Proposal for Physics Network on the theme of Structural Physics

1. Scientific background: Structural Physics research in the UK

The theme of "Structural Physics" encompasses the area of condensed matter physics in which physical properties of solids are related to their atomic structure. Implicit in this are questions of what determines the structure, how the structure changes with external conditions such as temperature, pressure or applied electric field, and how properties can be very sensitive to small changes in structure. The area of Structural Physics is one of the major themes of condensed matter physics, no less important than the areas of electronic structure, magnetic properties, and highly-correlated electronic systems, and certainly as important for technological applications (non-linear optical properties, electro-optic, electro-mechanical, and electro-thermal coupling). The UK has consistently maintained a prominent lead in this work, although this fact has not always been fully appreciated by the research funding agencies.

The basis for much of the present work in structural physics was laid down in the 1960's, which saw the development of the modern theory of lattice dynamics, neutron scattering methods, accurate X-ray diffraction measurements, and the soft-mode theory of displacive phase transitions for example, all of which were pioneered by UK groups from which much of the present efforts in structural physics can be traced (e.g. Cochran and Megaw's groups in Cambridge. The last decade has seen a significant re-emergence in the interest in structural physics. In part this has been driven by new experimental technologies, such as those based at neutron scattering (ISIS and ILL) and synchrotron radiation (Daresbury and ESRF) facilities, modern NMR technologies, optical measurements, high-resolution X-ray diffraction techniques for measurements of diffuse scattering, high-pressure technologies etc. The earlier work was concerned with the properties of nominally perfect crystals (e.g. ferroelectrics, non-linear optical materials), but recently focus has moved to consider disordered crystalline materials (including high-temperature phases), and the effect of structure inhomogeneities over mesoscopic length scales (for example, domain walls). Present research is concerned with issues such as optimising the performance of materials by control of structure, understanding the structures of imperfect crystals, structures of high-pressure phases. Recent highlights of UK work in structure physics include:

- High-pressure work at ISIS and Daresbury. In particular, the facilities at ISIS are way ahead of anything else in the world.
- X-ray diffuse scattering facilities to measure structure inhomogeneities at domain walls.
- New developments in spectroscopic methods (NMR, infrared, optical)
- Development of time-resolved neutron diffraction at ISIS
- Determination of crystal structures of cuprate high-temperature superconductors and ordered phases of fullerenes — in both cases UK workers in Structural Physics played leading roles
- Observation of lattice melting in Na_2CO_3, where a structural phase transition is accompanied by a complete loss of the intensities of the Bragg peaks due to the divergence of the temperature factors
- Development of diffraction methods to determine short-range structures in disordered materials
- Rigid unit mode theory of phase transitions in silicates
- Experiments and theory of new negative thermal expansion ceramics
- Developments in computer simulations of disordered and defective crystals
- Development of *ab initio* electronic structure calculations for structural physics research

The proposal for a network programme in Structural Physics is particularly timely since the recent flourishing of new results, new techniques and new areas of work needs to be coordinated by those responsible, and information rapidly and easily disseminated between active members of the community. The network will be an effective and relatively inexpensive way to maximise the achievements of the work on structural physics in the UK.

The participating groups in this proposal all have a substantial track record in various aspects of Structural Physics. Some groups participate in the Physical Crystallography Group jointly organised within the Institute of Physics and the British Crystallographic Association. A number of groups are part of the GEM CRG at ISIS (funded by EPSRC).

2. The necessity of a network on the theme of Structural Physics

We have outlined above how a network would act to develop a coordinated activity of work amongst the major researchers in the UK. In Appendix 1 we list all the members of the network proposal, with their research interests, areas of expertise, and research facilities. The necessity of the network follows from some general objectives:

1. As the work on structural physics diversifies and develops into many new exciting areas of work, there is a need to bring these developments to the attention of all those active in the field as quickly as possible. For example, recent developments in solid-state NMR spectroscopy or optical measurements may be of crucial importance to problems being tackled by people whose expertise is in neutron diffraction, and it is clear that the network will enable important scientific problems to be tackled be several groups to give a more holistic approach.

