

AU8708627 - AU8708657

INIS-mf--10998

C O N T E N T S

	<u>PAGE NO.</u>
PROGRAMME SUMMARY	1
PROGRAMME	2
ABSTRACTS	7
GENERAL INFORMATION	37
LIST OF PARTICIPANTS	41

S U M M A R YThursday 6th November, 1986

10.30 - 10.40 a.m.

Opening Remarks - Conference President
Prof. E.O. Hall (Uni. of Newcastle)SESSION I

10.40 - 12.20 p.m.

Hydrogenous and Biological Materials
Chairman:- Dr. P.W. Smith (Uni. of Tasmania)

12.20 - 1.40

CONFERENCE LUNCH - Stevens Hall

SESSION II

1.40 - 3.00

Industrial Applications - A.
Chairman:- Dr. D.R. McFarlane (Monash Uni.)

3.00 - 3.20

AFTERNOON TEA

SESSION III

3.20 - 4.40

Industrial Applications - B.
Chairman:- Dr. R.L. Davis (AINSE)SESSION IV

4.40 - 6.15

6.15 - 7.45

7.45 onwards

POSTER SESSION

CONFERENCE DINNER

Conference Address:- Prof. R.E. Collins
(Uni. of Sydney)Friday 7th November, 1986SESSION V

9.00 - 10.20 a.m.

Phase TransitionsChairman:- Prof. H. Freeman (Uni. of Sydney)

10.20 - 10.40

MORNING TEA

SESSION VI

10.40 - 12.20 p.m.

MagnetismChairman:- Dr. A.M. Stewart (A.N.U.)

12.20 - 1.20

CONFERENCE LUNCH - Stevens Hall

SESSION VII

1.20 - 2.40

Small Angle Neutron ScatteringChairman:- Dr. S.J. Campbell (Aust. Defence
Force Academy)

2.40 - 3.00

AFTERNOON TEA

SESSION VIII

3.00 - 4.00

New DevelopmentsChairman:- Prof. E.O. Hall (Uni. of Newcastle)CLOSING DISCUSSIONS

4.00 - 4.10

Prof. E.O. Hall - Conference President

Thursday 6th November, 1986 - Lucas Heights

<u>TIME</u>	<u>PAPER NO.</u>	
10.30 - 10.40		<u>Opening Remarks</u> - Prof. E.O. Hall (Uni. of Newcastle) Conference President
<u>SESSION I</u>		<u>HYDROGENOUS AND BIOLOGICAL MATERIALS</u> <u>Chairman:</u> Dr. P.W. Smith (Uni. of Tasmania)
10.40 - 11.20	1R <u>Review</u>	Applications of Neutron Scattering Techniques to Molecular Biology. <u>B.A. Cornell</u> (CSIRO), R. Knott (AAEC)
11.20 - 11.40	2	Weak Hydrogen Bonding in some Chlorometallates? <u>B.D. James</u> (La Trobe Uni.)
11.40 - 12.20	3R <u>Review</u>	Electrical Ordering in the Alkali Hydroxides. <u>T.J. Bastow</u> (CSIRO)
12.20 - 1.40		CONFERENCE LUNCH - Stevens Hall
<u>SESSION II</u>		<u>INDUSTRIAL APPLICATIONS - A.</u> <u>Chairman:</u> Dr. D.R. McFarlane (Monash Uni.)
1.40 - 2.20	4R <u>Review</u>	Industrial Applications of Neutron Scattering. <u>R.J. Hill</u> (CSIRO)
2.20 - 2.40	5	Quantitative Analysis of a Partially Stabilised Zirconia. R.J. Hill (CSIRO), <u>C.J. Howard</u> (AAEC), C.S. Blake, B.E. Reichert (ICI Aust)
2.40 - 3.00	6	Spin Reorientation in $Tm_2 Fe_{14} B$. R.K. Day, J.B. Dunlop (CSIRO), R.L. Davis (AINSE)
3.00 - 3.20		A F T E R N O O N T E A
<u>SESSION III</u>		<u>INDUSTRIAL APPLICATIONS - B.</u> <u>Chairman:-</u> Dr. R.L. Davis (AINSE)
3.20 - 4.00	7R <u>Review</u>	Transition-Metal Hydride Complexes: Characterisation and Role in Catalysis. <u>G.B. Robertson</u> (ANU)
4.00 - 4.20	8	Determination of Hydrogen Content by Polarization Analysis. <u>J.C. Osborn</u> , T.J. Hicks (Monash Uni.)
4.20 - 4.40	9	Measurements of Residual Stress by Neutron Powder Diffraction. <u>C.J. Howard</u> (AAEC), T.F. Smith, P. Lambrineas, T.R. Finlayson, J.R. Griffiths (Monash Uni.)

Thursday 6th November, 1986 - Lucas Heights

<u>TIME</u>	<u>PAPER NO.</u>	
<u>SESSION IV</u>		<u>POSTER SESSION</u>
4.40 - 6.15	10	Thermal Phase Transformations in Sodium Sulphate and Sodium Chromate. <u>J.K. Nimmo</u> (Uni. of Queensland)
" "	11	Rietveld Refinement of Ternary Gamma Brass Structures and Associated Binary Alloys. <u>E. Kisi</u> (Uni. of Newcastle)
" "	12	Neutron Small Angle Scattering from Nucleating ZSM-5 Catalysts. <u>L. Iton, S. Henderson, J.W. White</u> (ANU)
" "	13	Diffuse Scattering on the Niobium-Deuterium System. <u>J.C. Osborn, T.J. Hicks</u> (Monash Uni.)
" "	14	Polarization Analysis using a Time of Flight Technique. <u>J.C. Osborn, L.D. Cussen, T.J. Hicks</u> (Monash Uni.)
" "	15	Powder Refinements of Larger Structures. <u>J.C. Taylor, S.A. Miller</u> (CSIRO)
" "	16	The Structure of KSCN by Powder Neutron Diffraction. <u>D.J. Cookson</u> (Monash Uni.), <u>M.M. Elcombe</u> (AAEC)
" "	17	Anomalous Line Broadening in HRPD Patterns of Rubidium Deuterioxide. <u>M.M. Elcombe, C.J. Howard</u> (AAEC).
" "	18	Neutron Diffraction Studies of Super-Cooled Liquid Heavy Water. <u>M.A.M. Sufi</u> (Nuc. Energy Unit, Puspati, Malaysia), <u>J.C. Dore</u> (Uni. of Kent, Cant. England)
6.15		CONFERENCE DINNER
7.45		<u>Conference Address:-</u> Prof. R.E. Collins (Uni. of Sydney)

