello Ambiente</td>
</tr>
<tr>
<td>ASE</td>
<td>amplified spontaneous emission</td>
</tr>
<tr>
<td>ASiC</td>
<td>application-specific integrated circuit</td>
</tr>
<tr>
<td>ATC</td>
<td>Anderson-Tsao-Curnutte (theory)</td>
</tr>
<tr>
<td>BAS</td>
<td>beam angular stability</td>
</tr>
<tr>
<td>BET</td>
<td>Brunauer-Emmett-Teller (technique)</td>
</tr>
<tr>
<td>BTN</td>
<td>Baia Terranova</td>
</tr>
<tr>
<td>BUU</td>
<td>Boltzmann-Uehling-Uhlenbeck (collision integrals)</td>
</tr>
<tr>
<td>CARS</td>
<td>coherent anti-Stokes Raman scattering</td>
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<tr>
<td>CCD</td>
<td>charge coupled device</td>
</tr>
<tr>
<td>CINECA</td>
<td>Interuniversity Computation Centre of North-East Italy</td>
</tr>
<tr>
<td>CIRB</td>
<td>Centro Interdipartimentale per le Ricerche in Biotecnologie (Bologna University)</td>
</tr>
<tr>
<td>CMS</td>
<td>compact muon solenoid</td>
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<tr>
<td>CNR</td>
<td>Consiglio Nazionale di Ricerca</td>
</tr>
<tr>
<td>CSE</td>
<td>coherent spontaneous emission</td>
</tr>
<tr>
<td>CVD</td>
<td>chemical vapour deposition</td>
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### Abbreviations and Acronyms

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DFEE</td>
<td>digital front-end electronics</td>
<td>ICP</td>
<td>inductively coupled plasma</td>
</tr>
<tr>
<td>DFWM</td>
<td>degenerate four-wave mixing</td>
<td>id</td>
<td>internal diameter</td>
</tr>
<tr>
<td>DIAL</td>
<td>differential absorption lidar</td>
<td>ILL</td>
<td>Institute Laue Langevin - France</td>
</tr>
<tr>
<td>EC</td>
<td>electrochromic</td>
<td>IMS</td>
<td>Istituto Materiali Speciali (CNR)</td>
</tr>
<tr>
<td>ECAL</td>
<td>electromagnetic calorimeter</td>
<td>INF</td>
<td>Istituto Nazionale di Fisica della Materia</td>
</tr>
<tr>
<td>ECRH</td>
<td>electron cyclotron resonance heating</td>
<td>INFN</td>
<td>Istituto Nazionale di Fisica Nucleare</td>
</tr>
<tr>
<td>EGR</td>
<td>exhaust gas recirculation</td>
<td>INMRI</td>
<td>Istituto Nazionale di Metrologia delle Radiazioni Ionizzanti</td>
</tr>
<tr>
<td>ESA</td>
<td>European Space Agency</td>
<td>INTEGRAL</td>
<td>International Gamma-Ray Astrophysics Laboratory</td>
</tr>
<tr>
<td>ESTEC</td>
<td>European Space Research and Technology Centre</td>
<td>IORT</td>
<td>intra-operative radiation therapy</td>
</tr>
<tr>
<td>ETM</td>
<td>electron transparent mirror</td>
<td>ISS</td>
<td>Istituto Superiore di Sanità</td>
</tr>
<tr>
<td>EUM</td>
<td>equivalent uncoated material</td>
<td>ITER</td>
<td>International Thermonuclear Experimental Reactor</td>
</tr>
<tr>
<td>FBP</td>
<td>filtered backprojection</td>
<td>JAERI</td>
<td>Japan Atomic Energy Research Institute</td>
</tr>
<tr>
<td>FEL</td>
<td>free electron laser</td>
<td>JET</td>
<td>Joint European Torus - Culham - U.K.</td>
</tr>
<tr>
<td>FEM</td>
<td>finite-elements model</td>
<td>KdF</td>
<td>Kampé de Ferièt (polynomials)</td>
</tr>
<tr>
<td>FIR</td>
<td>far infrared</td>
<td>LAMEL</td>
<td>Institute for Material Technology and Electronic Components (CNR)</td>
</tr>
<tr>
<td>FOTO</td>
<td>Centro per lo Sviluppo di Tecnologie dei Materials per il Settore FOTOvoltaico e microelettronico (project)</td>
<td>LHC</td>
<td>large hadron collider</td>
</tr>
<tr>
<td>FOTO</td>
<td>Centro per lo Sviluppo di Tecnologie dei Materials per il Settore FOTOvoltaico e microelettronico (project)</td>
<td>LIBS</td>
<td>laser-induced breakdown spectroscopy</td>
</tr>
<tr>
<td>FW</td>
<td>first wall</td>
<td>lidar</td>
<td>light detection and ranging</td>
</tr>
<tr>
<td>FWHM</td>
<td>full width at half maximum</td>
<td>LIF</td>
<td>laser-induced fluorescence</td>
</tr>
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<td>FZK</td>
<td>Forschungszentrum Karlsruhe - Germany</td>
<td>LIM</td>
<td>limiter</td>
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<tr>
<td>GOE</td>
<td>Gaussian Orthogonal Ensemble</td>
<td>linac</td>
<td>linear accelerator</td>
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<td>GKSS</td>
<td>Forschungszentrum Geesthacht - Germany</td>
<td>LIVVS</td>
<td>laser in-vessel viewing system</td>
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<tr>
<td>GPS</td>
<td>global positioning system</td>
<td>LNB</td>
<td>Laboratoire Leon Brillouin - France</td>
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<tr>
<td>GSFUR</td>
<td>generalised self-filtering unstable resonator</td>
<td>LND</td>
<td>log-normal distribution</td>
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<td>GSO</td>
<td>gadolinium silicate ortho</td>
<td>LNT</td>
<td>liquid nitrogen temperature</td>
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<td>HVAC</td>
<td>heat-ventilation air conditioning</td>
<td>ML</td>
<td>monolayer</td>
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<tr>
<td>IBB</td>
<td>inboard baffle</td>
<td>MPI</td>
<td>message-passing interface</td>
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<td>IBIS</td>
<td>imager on-board integral satellite</td>
<td>MPW</td>
<td>multiproject wafer</td>
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<td>Interacting Boston Model-2</td>
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<td>Abbreviation</td>
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<td>NDT</td>
<td>nondestructive testing</td>
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<td>OB B</td>
<td>outboard baffle</td>
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<tr>
<td>PAM</td>