2. There are many exciting projects being pursued by the members of the proposed network, with overlap of interests. The network should be used to help chart an agenda for some of this work, i.e. to focus some of the common issues being tackled throughout the network, and in particular to link those involved in the scientific programmes to the users.

3. The network can also be used to further encourage diversity of the work. A lot of the experience of the members of the network could be (and in some cases is currently being) used to tackle new scientific problems where new expertise could usefully be brought into play. For example, work on the physics of crystalline silicates has recently been used to provide new insights into the properties of glasses, zeolites, and materials with negative thermal expansion.

4. There is an inevitable trend towards individual groups having specialised equipment, and investing to ensure that this equipment remains world class. For example, some of the network laboratories have specialised NMR, X-ray diffraction, spectroscopic and optical equipment, and the Central Site Laboratories (CLRC) are clear examples of this. The network will stimulate members of the network to form collaborations with other laboratories who have specialised equipment.

5. Parallel to the developments in experimental work are developments in computational methods and theory. It should be noted that these developments are in a particularly exciting stage. If theory and computer simulations are to have maximum effect, it is essential that there is close coordination with the experimentalists in the community. The network will provide this coordination.

6. The network will also act to focus work that requires the facilities of the Central Laboratories. The trend within the Research Councils is to support major programmes of work at CLRC facilities instead of the small experiments that previously were more typical of the work in Structural Physics. The network will provide the necessary experience for the development of these programmes, and the network itself will provide the forum for the collaboration involved in these larger programmes.

7. A lot of the work of the network has considerable relevance for high-technology industries that exploit the optical (particularly non-linear), piezoelectric and pyroelectric properties of ceramics, and also for battery technology and silicate ceramics. The network will act as a focus for industries to tap into the expertise that exists within the Structural Physics community.

We see the proposed network on Structural Physics following and developing a model that has operated within the area of Mineral Physics over the past decade. Briefly, a small network based on 4-5 sites of groups who are using condensed matter physics methods and insights to tackle problems in the mineral sciences have held informal meetings twice a year. These meetings have each had a different focus, for example on computational methods, and the relationship between lattice relaxation and ordering processes. In these meetings different members of the Mineral Physics community have presented recent developments in the field. These meetings have stimulated a great deal of informal contact between the members of the community, with the result of fostering collaborations between institutes, and spreading information on developments relatively quickly. The proceedings of some of these meetings have been published in Mineralogical Magazine. Following this model Prof Salje has coordinated an ESF Network Programme on Kinetic Processes in Minerals and Ceramics. The proceedings of all of these meetings have been published in Phase Transitions. We plan that the network will hold a similar series of information meetings, with published proceedings.

3. Network Objectives

The objectives listed here summarise some of the ideas outlined in the preceding sections.

1. The primary objective of the network will be to maintain the position of the UK Structural Physics community at the forefront of international science through the interchange of information and expertise, and the stimulation of communication and collaboration.

2. The scientific objective of the network in Structural Physics is to continue to enhance the understanding of the link between microscopic structure and macroscopic properties, particularly in the light of many recent developments such as new understanding of structural inhomogeneities, mesoscopic inhomogeneities, new theories of phase transitions, new experimental techniques enabling new experiments to be performed (e.g. high pressures).

3. The network will ensure the healthy future of Structural Physics in the UK through nurturing and training of new talent, and through the transfer of skills between groups.

4. The network will establish a clear funding base for the excellent research activities in Structural Physics.

5. The network will work to raise the profile of the Structural Physics community within the broader area of Condensed Matter Physics in the UK. For example, it will seek to establish a greater presence at the CMMP meetings of the Institute of Physics.

6. The network will significantly optimise use of CLRC facilities for experiments in Structural Physics.

7. The network will be instrumental in disseminating information about new experimental techniques, both lab based and in CLRC facilities, to the Structural Physics community, in order to keep the community abreast of new developments and to ensure that the community remains in the forefront of research maximising the use of the best techniques.