Friday 7th November, 1986 - Lucas Heights

<u>TIME</u>	<u>PAPER NO.</u>	
<u>SESSION V</u>		
		<u>PHASE TRANSITIONS</u>
		<u>Chairman:</u> Prof. H. Freeman (Uni. of Sydney)
9.00 - 9.40	19R <u>Review</u>	Neutron Scattering from Premartensitic Metal Alloys. <u>T.R. Finlayson</u> (Monash Uni.)
9.40 - 10.00	20	Phase Transitions and Ferroelectricity in Potassium Iodate. <u>B.W. Lucas</u> (Uni. of Qld)
10.00 - 10.20	21	The Lattice Dynamics of the Alkali Thiocyanates. <u>D.J. Cookson</u> , <u>T.R. Finlayson</u> (Monash Uni.) <u>M.M. Elcombe</u> (AAEC)
10.20 - 10.40		M O R N I N G T E A
<u>SESSION VI</u>		
		<u>MAGNETISM</u>
		<u>Chairman:</u> Dr. A.M. Stewart (A.N.U.)
10.40 - 11.20	22R <u>Review</u>	Doing More with Polarised Neutrons <u>T.J. Hicks</u> (Monash Uni.)
11.20 - 11.40	23	The Distribution of Magnetic Moment in Antiferromagnetic Fe Mn_{1-x} Alloys. <u>S.J. Kennedy</u> , <u>T.J. Hicks</u> (Monash Uni.)
11.40 - 12.00	24	The Distribution of Magnetic Moment in Ferromagnetic $\text{Fe}_{3-x}\text{Mn}_x\text{Si}$ Alloys. <u>H.Kepa</u> , <u>T.J. Hicks</u> (Monash Uni.)
12.00 - 12.20	25	Convalence, Transition Metal Complexes, and Polarised Neutron Diffraction. <u>P.A. Reynolds</u> , <u>B.N. Figgis</u> , <u>R. Deeth</u> (Uni. of W.A.)
12.20 - 1.20		CONFERENCE LUNCH - Stevens Hall
<u>SESSION VII</u>		
		<u>SMALL ANGLE NEUTRON SCATTERING</u>
		<u>Chairman:-</u> Dr. S.J. Campbell (Aust. Defence Force Academy)
1.20 - 2.00	26R <u>Review</u>	Neutron Scattering in Surfactant Systems. <u>T.N. Zemb</u> (C.E.N. Saclay, France)
2.00 - 2.20	27	The Malaysian Neutron Beam Research Program <u>A.G. Ramli</u> (Kompleks Puspatti, Bangi, Malaysia)
2.20 - 2.40	28	Small-Angle Neutron Scattering at Lucas Heights-Past, Present and Future. <u>E.M. Gray</u> (Uni. of Qld)
2.40 - 3.00		A F T E R N O O N T E A

Friday 7th November, 1986 - Lucas Heights

<u>TIME</u>	<u>PAPER NO.</u>	
<u>SESSION VIII</u>		<u>NEW DEVELOPMENTS</u>
		<u>Chairman:-</u> Prof. E.O. Hall (Uni. of Newc.)
3.00 - 3.40	29R <u>Review</u>	The Neutron Kikuchi Effect. <u>M.M. Elcombe</u> (AAEC)
3.40 - 4.00	30	Plans for the Future Development of Neutron Scattering Facilities on HIFAR. R.L. Davis (AINSE), C.J. Howard (AAEC)
<u>CLOSING DISCUSSIONS</u>		Prof. E.O. Hall - Conference President
4.00 - 4.10		

ABSTRACTS

APPLICATIONS OF NEUTRON SCATTERING TECHNIQUES
TO MOLECULAR BIOLOGY

by

B.A. Cornell¹ and R. Knott²

¹ Commonwealth Scientific and Industrial
Research Organisation
North Ryde, N.S.W., Australia

² Australian Atomic Energy Commission
Lucas Heights, N.S.W., Australia

Abstract

Neutron diffraction has provided a unique probe into the organisation of biological systems. In particular it has been employed to study a range of synthetic and biological membranes. An essential part of this work has been the development of techniques to produce aligned multilamellar membrane stacks. Multilamellar membranes can occur naturally (the myelin sheath of nerve fibres, the grana stacks in the photosynthetic apparatus of green plants and the rod cells lining the retina of the eye) or may be formed from either synthetic or extracted organic material (the retinal rod outer segment membranes, the photosynthetic membrane patches of the bacteria Halobacterium halobium, the gap junction membranes of nerve synapses or various lipids with or without proteins).

Appropriate analysis of the neutron diffraction pattern produced by these stacks yields the neutron scattering density distribution perpendicular to the plane of the membrane. Deuterium-hydrogen isotope exchange provides a convenient solution to the phase problem. The large difference between the coherent scattering amplitude of hydrogen and deuterium is used in an analogous manner to the heavy atom phase shift in X-ray crystallography. A similar approach has been used to contrast the scattering amplitude of Ca^{44} and Ca^{40} across synthetic membranes, and thus the distribution of Calcium ions. The membrane distribution of many molecules has now been reported, including cholesterol, small hydrocarbons such as hexane, and intrinsic membrane proteins such as cytochrome b_5 and bacteriorhodopsin.

The installation of a linear position sensitive detector and computer based data acquisition system have very significantly improved the facilities on the AAEC HIFAR reactor for small angle diffraction from biological membranes. Each reflection is now collected in $\omega/2$ - θ space. Appropriate integration of the data dramatically improves the statistics of each reflection.

Neutron diffraction experiments have been undertaken at Lucas Heights to determine the location of the ionophore, gramicidin A, and the electron/proton carrier, ubiquinone, within phospholipid membranes. These studies provide structural information which could only be obtained using neutron diffraction.

WEAK HYDROGEN BONDING IN SOME CHLOROMETALLATES?

by

B.D. James

Dept. of Chemistry, La Trobe University, Bundoora, Vic.

Abstract

In comparison with $-O-H\cdots O$ or $-F-H\cdots F$ interactions, the $-N-H\cdots Cl$ hydrogen bonding interaction is generally regarded as rather weak. On the other hand, in the chlorostannate (IV) series, such interactions are not only a source of the bifurcated variety of hydrogen bonds but examples are found in which the $SnCl_6^{2-}$ octahedra have been induced into marked distortions. The energies involved appear to be very large in such processes, suggesting that the hydrogen bonds responsible are not weak after all.

In an attempt to study these interactions in a systematic manner, two series of compounds are being investigated: substituted pyridinium salts of chlorothallates (III) and chlorostannates (IV). The planar pyridinium ring is sufficiently large to impose "open-ness" on the solid structure such that the hydrogen bonds are able to come about as a result of intrinsic bonding interactions rather than as a result of structural compactness. Also, the availability of substituted pyridines provides a wide range of basicities at the ring nitrogen atom, which allows for the variation of the partial positive charge on the acid proton. The Group IIIB metal thallium provides a series of anions $TlCl_4^-$, $TlCl_5^{2-}$ and $TlCl_6^{3-}$ on which the partial negative charge on the chlorine is successively increased. In this way, a range of compounds having a spectrum of hydrogen bond strengths may be obtained which can be investigated by methods such as ^{14}N and ^{35}Cl NQR, differential scanning calorimetry and infrared spectroscopy. It is expected that a correlation will exist between such bond strength measurements and the $-N-H\cdots Cl$ bond parameters measured via powder neutron diffraction.

ELECTRICAL ORDERING IN THE ALKALI HYDROXIDES

by

T.J. Bastow

CSIRO Division of Chemical Physics, Clayton 3168.

Abstract

Ferroelectricity in insulators is analogous to ferromagnetism in metals; ordering of electric dipoles in the former corresponding to ordering of electronic spins in the latter.

We have discovered in the alkali hydroxides MOH and their deuterated analogues MOD (M: Na,K,Rb,Cs) an entirely new group of electrically ordered compounds exhibiting both ferroelectric (FE) and antiferroelectric (AFE) ordering. The latter is characterised by antiparallel ordering of the electric dipoles. The transitions were found by nuclear resonance, dielectric constant and DTA measurements. The structures were determined by high-resolution powder neutron diffraction.

At present we have complete structures for the sodium and potassium and caesium compounds, both above and below the ordering temperature. For NaOD, KOH(D) and CsOH(D) the nature of the ordering is antiferroelectric; NaOH being anomalous in this respect and remaining in the room temperature orthorhombic phase down to at least 6K. A determination of the structure of the electrically ordered phases of RbOH(D) is in progress. It has been established that the stable phase of both compounds at 77K is ferroelectric.