<td>pulse amplitude modulation</td>
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<td>PAS</td>
<td>positron annihilation spectroscopy</td>
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<td>PBUR</td>
<td>positive-branch unstable resonator</td>
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<tr>
<td>PCA</td>
<td>principal component analysis</td>
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<td>PCGM</td>
<td>preconditioned conjugate gradient method</td>
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<tr>
<td>PD</td>
<td>photodiode</td>
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<td>PET</td>
<td>positron emission tomography</td>
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<td>PFW</td>
<td>poloidal first wall</td>
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<td>PICsT</td>
<td>Pixellated Imaging CsI Telescope</td>
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<tr>
<td>PIN</td>
<td>positive intrinsic negative (photodiode)</td>
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<td>PIGE</td>
<td>particle-induced γ-ray emission</td>
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<td>PIXE</td>
<td>particle-induced x-ray emission</td>
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<td>PL</td>
<td>photoluminescence</td>
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<td>PLOZT</td>
<td>lanthanum-doped lead zirconate titanate</td>
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<td>phase-matching section</td>
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<td>passive optics module</td>
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<td>PSC</td>
<td>polar stratospheric cloud</td>
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<td>QTS</td>
<td>Quality Targeting System</td>
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<td>radar electronics</td>
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<td>rare gas halide</td>
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<td>RKE</td>
<td>relativistic kinetic equation</td>
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<td>rms</td>
<td>root mean square</td>
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<td>RMT</td>
<td>Random Matrix Theory</td>
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<tr>
<td>RT</td>
<td>room temperature</td>
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<td>SANS</td>
<td>small-angle neutron scattering</td>
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<tr>
<td>SASE</td>
<td>self-amplified spontaneous emission</td>
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<td>SDC</td>
<td>silicon drift chamber</td>
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<td>SCDTL</td>
<td>side-coupled drift tube linac</td>
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<td>SEM</td>
<td>scanning electron microscopy</td>
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<tr>
<td>sf</td>
<td>similarity factor</td>
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<tr>
<td>SIMD</td>
<td>single-instruction multiple-data</td>
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<tr>
<td>S/N</td>
<td>signal-to-noise</td>
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<tr>
<td>SOBP</td>
<td>spread-out Bragg peak</td>
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<td>SPECT</td>
<td>single-photon emission tomography</td>
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<td>SSOT</td>
<td>symmetric split operator technique</td>
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<td>STI</td>
<td>sawtooth instability</td>
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<td>SV</td>
<td>sensitive volume</td>
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<td>TDL</td>
<td>times diffraction limit</td>
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<td>transmission electron microscopy</td>
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<td>Institute for Extraterrestrial Radiation (CNR)</td>
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<td>tungsten inert gas (welding)</td>
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<td>Terapia Oncologica con Protoni (project)</td>
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<td>UNISAT</td>
<td>University Satellite (project)</td>
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<tr>
<td>UV</td>
<td>ultraviolet</td>
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<td>VASARI</td>
<td>Visual Arts System for Archiving and Retrieval of Images</td>
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<tr>
<td>VLSI</td>
<td>very large scale integration</td>
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<td>VME</td>
<td>Versa Module Europe</td>
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<tr>
<td>VPU</td>
<td>variably polarising undulator</td>
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<tr>
<td>VUV</td>
<td>vacuum ultraviolet</td>
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<td>VV</td>
<td>vacuum vessel</td>
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<td>XRD</td>
<td>x-ray diffraction</td>
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<tr>
<td>XUV</td>
<td>extreme ultraviolet</td>
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<td>YAP</td>
<td>yttrium aluminium perovskite</td>
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<tr>
<td>2D-ACAR</td>
<td>2-dimensional angular correlation of annihilation radiation</td>
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