8. The network will bring together experimentalists, theorists and computer modellers in order to provide more coherent programmes of work.

9. The network will provide a forum for industrial partners to learn of the work of the Structural Physics academic community, and for the academic community to learn of the interests and priorities of related industrial research.

4. Network activities (costed)

The primary focus of the network will be two meetings each year that each group will participate in. One with be a one-day event devoted to a single theme, and the other will be a more-general two-day meeting where each group will be able to report its progress. These meetings will only require funding for meals, accommodation and travel for the academic participants. These meetings will be organised from Cambridge, but will be hosted (at no cost for lecture theatres etc.) around the different institutes involved in the network. Industrial contacts will be encouraged to attend in order to gain maximum exposure to the work of the Structural Physics community. (Cost £15,000)

In order to foster specific collaborations we will plan four informal one-day meetings each year, each with approximately ten participants from 3–4 institutes. These will be organised by the participants themselves. Each of these meetings will conclude with a short report that will be posted to each participating institute in the network and available on the WWW. Some of these meetings will take the form of working parties aiming to stimulate ‘best practice’ use of central site facilities or laboratory techniques. (Cost £6,000)

We anticipate that in order to make progress with collaborative research programs members of the network will need to spend periods of time (average one week) at collaborating laboratories. We anticipate five such visits each year. These will be organised locally by the participants, and each visit will conclude with a short report that will be posted to each participating institute in the network and available on the WWW. (Cost £6,000)

The final component of the network will be a one-week workshop, held during the third year, which will be used to provide thorough teaching in the wide range of techniques available for Structural Physics research, which will be aimed at scientists from all levels of experience (graduate students to Professors), with the aim of providing a firm foundation for the community to develop from in the next century (!), with high-quality training for the next generation of scientists and their mentors. We anticipate 40 participants. It is felt that this workshop will best be held later in the duration of the network rather than at the beginning since it will build upon the experience gained in the network. A

significant teaching The proceedings will be published as an edited text book, negotiated with a publisher to produce at a price that is affordable to graduate students. The running of the workshop and the editing of the final book will be coordinated from Cambridge. (Cost £14,000)

The network will be coordinated and managed from Cambridge. This will involve regular communication to members of the networks, organisation of meetings (as noted above), editing of meeting transcripts, and coordination and distribution of reports. In order to ensure effective communications between members of the network (information about meetings, bookings of accommodation etc.) and maintenance of the network's WWW pages, we will need secretarial support and computer officer support. We anticipate that this will require the equivalent of 4 months work over the three-year duration of the network. (Cost £7250 including overheads)

We will also require support for consumables such as postage and photocopies. (Cost £1250)

5. Support for existing research programmes within the proposed network

The members of the network hold a number of current research grants and contracts, some of which are listed in Appendix 2. Some of these are high-profile projects, such as support for a CRG on diffraction at ESRF, development of high-pressure research at CLRC facilities, and NMR facilities at Warwick.

6. Exploitation of results

This depends on our objectives!!

7. Dissemination of results

1. Research results will be disseminated by publication of the proceedings of our twice-yearly workshops.

2. Reports produced by the network will be posted on the network page on the WWW, and to maximise this route this page will be accessible through links from all the WWW pages of the participating members and from the research councils.

3. The experience of the network will culminate in a workshop, with proceedings being published as an affordable text book.

4. All the members of the proposed network have an excellent record of publishing the results of their research in top quality journals of physics and related subjects, and it is common practice to target publications towards likely beneficiaries.

5. A number of participating groups have in place facilities to disseminate research results to industrial partners.

6. Industrial partners will be encouraged to attend the meetings of the network in order to learn first hand about the results of the members of the network.

7. All the members of the proposed network already receive regular invitations to present their work at international conferences and workshops.