A common characteristic of all these structures is the existence of zig-zag chains of oxygen atoms running in the [010] direction (the unique b-axis in the monoclinic phases). Displacement of the H(D) atoms in the b-direction relative to the oxygen chain gives the latter an electrical polarisation.

A review will be given of the structures and properties of these compounds and the nature of the phase transitions to the ordered state.

INDUSTRIAL APPLICATIONS OF NEUTRON SCATTERING

R.J. HillCSIRO Division of Mineral Chemistry
PO Box 124, Port Melbourne, Vic 3207, AustraliaAbstract

We are entering an era when technological progress is limited only by our ability to discover and fabricate new materials. It is the business and responsibility of Industry to invent and develop these materials (either alone or in collaboration with others) and then to produce and market them profitably.

The utilization and optimization of the properties of these commodities follows most effectively from a detailed knowledge and understanding of the positions and energetics of their constituent atoms, generally obtained from experiments involving the scattering of electrons or electromagnetic radiation. Most of these techniques are now commonplace in Industrial laboratories. However, in the last decade or so, it has become clear that neutrons have a unique and complementary/synergistic role to play as a probe for the study of the complex materials and processes on which future technologies will be based. The exciting new dimensions of this role are founded on the neutron's large penetration depth, light-element sensitivity, magnetic moment and wide range of energies, in company with minimal sample damage.

The present talk will highlight properties of condensed matter that are of significance in Industrial applications and can be accessed only, or far more easily, by neutron scattering experiments. In particular, examples will be given of studies of microporosity in coals, creep cavitation in metals and ceramics, textures in cold-worked metals, residual stress in welds, hydrogen embrittlement, metal hydrides, battery failure modes, crystallization of amorphous materials, phase nucleation and growth in cement, structure of catalysts, surfactants and polymers, diffusion, phase transitions, ionic conduction, minerals characterization, disposal of nuclear wastes, silicon doping by transmutation, quality control in computer memory units, and the authentication of artefacts.

Since the above scattering experiments require neutron sources of substantial intensity, objects intended for interrogation in Australia must be studied at Lucas Heights. The required expertise and much of the instrumentation is already in place there; all that remains is for the Industrialists and the Nuclear Scientists to get together.

QUANTITATIVE ANALYSIS OF A PARTIALLY STABILISED ZIRCONIA

by

C. S. Blake and B. E. Reichert
ICI Australia Research Group, Ascot Vale

R. J. Hill
CSIRO Division of Mineral Chemistry, Port Melbourne

and

C. J. Howard
Applied Physics Division,
Australian Atomic Energy Commission, Lucas Heights

Abstract

Zirconia (ZrO_2) has three well known phases - a monoclinic phase at room temperature, a tetragonal phase above $1200^\circ C$, and a cubic phase stable above $2370^\circ C$. By the use of certain additives, the tetragonal and cubic phases can be stabilised at room temperature. It is also possible to produce partially stabilised zirconias (PSZs), which are toughened ceramics attracting great interest.

The PSZ ceramics may contain all three phases of ZrO_2 , and it is certainly desirable to know the proportions of these three phases in any PSZ. This information should be derivable from the neutron powder diffraction pattern. Here we report the quantitative analysis of a magnesium partially stabilised zirconia (Mg-PSZ) using high resolution neutron powder diffraction. We outline the methods we have developed for analysing the diffraction patterns, and compare our results with those obtained using X-ray techniques.

SPIN REORIENTATION IN $Tm_2 Fe_{14} B$

by

R.K. Day, J.B. Dunlop and R.L. Davis
CSIRO and AINSEAbstract

The magnetic structures of $Tm_2 Fe_{14} B$ above and below its spin reorientation temperature have been obtained from high resolution neutron powder diffraction. This work supports a model of $Tm_2 Fe_{14} B$ as a basal plane ferrimagnet at 294K and a c-axis ferrimagnet above 340K.

This contribution to our understanding of isostructural $R_2 Fe_{14} B$ compounds is of particular significance for $Nd_2 Fe_{14} B$ which has outstanding permanent magnetic properties. The latter material is currently being developed for commercial production in Australia at the CSIRO Applied Physics Division in Sydney.

TRANSITION-METAL HYDRIDE COMPLEXES: CHARACTERISATION
AND ROLE IN CATALYSIS

by

G.B. Robertson,

Research School of Chemistry
Australian National University
GPO Box 4, Canberra, A.C.T. 2601

Abstract

Transition-metal hydride complexes are of importance as initiators or intermediates in both catalytic and stoichiometric reactions. Commercially significant examples include $\text{CoH}(\text{CO})_4$ and $\text{RhH}(\text{CO})(\text{PPh}_3)_3$ in the hydroformylation or 'Oxo' process [olefins \rightarrow aldehydes], $\text{RuHCl}(\text{PPh}_3)_3$ and $\text{RhH}_2\text{Cl}(\text{PPh}_3)_3$ in olefin hydrogenation, and $\text{NiH}(\text{CN})\{\text{P}(\text{O}-\text{Ar})_3\}_3$ in olefin hydrocyanation.

Modern transition-metal hydride chemistry dates from ca. 1955 with the syntheses of $\text{ReH}(\text{C}_5\text{H}_5)_2$ ¹ and $\text{MH}(\text{C}_5\text{H}_5)(\text{CO})_3$ (M=Cr, Mo)² and, shortly thereafter, of trans-PtHCl(PEt₃)₂³. The first successful location of a hydride ligand [in $\text{RhH}(\text{CO})(\text{PPh}_3)_3$]⁴ by X-ray diffraction was reported in 1963. The first neutron diffraction studies [of K_2ReH_9 and $\text{MnH}(\text{CO})_5$]^{5,6} were reported in 1964 and 1969. Many hundred of such complexes are now known and instances of terminal, bridging (μ_2 and μ_3) and encapsulated (interstitial) hydride ligands have been fully characterised by diffraction methods.

Encapsulated hydrogens have similar environments to those in the binary metallic hydrides and the triply bridging μ_3 -hydrides found in metal-clusters have parallels in chemisorption. Complexes involving weak M...H-C interactions have been known for some time. Recently a new class of complexes involving 'strong' M-H-C interactions has attracted interest because of possible catalytic implications. M-H and C-H distances are each ca. 0.1Å longer than for terminally bound hydrogen.^{7,8} Examples of these and other relevant complexes will be described.

References

- [1] G. Wilkinson & J.M. Birmingham, J. Am. Chem. Soc., 1955, 77, 3421.
- [2] E.O. Fischer et al., Z. Anorg. Allg. Chem., 1955, 282, 47.
- [3] J. Chatt et al., Proc. Chem. Soc., 1957, 343.
- [4] S.J. La Placa & J.M. Ibers, J. Am. Chem. Soc., 1963, 85, 3501.
- [5] A.P. Ginsberg et al., Inorg. Chem. 1964, 3, 558.
- [6] J.M. Ibers et al., Inorg. Chem., 1969, 8, 1928.
- [7] J.M. Williams et al., J. Am. Chem. Soc., 1980, 102, 981.
- [8] J.M. Williams et al., Science, 1983, 220, 197.

DETERMINATION OF HYDROGEN CONTENT BY POLARIZATION ANALYSIS

by

J. C. Osborn, T. J. HicksDepartment of Physics
Monash University
Clayton Vic. 3168.

and

R. J. Hill

Division of Mineral Chemistry
C.S.I.R.O.
Box 124, Port Melbourne Vic. 3207.Abstract

The large spin-incoherent cross-section of hydrogen can be used to determine the bulk hydrogen content of materials by neutron scattering [1]. Polarization analysis is required to distinguish the scattering from hydrogen, two-thirds of which is neutron spin-flip scattering, from other nuclear scattering which occurs without spin-flip. An alternative method of hydrogen determination by neutron attenuation measurements [2] suffers from errors due to an inability to distinguish between these types of scattering.