Appendix 1: Expertise and facilities offered by the participating research groups

Here we list the participating groups that will form the proposed network, together with their special facilities and areas of expertise. Of particular note are the NMR facilities at Warwick and Kent, the high-pressure facilities at ISIS, Daresbury and Edinburgh, the X-ray facilities for structure determination and measurements of diffuse scattering in many groups, the optical measurement facilities at Oxford and Warwick, and the computational facilities at Edinburgh and Cambridge for simulation studies. These complement the world-leading facilities for neutron scattering at ISIS and synchrotron-based techniques at Daresbury. Additional expertise lies in structural phase transitions, mesoscopic scale structures, structure analysis for ideal and disordered materials, optical properties, ferroelectric materials, high-temperature superconductors, and computer simulations.

Birmingham Physics (Darlington): Phase transitions in perovskites, X-ray diffraction, diffraction at CLRC facilities

Cambridge Earth Sciences (Dove, Farnan, Redfern, Salje): Phase transitions in silicates and high-temperature superconductors, High-resolution X-ray diffuse scattering, powder diffraction, computer simulations, IR spectroscopy, TEM, 2nd harmonic generation, theory of phase transitions, mesoscopic structures

CLRC Daresbury (Cernik): High-resolution diffraction, high-pressure

CLRC ISIS (David, Harris, Hull, Keen, Knight, Wilson): High-resolution neutron powder diffraction, high-pressure facilities, single-crystal neutron diffraction, total scattering to large scattering vectors, inelastic neutron scattering, data analysis, modelling of disordered systems, structural phase transitions, perovskites, fast-ion conductors

Cranfield Physics (Whatmore): Inhomogeneous structures, ferroelectrics, fabrication and sample preparation, structure analysis, microengineering/nanotechnology laboratory with large clean room.

Edinburgh Physics (Ackland, Allan, Nelmes): High-pressure studies, electronic structure calculations, computer simulations

Keele Physics (Hagen): High-resolution X-ray diffraction, time-resolved neutron diffraction

Kent Physics (Nield, Smith, Strange, van Eck): Diffuse scattering and structures of disordered materials, NMR, modelling of disordered systems

Liverpool Physics (McMahon, Stirling): High-resolution X-ray diffraction, high-pressure, synchrotron radiation

Oxford Physics (Cowley, Glazer): High-resolution single-crystal and powder X-ray diffraction, neutron scattering, optical properties, phase transitions, domain walls

Philips (Fewster): Diffraction from imperfect materials

UCL Physics (Skipper): Clays and layered structures

Warwick Physics (Dupree, Thomas): NMR, X-ray diffraction, optical properties, phase transitions

Appendix 2: Support for research programmes

The members of the proposed network have a number of research grants. Some representative (not exhaustive) examples of current grants:

Oxford/Cranfield: EPSRC support for PZT ceramics and crystals; X-ray work including structural phase transitions

Keele/ISIS: EPSRC support for building a detector for critical scattering measurements at ISIS (£60k + neutron tickets)

Liverpool: EPSRC grant for CRG diffraction instrument at ESRF (£2.3M construction, GR/J79363, £2.5M for five years operating programme, GR/L39698)

Kent: EPSRC grant on Atomic scale studies of dynamics and structure of technologically significant oxides (£217,336, GR/K74876), Development of an advanced characterisation methodology for gel-produced materials (£539,586, GR/L28647), Microdynamics and Phase Equilibria in Nanocrystals (£84,434, GR/K62347). Unilever support for Generic Research Investigation by NMR of Heterogeneous Materials (£75k, UKC R15.126).

Warwick: EPSRC support for Investigation of the Optical Constants of Crystalline and Amorphous Materials (£121k, GR/L02616), High-resolution diffraction studies of Periodically Domain-inverted Crystals (£99k, GR/K92955), NMR facilities (£600k). Support from DRA Fort-Halstead (£30k). Support from Leverhulme Trust for Inorganic Nonlinear Optical Crystals (£80k, F215AK)

Edinburgh: EPSRC support for New techniques for high pressure diffraction studies of structures and transitions at SRS (£196,882 + beam tickets, GR/K24215), Novel instrumentation for neutron diffraction to very high pressures (£827,470 + neutron tickets, GR/J91760).