The hydrogen contents of some lead oxide samples have been determined using polarization analysis. The method has also been used to determine the hydrogen fraction in the deuterium in deuterated niobium crystals. The technique is applicable to a wide range of materials.

References

- [1] O. Moze, T. J. Hicks and A. C. McLaren, Phys. & Chem. Miner. 5, 309-314 (1980).
- [2] P. T. Moseley, J. L. Hutchison et al., J. Electrochem. Soc. 130, 829-834 (1983).

MEASUREMENTS OF RESIDUAL STRESS
BY NEUTRON POWDER DIFFRACTION

by

C.J.Howard,# T.F. Smith,*
P. Lambrineas,* T.R. Finlayson,* J.R.Griffiths[†]#Applied Physics Division,
Australian Atomic Energy Commission*Department of Physics
Monash University[†]Department of Materials Engineering
Monash UniversityAbstract

Neutron powder diffraction techniques have been employed in the investigation of residual stress in a number of model systems. The increased penetration of neutrons compared with that of X-rays provides the means for the direct measurement of stress in bulk material, but it also leads to the need for particular care in the interpretation of the data. Results from neutron powder diffraction have been compared with results obtained using other techniques.

The residual stresses in a thin (4mm) thermally stressed steel plate have been studied in considerable detail. The measurements have been made using a neutron diffraction version of the well known (X-ray) $\sin^2\psi$ technique. Measurements have been made in both transmission and reflection geometries. Stress measurements made in a particular sample orientation are reproducible to within ± 10 MPa. The principal stresses determined from a series of such measurements have an uncertainty of ± 30 MPa, which is comparable to the ± 20 MPa commonly quoted for the X-ray technique.

Further measurements have been made on steel plates fitted with normal and inclined plugs, and on alloys containing second phase precipitates.

**THERMAL PHASE TRANSFORMATIONS IN
SODIUM SULPHATE AND SODIUM CHROMATE**

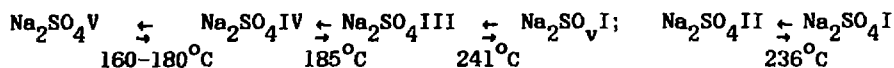
by

J. K. Nimmo

Department of Physics
University of Queensland
St. Lucia, Australia

Abstract

Sodium sulphate has complicated and controversial thermal phase transformation behaviour. In 1929 and 1930 Kracek and various collaborators (1) published four papers detailing their investigations (thermal analysis, density studies, dilatometry and x-ray analysis). They proposed the following transformation system:



The inversions were found to exhibit varying degrees of promptness, depending largely on the presence or absence of traces of moisture, or other catalysts. The thoroughly dry salt tended to persist in metastable modifications. They suggested $\text{Na}_2\text{SO}_4^{\text{II}}$ and $\text{Na}_2\text{SO}_4^{\text{IV}}$ may be pressure forms unstable at atmospheric pressure; their x-ray powder diffraction studies revealed no evidence of these phases.

Since the work of Kracek et al. there have been many conflicting claims about how many and which phases occur at atmospheric pressure (up to 8 phases), what factors influence their occurrence, which transitions are reversible, what are the transition temperatures and what are the appropriate crystal systems, space groups and structures.

The present study aims to achieve some clarification of the situation using neutron and x-ray single crystal and powder diffraction techniques. Na_2CrO_4 is thought to have two phases which are isostructural with Na_2SO_4 phases and so it too is being studied, principally as an aid to understanding the Na_2SO_4 transformations.

To date the structures of $\text{Na}_2\text{SO}_4^{\text{V}}$ (2 temperatures) and $\text{Na}_2\text{CrO}_4^{\text{II}}$ (2) have been determined from neutron single crystal data, and the structure of $\text{Na}_2\text{SO}_4^{\text{III}}$ from neutron powder data using profile refinement techniques. These same techniques are currently being used in an attempt to tease a structure from marginal (only a few weak peaks observable) high resolution (neutron) powder diffractometer data for $\text{Na}_2\text{SO}_4^{\text{I}}$; the complication is considerable disorder of the SO_4 . Many neutron powder scans have been made searching for other phases (II and IV particularly) but no compelling evidence for their existence has been found.

-
- (1) F. C. Kracek et al., *J Phys.Chem.*(1929)33, 1281-1303, 1304-1308; (1930)34, 188-206, 1741-1744.
(2) J. K. Nimmo, *Acta Cryst.* (1981)B37, 431-433.

17.

RIETVELD REFINEMENT OF TERNARY GAMMA BRASS STRUCTURES
AND ASSOCIATED BINARY ALLOYS

by

E. Kisi

Chemical & Materials Engineering Dept.
University of Newcastle

Abstract

The prototypical gamma brass Cu_5Zn_8 is b.c.c. (space group $I\bar{4}3m$) whilst the phase in the Cu-Al alloy system exhibiting a gamma brass structure, Cu_9Al_4 , is primitive (space group $P\bar{4}3m$). In the ternary Cu-Al-Zn system, a continuous intermediate phase links the two.

High resolution neutron powder diffraction data as well as some single crystal data have been collected from a series of alloys spanning the ternary phase field.

Of interest are the sites where substitution of Zn for Cu and Al in the Cu_9Al_4 structure occurs as the composition is progressively varied between Cu_9Al_4 and Cu_5Zn_8 with a view to determining a rationale for the occurrence of this structure type and comparison with current thinking on intermetallic compound formation.

Rietveld analysis of the powder data is shown to give promising results in this area.

NEUTRON SMALL ANGLE SCATTERING
FROM NUCLEATING ZSM-5 CATALYSTS

by

L. Iton, S. Henderson, J.W. White

Research School of Chemistry
Australian National UniversityAbstract

ZSM-5 is a highly siliceous material closely related to the new form of silica-silicalite which possesses regular criss-cross channels accessible to hydrocarbon molecules. In the ZSM-5 form a small quantity of substituted aluminium leads to important catalytic activity and is, for example, the basis of the Mobil methanol-petrol process.

There are rival mechanisms for the production of this catalyst but it appears that for both of the two main contenders -

- a. The solid hydro gel reformation and
- b. The liquid phase transport mechanism

there is a key role played by template molecules - typically the tetropropyl ammonium ion.

Neutron small angle scattering has been shown by us in reference 1 to be a promising way of elucidating the role of the template in both the above mechanisms.

The poster will present evidence for template action on silicate gels and will show how the kinetics and the competition of competing zeolite products is modified in the early stages of ZSM-5 growth in the presence of template molecules.

Ref. 1 L.Iton, S.Henderson and J.W.White, Proc Zeolite Conf. Japan, August 1986

DIFFUSE SCATTERING ON THE NIOBIUM-DEUTERIUM SYSTEM

by

J. C. Osborn and T. J. HicksDepartment of Physics
Monash University
Clayton Vic. 3168.Abstract

The absorption of hydrogen by metals is important for two reasons: the embrittlement caused by hydrogen, and the possibility of storing hydrogen in metals for fuel. The niobium-hydrogen system is considered a prototype for bcc metal hydrides. The low concentration, alpha phase of this system is a disordered solution of deuterium in the tetrahedral interstitial sites of the niobium lattice. The displacement field of niobium atoms around a deuterium atom and the possibility of short range ordering of the deuterium can both be studied by diffuse elastic neutron scattering. The displacement field has previously been studied by diffuse neutron scattering [1,2] and other techniques [3].

We present diffuse scattering measurements on single crystals containing 2.5 at.% deuterium, obtained with the LONGPOL diffractometer at Lucas Heights. Time of flight experiments showed both elastic and inelastic scattering to be present. The latter was removed by a beryllium filter. We are attempting to model the system using Kanzaki forces, applied to niobium near neighbours of the deuterium atom, and short range order parameters.

References

- [1] G. S. Bauer, W. Schmatz and W. Just, Proc. 2nd Int. Cong. on Hydrogen in Metals, Paris, 1977, paper 2C15.
- [2] H. Dosch and J. Peisl, Phys. Rev. Letts. 56, 1385-1388 (1986).
- [3] J. Peisl, Festkorperprobleme XXIV, 45-72 (1984).

POLARIZATION ANALYSIS USING A TIME OF FLIGHT TECHNIQUE

by

J. C. Osborn, L. D. Cussen and T. J. HicksDepartment of Physics
Monash University
Clayton Vic. 3168.Abstract

The LONGPOL diffractometer at Lucas Heights is a polarization analysis instrument which uses a neutron spin flipper as a time of flight (TOF) chopper. The TOF spectrum is obtained by gating the flipper with a pseudo-random sequence. The difference between non-spin-flip and spin-flip cross-sections is obtained as a function of energy. The technique is analogous to the use of a 'statistical' rotating disc chopper for TOF experiments. It differs from that method in that separation of the scattering into spin-flip and non-spin-flip cross-sections is achieved and that the neutron beam is used continuously, with the polarization direction being alternated by the flipper instead of the beam being chopped.

Two methods of analysis of such spectra to determine the spin-flip and non-spin-flip cross-sections will be discussed. The first relies on calculating the area under each peak while the second involves fitting the spectrum with a lineshape comprising the convolution of the pseudo-random sequence autocorrelation function with the wavelength distribution of the incident beam. Both methods have been tested using spectra collected on vanadium and both give a spin-flip scattering fraction close to the expected value.

POWDER REFINEMENTS OF LARGER STRUCTURES

J.C. Taylor and S.A. Miller
Division of Energy Chemistry
CSIRO Private Mail Bag 7,
Sutherland, NSW, 2232, Australia.

Refinement of large structures is of interest in neutron scattering where high-resolution neutron diffractometers have been developed. So far, the largest structure refined by powders is TPA-ZSM5 (Baerlocher 1983), with 49 atoms in the asymmetric unit (an X-ray analysis, but the principle is the same except for the scattering factors). We have refined both H^+ -ZSM5 and coked ZSM5 to $R(\text{profile}) = 0.13$ (38 atoms in the asymmetric unit) with X-ray powder data ($CoK\alpha_1$ and α_2) by the method of Toraya et al. (1984). Refinements of ZSM5- C_6D_6 by the same method (124 atoms in the asymmetric unit), with neutron powder data collected at 77 K, gives at this stage $R(\text{profile}) = 0.2$ and $R(F) = 0.07$.

THE STRUCTURE OF KSCN BY POWDER NEUTRON DIFFRACTION

by

D. J. Cookson[†] and M. M. Elcombe*[†]Physics Department, Monash University
*Applied Physics Division,
Australian Atomic Energy CommissionAbstract

There is conflicting data in the literature concerning the lattice parameters and internal coordinates of potassium thiocyanate (KSCN). A room temperature, high resolution neutron powder pattern has been collected and used to refine the structure. The lattice parameters agree with our own X-ray measurements. The internal coordinates of the carbon and nitrogen atoms are significantly different from the X-ray values. This is correlated with the fact that these atoms are weak X-ray scatterers when compared with potassium and sulphur, but are strong neutron scatterers. The structural details and some interatomic distances will be presented.

ANOMALOUS LINE BROADENING IN HRPD PATTERNS
OF RUBIDIUM DEUTEROXIDE

by

M. M. Elcombe and C. J. HowardApplied Physics Division
Australian Atomic Energy Commission
Lucas Heights Research LaboratoriesAbstract

Rubidium deuteroxide (RbOD) undergoes a phase transition at ~ 270 K and another at ~ 308 K. The phase which is found between 270 K and 308 K is monoclinic. We have observed that the high resolution neutron powder diffraction pattern recorded from this monoclinic phase of RbOD (at room temperature) shows peak broadening which depends markedly on the reflection indices. We have postulated that, with $c \sin \beta$ remaining constant, the value of β has a significant range of values ($\Delta\beta$). The contribution from $\Delta\beta$ to the peak width has been incorporated into a Rietveld refinement of the observed neutron pattern, and excellent agreement obtained.

NEUTRON DIFFRACTION STUDIES OF
SUPER-COOLED LIQUID HEAVY WATER

by

M.A.M. Sufi* and J.C. Dore

University of Kent, Canterbury, England
*Permanent address; UTN, Puspati, MalaysiaAbstract

Neutron diffraction experiments have been carried out on liquid heavy water in the temperature ranges -14°C to 36°C , using the D4B diffractometer at the Institut Laue-Langevin, Grenoble, France. Data has been collected to a high statistical accuracy out to large Q -values. A first-order difference function method had been used to determine the changes in the molecular structure factor of heavy water with temperature. Fourier transformation is used to give the changes in the real-space distribution functions, $\Delta d_L(r,t)$. The result obtained is in good agreement with previous observations from an earlier experiment and give a more precise indication of the structure variations. The present analysis shows that the inter-molecular OD and DD separations increase as the temperature changes from 11°C , which corresponds to maximum density of liquid D_2O . The variation in the hydrogen bond configurations for the super-cooled liquid may be explained by the present of 'bifurcated' hydrogen bonds.

NEUTRON SCATTERING FROM PREMARTENSITIC
METAL ALLOYS

by

T.R. Finlayson

Department of Physics
Monash University
Clayton, Australia

Abstract

There is an increasing body of experimental data concerning the physical properties of materials exhibiting martensitic transformations to suggest that the premartensitic regime (usually the temperature range slightly above the martensite start temperature, M_s) is a unique one. Studies of properties in this regime have provided an improved understanding of transformation mechanisms and kinetics.

Specifically, from the study of neutron scattering from the metal and metal alloy martensitic materials two distinct patterns of behaviour have emerged involving the softening of either zone-centre phonons or phonons with wave vectors out into the zone. In some of the latter cases the precise soft phonon mode can be related to the martensite crystallography.

This paper will comprise a review of some of the recent data. Critical comment, by way of comparisons among the different metal systems will be attempted.

THE LATTICE DYNAMICS OF THE ALKALI THIOCYANATES

by

D.J. Cookson^{*}, M.M. Elcombe[†], T.R. Finlayson^{*}

^{*}Department of Physics, Monash University, Vic.

[†]A.A.E.C. Lucas Heights Research Laboratories N.S.W.

Abstract

The spherical cations and 'rod like' molecular anions in the lattice structure of potassium thiocyanate [1] make the lattice dynamics of this crystal interesting.

Phonon measurements have been made on a large single crystal of potassium thiocyanate on the triple axis spectrometer at Lucas Heights. These experimental data have been used in developing a uniaxial nearest neighbour force-constant model for the vibrational modes of the crystal.

The frequencies calculated from the model will be compared with those determined experimentally and possible ways of improving the model will be discussed.

References

[1] Akers, C., Peterson, S.W., Willet, R.D., Acta Cryst.

B24 1125-1126 (1968)

Session V

Friday 10.00 - 10.20 a.m.

DOING MORE WITH POLARISED NEUTRONS

by

T. J. HicksDepartment of Physics
Monash University
Clayton 3168Abstract

The neutron scatters from condensed matter primarily by two interactions; that of the neutron with the nucleus, and that with the local magnetisation. These are, at least partly, vector interactions and give rise to neutron spin flipping on scattering. To completely characterise these interactions, it is necessary to determine polarisation before and after scattering. In particular, with the neutron polarisation along the scattering vector, all magnetic scattering is with spin flip.