Cambridge/ISIS: EPSRC support for “Low energy excitations in glasses” (£135k + neutron tickets)

In addition, several groups are members of the GEM CRG supported by EPSRC

Appendix 3: Industrial interest

Individual establishments have collaborations with a number of industrial groups. These include Unilever (CLRC, Kent), Redland (Cambridge, Kent), ICI (CLRC), Shell (CLRC, Cambridge), Castle Cement (CLRC), Oxford Cryosystems (Oxford), MSI (Cambridge, Edinburgh), Oxford Instruments (Kent), Siemens (Warwick, Cambridge). Of note is the CLRC Daresbury Research and Technology Services, which provides facilities for industrial use.

Appendix 4: Selected publications

This list is a brief selection of publications in the area of structural physics by members of the network, illustrating the scope of the research.

Structural study of barium titanate between 150 and 425 K. Darlington, CNW, David, WIF, Knight, KS. Phase Transitions, 1994, 48, 217-236

Mesoscopic structures in ferroelastic crystals: needle twins and right-angled domains. Salje, EKH, Ishibashi, Y. Journal Of Physics: Condensed Matter, 1996, 8, 8477-8495

Hard mode spectroscopy for the investigation of structural and superconducting phase-transitions. Salje, EKH, Yagil, Y. Journal Of Physics And Chemistry Of Solids, 1996, 57, 1413-1424

High-temperature study of octahedral cation-exchange in olivine by neutron powder diffraction. Henderson, CMB, Knight, KS, Redfern, SAT, Wood, BJ. Science, 1996, 271, 1713-1715

Origin of the negative thermal expansion in ZrW_2O_8 and ZrV_2O_7. Pryde, AKA, Hammonds, KD, Dove, MT, Heine, V, Gale, JD, Warren, MC. Journal Of Physics-Condensed Matter, 1996, 8, 10973-10982

Low-frequency floppy modes in β-cristobalite. Swainson, IP, Dove, MT. Physical Review Letters, 1993, 71, 193-196

A near-ambient-temperature-control cell for use with synchrotron x-ray powder diffraction. Cernik, RJ, Craig, SR, Roberts, KJ, Sherwood, JN. Journal Of Applied Crystallography, 1995, 28, 651-653

High-resolution neutron powder diffraction: a case study of the structure of C_{60}. David, WIF, Ibberson, RM, Matsuo, T. Proceedings Of The Royal Society Of London, 1993, 442, 129-146

Structural evidence for a past-ion transition in the high-pressure rock-salt phase of silver iodide. Keen, DA, Hull, S, Hayes, W, Gardner, NJG. Physical Review Letters, 1996, 77, 4914-4917

The interpretation of single-crystal diffuse scattering using reverse Monte Carlo modeling. Nield, VM, Keen, DA, Mcgreevy, RL. Acta Crystallographica Section A, 1995, 51, 763-771

Crystal dynamics by neutron time-of-flight laue diffraction in olivine up to 1573 K using single frame methods. Rinaldi, R, Wilson, CC. Solid State Communications, 1996, 97, 395-400

Perovskite solid electrolytes: structure, transport properties and fuel-cell applications. Bonanos, N, Knight, KS, Ellis, B. Solid State Ionics, 1995, 79, 161-170

A neutron diffraction study of the order-disorder phase transition in sodium nitrate. Payne, SJ, Harris, MJ, Hagen, ME, Dove, MT. Journal Of Physics-Condensed Matter, 1997, 9, 2423-2432

Observation of lattice melting at the ferroelastic phase transition in Na_2CO_3. Harris, MJ, Cowley, RA, Swainson, IP, Dove, MT. Physical Review Letters, 1993, 71, 2939-2942

Phase transition induced defect formation in iii-v semiconductors. Crain, J, Ackland, GJ, Piltz, RO, Hatton, PD. Physical Review Letters, 1993, 70, 814-817

Hidden high-to-low cristobalite type transition in HgSe and HgTe at high-pressure. Mcmahon, MI, Nelmes, RJ, Liu, H, Belmonte, SA. Physical Review Letters, 1996, 77, 1781-1784

Ordered superstructure of InSb-iv. Nelmes, RJ, Mcmahon, MI. Physical Review Letters, 1995, 74, 106-109

Observation of inverted-molecular compression in boron carbide. Nelmes, RJ, Loveday, JS, Wilson, RM, Marshall, WG, Besson, JM, Klotz, S, Hamel, G, Aselage, TL, Hull, S. Physical Review Letters, 1995, 74, 2268-2271

Crystal-structure of ZnTe-iii at 16 GPa. Nelmes, RJ, Mcmahon, MI, Wright, NG, Allan, DR. Physical Review Letters, 1994, 73, 1805-1808

Time-resolved studies on a millisecond time-scale by elastic neutron scattering: transient properties of the ferroelectric phase transition in Rb_2ZnCl_4. Steigenberger, U, Eckold, G, Hagen, M. Physica B, 1995, 213, 1012-1016

The structure of ice ih from analysis of single-crystal neutron diffuse-scattering. Nield, VM, Whitworth, RW. Journal Of Physics-Condensed Matter, 1995, 7, 8259-8271

NMR techniques in materials physics - a review. Smith, ME, Strange, JH. Measurement Science & Technology, 1996, 7, 449-475

Characterization of porous solids by NMR. Strange, JH, Rahman, M, Smith, EG. Physical Review Letters, 1993, 71, 3589-3591

High-temperature defect spectroscopy in ionic crystals. Xie, ZH, Smith, ME, Strange, JH, Jaeger, C. Journal Of Physics-Condensed Matter, 1995, 7, 2479-2487

Q-dependence of the central peak in the inelastic neutron scattering spectrum of $SrTiO_3$. Shirane, G, Cowley, RA, Matsuda, M, Shapiro, SM. Physical Review B-Condensed Matter, 1993, 48, 15595- 15602

The phase transition of strontium titanate. Cowley, RA. Philosophical Transactions Of The Royal Society, 1996, 354, 2799-2814

A re-investigation of the crystal structure of the perovskite $PbZrO_3$ by X-ray and neutron diffraction. Corker, DL, Glazer, AM, Dec, J, Roleder, K, Whatmore, RW Acta Crystallographica Section B-Structural Science, 1997, 53, 135-142

Structure and optical nonlinearity of $PbO.2B_2O_3$. Corker, DL, Glazer, AM. Acta Crystallographica Section B-Structural Science, 1996, 52, 260-265

X-ray-analysis of thin-films and multilayers. Fewster, PF. Reports On Progress In Physics, 1996, 59, 1339-1407

High dielectric-constant ceramics in the $PbSc_{0.5}Ta_{0.5}O_3$-$PbZrO_3$ and $PbSc_{0.5}Ta_{0.5}O_3$-$PbTiO_3$ systems. Osbond, PC, Whatmore, RW. Journal Of Materials Science, 1993, 28, 1377-1384

Negative thermal-expansion and phase-transitions in the $ZrV_{2-x}P_xO_7$ series. Korthuis, V, Khosrovani, N, Sleight, AW, Roberts, N, Dupree, R, Warren, WW. Chemistry Of Materials, 1995, 7, 412-417

A new Kosters prism interferometer for simultaneous determination of refractive index and thermal expansion of crystals as a function of temperature. Womersley, MN, Thomas, PA. Journal Of Applied Crystallography, 1996, 29, 574-583

Monte Carlo and molecular dynamics simulations of interfacial structure in lithium-montmorillonite hydrates. Chang, FRC, Skipper, NT, Sposito, G. Langmuir, 1997, 13, 2074-2082