For the first almost fifteen years that they were routinely available, polarised beams were used exclusively for measuring the two cross-sections with polarisation parallel and antiparallel to a preferred direction in the sample. Usually the sample was ferromagnetic and rarely the sample was an aligned paramagnet.

For about the last sixteen years the polarisation of the scattered beam has also been measured by various groups. LONGPOL, at Lucas Heights, has been one of the major sources of the polarisation analysis data. This data has included magnetic cross-sections from paramagnets, spin glasses, and antiferromagnets, which have been isolated from the rest of the scattering. It has also included the measurement of the spin part of the incoherent scattering from several nuclei, as well as the determination of hydrogen content using the proton's large spin incoherent cross-section. LONGPOL has also pioneered the use of time of flight spectroscopy incorporating polarisation analysis, tagging the beam by fast pulsing of the polarisation.

It is important to isolate the magnetic scattering in cases where it, and the nuclear scattering which it overlays, can both vary with scattering vector. This happens in binary magnetic alloys, of which the spin glass CuMn, and the antiferromagnet Mn-Ni are examples which will be discussed. The method of time of flight analysis with polarisation analysis and its application to the measurement of low energy antiferromagnons will also be described.

THE DISTRIBUTION OF MAGNETIC MOMENT IN
ANTIFERROMAGNETIC $\text{Fe}_x\text{Mn}_{1-x}$ ALLOYS

by

S J. Kennedy, and T. J. Hicks

Department of Physics
Monash University
Clayton 3168

ABSTRACT

γ -Fe-Mn is a face centred cubic, antiferromagnetic alloy. The magnetic structure has been shown to consist of four magnetic sublattices with spins all making a common angle with respect to the cube axis [1], and more recently [2] this has been narrowed down to either $\langle 110 \rangle$ or $\langle 111 \rangle$ spin structures.

The nuclear and magnetic neutron bragg scattering, and the nuclear and magnetic neutron diffuse cross-sections have been measured for a series of polycrystalline alloys with $x = 0.66, 0.58, 0.50, 0.42$. In these alloys the γ phase is stable at 77 Kelvin.

The elastic diffuse cross-sections were isolated using time of flight spectroscopy. Polarisation analysis was used to separate the magnetic and nuclear diffuse cross-sections.

The bragg scattering measurements indicate an average magnetic moment which increases with manganese concentration in contrast to the earlier measurements by Ishikawa et. al. [3] The diffuse scattering measurements indicate that the alloys are substantially random.

The magnetic moment on the iron atoms is small and fairly constant over the measured range, whereas the magnetic moment on the manganese atoms is large.

REFERENCES

- [1] H Umebayashi and Y Ishikawa, J Phys. Soc. Japan 21, 1281 (1966)
- [2] S Kennedy and T J Hicks, to be published
- [3] Y Ishikawa and Y Endoh, J Appl. Phys. 39, 1318 (1968)

Session VI

Friday 11.20 - 11.40 a.m.

THE DISTRIBUTION OF MAGNETIC MOMENT IN
FERROMAGNETIC $\text{Fe}_{3-x}\text{Mn}_x\text{Si}$ ALLOYS

by

H. Kepa, and T. J. Hicks

Department of Physics
Monash University
Clayton 3168

and

R. L. Davis

AINSE Neutron Diffraction Group
Private Mailbag
Sutherland 2232

Abstract

Fe_3Si is an ordered ferromagnetic compound in which two iron sites are equivalent and carry a moment of $1.35 \mu_B$ while the third has a moment of $2.2 \mu_B$ [1]. Manganese substitutes for iron on the latter site in a non ordered manner with a moment of $2.3 \mu_B$ [2]. For $x > 0.75$ there is a low temperature reordering of the magnetic structure which acquires an antiferromagnetic component [2].

Diffuse magnetic scattering data collected from a polycrystalline alloy with $x=0.1$ [3], suggest that even at these low manganese concentrations there may be a non-collinear component to the magnetic structure. The measured magnetic diffuse cross-section is much larger than would be expected if the defect caused by the Mn atom were collinear with the ferromagnetic direction. The larger cross-section could be explained if the magnetic defect also had components of magnetic moment perpendicular to the ferromagnetic direction.

The present data, taken on single crystals with $x=0.19$ and $x=0.4$, confirms the data of [3] that the Mn cluster strongly on their preferred site. The magnetic diffuse cross-section per Mn atom is not as large at small angles as that determined by [3] but is still larger, at least for $x=0.19$, than would be expected for a collinear moment defect. The variation of cross-section with scattering angle is also not what would be expected for a collinear moment defect at the substituted site and the iron first neighbour sites.

References

- [1] A Paoletti and L Passari, Nuovo Cimento 32, 1450 (1964).
- [2] S Yoon and J G Booth, J Phys F7, 1079 (1977).
- [3] B Maguire and T J Hicks, unpublished.

COVALENCE, TRANSITION METAL COMPLEXES,
AND POLARISED NEUTRON DIFFRACTION

by

P. A. Reynolds, B. N. Figgis, and R. Deeth

School of Chemistry
University of Western Australia,
Nedlands, W.A. 6009.

Abstract

Polarised Neutron and X-ray diffraction experiments have been performed on the Elpasolite $\text{Cs}_2\text{KCr}(\text{CN})_6$ [1,2]. Spin and Charge density maps and parameters have been extracted by least-squares modelling of the respective data. These show substantial spin and charge transfers between the chromium and cyanide ligands in the $[\text{Cr}(\text{CN})_6]^{3-}$ complex ion including significant negative spin density in regions on the cyanide ion. This means that electron-electron correlation effects are as important as simple covalent spin and charge transfers.

Theories, such as Restricted Hartree-Fock ab-initio calculations [3], which do not include such correlation cannot fit the spin density results. However, Unconstrained DV-X α calculations [4], which partly incorporate electron-electron correlation are in reasonable qualitative agreement with both spin and charge density results.

The P.N.D. experiment provides a sensitive test of bonding theory because small effects on the ligands can be separated from changes in the metal "3d" region because of the spatial nature of the diffraction experiment. This is in contrast to spectroscopy where the energies are dominated by "3d" effects.

The Charge density results although, for experimental reasons, much less accurate than the spin density, are more sensitive to intermolecular effects causing polarisation of the complex ion. It thus provides complementary information to the P.N.D. experiment.

References

- [1] B. N. Figgis, J. B. Forsyth, and P. A. Reynolds, *Inorg. Chem.* (1986), in press.
- [2] B. N. Figgis and P. A. Reynolds, *J. Chem. Soc. Dalton Trans.* (1986), in press.
- [3] L. G. Vanquickenborne, L. Haspelagh, J. Hendrickx and J. Verhulst, *Inorg. Chem.* (1984), 23, 1677.
- [4] M. Sano, H. Adachi, and H. Yamatera, *Bull. Chem. Soc. Japan* (1981), 54, 2898.

Session VI

Friday 12.00 - 12.20 p.m.

NEUTRON SCATTERING IN SURFACTANT SYSTEMS

Thomas N. ZEMB
 Research School of Chemistry
 Australian National University CANBERRA
 permanent address : Departement de Physico-Chimie
 91191 CEN Saclay (FRANCE)

Abstract :

All surface active molecules, called surfactants, share the property of forming dynamic aggregates once in solution. These aggregates are dynamic entities, subject to chemical exchange processes in the timescale of nanoseconds. At least one of the dimensions of the aggregates is always of the order of one molecular length; the actual shape can vary from spheres, lamellas, cylinders, ellipsoids and bicontinuous random networks. These labile structures, known by the chemists as micelles, microemulsions, mesophases and lyotropic liquid crystals, cannot be observed in the optical or electron microscopes.

Neutron and X-ray scattering are the only "direct" methods for studying these structures.

These are studied by the physicist since the surfactant aggregates behave as complex liquids, made of interacting aggregates and reproducing the full range of liquid properties (critical points, liquid-gas phase transitions etc..). Phase diagrams are more complicated than for molecular liquids since the interaction between these colloidal aggregates can be tuned by pH or salt concentration. For the chemist these heterogeneous media are model systems used for linking structure to the observed reactivity in colloidal media.

The main experimental methods of neutron small angle scattering data interpretation will be illustrated with examples in the litterature. First, the importance of spatial resolution will be emphasized.

Since diluted and non-interacting "particles" cannot be obtained in these media, the notion of Guinier radius cannot be used and should be replaced by the integral parameters introduced by Porod, such as "average cell length", "largest chord" or "characteristic distance". Absolute scaled measurements can, in favorable cases, be understand in terms of the "one-component macrofluid" introduced by Hayter and Penfold. Average mass, contact potentials and excluded volume can then be directly measured by neutron small angle scattering. The contrast variation method is used to localize any deuterium labelled molecule in the aggregate.

Session VII

Friday 1.20 - 2.00 p.m.

MALAYSIA'S ENTRY INTO A NEUTRON-SCATTERING PROGRAMME

by

Abdul Ghaffar Ramli and Mohamad Deraman

Nuclear Energy Unit
Kompleks Puspati, MalaysiaAbstract

The neutron-scattering programme in Malaysia had been planned and re-planned since 1982, soon after Malaysia's first research reactor was commissioned. Currently, and most definitely, the neutron-scattering programme will start off with small-angle neutron scattering (SANS). This seems to be in contrast with other nations' neutron scattering programmes where the usual activity would first be neutron diffraction. This paper gives the reasons behind the selection of SANS at a starting point. The design of Malaysia's SANS instrument and its expected applications will be explained. Other matters, especially those related to expected future developments or arrangements will also be discussed.

SMALL-ANGLE NEUTRON SCATTERING AT LUCAS HEIGHTS -
PAST, PRESENT AND FUTURE

by

E.M. Gray

Solar Energy Research Centre
University of Queensland
St. Lucia Queensland 4067
Australia

Abstract

The technique of small-angle neutron scattering (SANS) is almost as old as neutron scattering itself [1], but has only reached a high state of development in the past two decades. Some preliminary attempts at SANS were made at Lucas Heights in the 60's and 70's, and the author has made calibrated measurements with background corrections at scattering vectors down to about 0.04 \AA^{-1} in the last few years. There is, however, no facility dedicated to SANS in Australia.

Some examples of the work done so far at Lucas Heights will be given, and the future potential of the technique will be illustrated by discussing its use in magnetism and metal physics.

References

- [1] R.J. Weiss, Phys. Rev. 83, 379 (1951).

THE NEUTRON KIKUCHI EFFECT

by

M. M. Elcombe

Applied Physics Division
Australian Atomic Energy Commission
Lucas Heights Research Laboratories

Abstract

The Kikuchi effect arises from the secondary scattering of diffuse inelastic radiation generated in a crystal. It was first observed and formulated for electrons and has since been observed with X-rays and possibly γ -rays. For thermal neutrons the significant energy change that occurs on inelastic scattering complicates the geometry in that the incident and scattered wave vectors do not terminate on the same Ewald sphere. An exact formulation of the neutron Kikuchi effect will be presented.

The usual film techniques for observing the Kikuchi effect require intense radiation sources and very good angular resolution. Neutron sources are inherently large and diffuse and the efficiency of neutron film methods is very low, so an alternative strategy suitable for a neutron counting system has been evolved. Detailed measurements on lead (Pb), collected over the last 2 years on the Triple Axis Spectrometer at Lucas Heights, will be presented. From the analysis of this data it is reasonable to conclude that the neutron Kikuchi effect has been observed.

PLANS FOR THE FUTURE DEVELOPMENT OF
NEUTRON SCATTERING FACILITIES ON HIFAR

by

R. L. Davis⁺ and C. J. Howard*

⁺Australian Institute of Nuclear Science and Engineering

*Applied Physics Division, Australian Atomic Energy Commission

Abstract

The past year has seen a number of developments which may influence the future of neutron beam research at Lucas Heights. In November 1985, ASTEC tabled a report in which it recommended both increased funding for neutron beam facilities around HIFAR, and funding to facilitate access by Australian neutron beam scientists to advanced facilities overseas. Plans have been made to replace the AAEC by the Australian Nuclear Science and Technology Organisation (ANSTO), and a review has been undertaken to help define the objectives of the new organisation. Funding has been cut in many areas following the decline in the value of the dollar. We have also suffered the disaster at Chernobyl, and the political fallout from that.

In these circumstances, planning has been difficult. However, in response to the ASTEC report, the attempt has been made to develop a number of options for the development of the HIFAR facilities. The costs of these options range from practically nothing, to sums in excess of \$15 M! In this talk we outline future directions for Australian neutron beam research, identify the most important equipment requirements for progress in these directions, and describe some of the plans which have been developed.

GENERAL INFORMATIONCONFERENCE VENUE

The conference will be held in the AINSE Theatre, Lucas Heights (Institute Building) - see map page 39
Thursday 6th and Friday 7th November, 1986

PAPERS

Timing Green light shows for presentation of paper -
Warning light shows when 5 & 2 minutes are remaining -
Red light shows when presentation time has expired -
Discussion time of 5 minutes is then allowed by the
Chairman

Slides Authors using 35mm slides in conjunction with their talk are requested to place their slides in the projector magazine during the break preceding the session in which the paper is scheduled.

ACCOMMODATION

For out of Sydney participants whose nominations have been previously accepted, accommodation has been arranged in accordance with advised requirements, at Stevens Hall, Lucas Heights (adjacent to the Institute building, outside the Main Gate, Lucas Heights Research Laboratories) - or at the Sapphire Motel, 408 Princes Highway, Sylvania Heights - see map back cover. The Institute will make payment directly to the management for room only charges at Stevens Hall or the Sapphire Motel. Participants should make personal arrangements to pay cash for breakfast charges at Lucas Heights and the Sapphire Motel. Participants are requested to vacate Stevens Hall rooms by 10.30 a.m. Friday and to leave their luggage in the room marked 'luggage' adjacent to the theatre foyer, keys to be left in room door.

MEALS

Breakfast for Stevens Hall residents, breakfast is served in the AAEC Canteen from 7.30 a.m.
for Sapphire Motel residents, breakfast time to be advised.

Please note: Participants should make arrangements to pay cash for breakfast charges at Lucas Heights or the Sapphire Motel.

Conference Luncheons - Thursday & Friday 6th & 7th November, 1986
Luncheons for all participants will be held in the Stevens Hall Dining-room and Ante-room during the scheduled lunch periods on Thursday and Friday 6th & 7th November.

Evening Meals

Wednesday 5th November, 1986

Please advise the conference secretary, if you require an evening meal on this evening.

Conference Dinner - Thursday 6th November, 1986

5.30 p.m.	Pre-dinner drinks	Stevens Hall Lounge (included with Poster Session)
6.15 p.m.	Buffet Dinner	Bamboo Room - AAEC Canteen
7.45 p.m.	Conference Address	Prof. R.E. Collins - Uni. of Sydney

Note: No other meal service will be available at Lucas Heights on this evening.

TRANSPORT

Transport from Sydney Airport - Thursday 6th November, 1986
 An AAEC bus ('Z' number plate) will leave Australian Airlines Terminal (Sydney Airport) for Lucas Heights, at 9.25 a.m. If any difficulty is experienced in locating the bus, the Australian Airlines, Commonwealth Car Desk will advise details of its precise location.

Request to Participants arriving on AAEC Bus from Airport
As time will be limited, participants are asked to proceed directly to the AINSE Theatre and not to their rooms at Stevens Hall. Luggage may be left in a room adjoining the theatre foyer, marked 'Luggage'. Keys may be picked up from Stevens Hall Reception at any time during the day.

Transport from Sydney Airport (excluding special arrangements Thurs. 6th)

Taxis are available from the airport to -
 Lucas Heights
 Sydenham Railway Station - thence train to Sutherland Station.
 Sutherland Railway Station - thence bus to Lucas Hts. or taxi
 (ref. bus timetable below).

NOTE: Bookings must be made for all transport listed below - through AINSE - as transport only operates on demand.

Monday - Friday

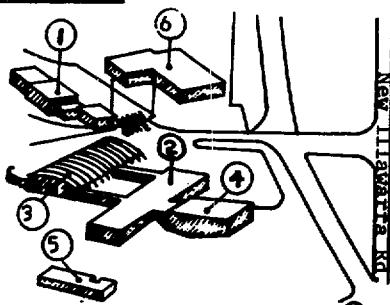
Depart Lucas Heights for Sutherland	Depart Sutherland for Lucas Heights
7.35 am	8.00 am
8.30 "	8.20 "
9.35 "	9.05 "
10.35 "	10.05 "
11.30 "	11.10 "
12.30 pm	12.00 pm
1.00 "	1.10 "
2.15 "	1.25 "
3.35 "	2.50 "
	4.00 "
* 8.20 "	8.40 "
* 9.20 "	9.40 "
* 10.25 "	11.00 "
11.35 "	12.05 am

Buses from Lucas Hts. leave from outside AAEC Main Gate.
 - - - - -

Buses from Sutherland leave from outside Post Office - Flora Street.
 - - - - -

* Upon request these buses will transport participants to the Sapphire Motel.

Lucas Heights N.S.W.



1. Main Gate
2. AINSE Building
3. Canteen
4. AINSE Theatre
5. Stevens Hall
6. Reception

Transport from Sapphire Motel to Lucas Heights

Transport will be arranged for participants on Thursday and Friday mornings. Please wait outside the motel reception office for transport leaving at 8.20 a.m. (approx). It would be appreciated if participants with their own transport could drive to Lucas Heights, and assist others if possible.

Transport from Lucas Heights to Sapphire Motel

Buses leaving Lucas Heights at the following times will transport participants to the Sapphire Motel - 8.20 p.m., 9.20 p.m., and 10.25 p.m. (see timetable).

* It is necessary, however, to book for these services - through AINSE, as transport is only provided if demand exists.

Transport from Lucas Heights to Sydney Airport - Friday 7th November, 1986

Transport will be arranged to take participants to Sydney Airport, after the conference concludes. *Please place your name on the list provided on the noticeboard outside the theatre, if you require this service.*

Participants leaving Stevens Hall - Friday 7th November, 1986

Participants are requested to vacate their rooms by 10.30 a.m. Luggage may be left in the room marked 'Luggage' adjacent to the AINSE Theatre Foyer. Room keys may be left in the Stevens Hall Reception Office or room door.

TELEPHONE MESSAGES

Telephone messages will be taken for conference participants on -

543-3411
(AINSE)

543-3436
(AINSE)

543-3111
(switchboard)

All enquiries concerning the conference arrangements should be directed to:-

Mrs. Joan Watson
Conference Secretary
A.I.N.S.E.
Private Mail Bag
SUTHERLAND. 2232

Phone: 543-3411 or 543-3111

L I S T O F P A R T I C I P A N T S

<u>OVERSEAS VISITORS</u>	<u>PAPER NO.</u>
Dr. T.N. Zemb C.E.N. Saclay, France (Visiting A.N.U.)	26R
Dr. A.G. Ramli Nuclear Energy Unit, Puspati, Malaysia (Visiting AAEC)	27
Mr. Mohd. Ali Sufi Nuclear Energy Unit, Puspati, Malaysia (Visiting AAEC)	18
<u>UNIVERSITY OF QUEENSLAND</u>	
(Department of Physics)	
Dr. B.W. Lucas	20
Dr. J.K. Nimmo	10
(Solar Energy Research Centre)	
Dr. E.M. Gray	28
<u>UNIVERSITY OF NEWCASTLE</u>	
(Department of Chemical & Materials Engineering)	
Professor E.O. Hall	
Assoc. Professor W.A. Oates	
Dr. J.D. Browne	
Mr. E. Kisi	11
<u>UNIVERSITY OF SYDNEY</u>	
(Department of Inorganic Chemistry)	
Professor H.C. Freeman	
Mr. B. Church	
Mr. H. Tong	
<u>UNIVERSITY OF NEW SOUTH WALES</u>	
(Uni. College, Aust. Defence Force Academy)	
Dr. S.J. Campbell	
Dr. G.A. Stewart	
Mr. D. Finkler	
Mr. P.W. Thompson	
<u>AUSTRALIAN ATOMIC ENERGY COMMISSION</u>	
(Applied Physics Division)	
Dr. J.W. Boldeman	
Dr. R. Bird	
Dr. C.J. Howard	5,9,17
Dr. M.M. Elcombe	16,17,21,29R
Mr. R. Knott	1R,30

PAPER NO.

<u>C.S.I.R.O.</u> (Division of Mineral Chemistry) Dr. R. Hill	4R,5,8
(Division of Chemical Physics) Dr. T.J. Bastow	3R
(Division of Energy Chemistry) Dr. J.C. Taylor	15
(Division of Applied Physics) Dr. J. Dunlop Dr. R. Day	6 6
(Division of Food Research) Dr. B. Cornell	1R
<u>A.I.N.S.E.</u> (Neutron Diffraction Group) Dr. R.L. Davis	6,30
<u>AUSTRALIAN NATIONAL UNIVERSITY</u> (Research School of Chemistry) Dr. S. Henderson Dr. G. Robertson	12 7R
(Department of Theoretical Physics) Dr. J. Mahanty	
(Department of Solid State Physics) Dr. A.M. Stewart	
<u>MONASH UNIVERSITY</u> (Department of Physics) Dr. T.J. Hicks Dr. T.R. Finlayson Dr. H. Kepa Mr. A. Abbas Mr. D. Cookson Ms. T. Fang Mr. S. Kennedy Mr. P. Lambrineas Mr. J.C. Osborn	8,13,14,22R,23,24 9,19R,21 24 16,21 23 9 8,13,14
(Department of Chemistry) Dr. D.R. MacFarlane Mr. L. Moore Mr. D. Wilkinson	

	<u>PAPER NO.</u>
<u>LA TROBE UNIVERSITY</u> (Department of Chemistry) Dr. B.D. James	2
<u>UNIVERSITY OF TASMANIA</u> (Department of Inorganic Chemistry) Dr. P.W. Smith	
<u>UNIVERSITY OF WESTERN AUSTRALIA</u> (Department of Chemistry) Dr. P.A. Reynolds	25
<u>N.S.W. INSTITUTE OF TECHNOLOGY</u> (Department of Physics) Dr. R. Cheary	
<u>NATIONAL STANDARDS COMMISSION</u> (Technical Services) Ms. S. Town	
<u>B.H.P.</u> (Melbourne Research Laboratories) Mrs. S. Hill	

