Proposal for Physics Network on the theme of Structural Physics

Case for Support

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, along with the areas of electronic structure, magnetic properties, and highly-correlated electronic systems, and is of fundamental importance for both condensed matter technological applications (non-linear optical properties, electro-optic, electro-mechanical, and electro-thermal coupling, silicate ceramics, low or negative thermal expansion ceramics, solid-state battery technology) and the Earth Sciences (properties of rock-forming minerals, environmental, waste containment). The UK has consistently maintained a prominent, and highly diverse, lead in this work, and we believe that funding for a network that is specifically aimed at bringing together the expertise and fostering collaborations will have wide-spread benefits across a range of disciplines.

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 broadening in the range of Structural Physics in the UK. 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 interest has widened substantially to include disordered crystalline materials (including high-temperature phases), the effect of structure inhomogeneities over mesoscopic length scales (for example, domain walls), thin film materials and multilayer structures (thin-film ferroelectrics, control of structure inhomogeneity in semiconductors). 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 Structural 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 measurements of structure inhomogeneities at domain walls
- New developments in spectroscopic methods (NMR, infrared, optical)
- Development of time-resolved neutron diffraction at ISIS
- Kinetics studies of phase transformations by X-ray and neutron diffraction
- Determination of crystal structures of cuprate high-temperature superconductors and ordered phases of fullerenes
- Theoretical prediction and experimental observation of displacive phase at which there is 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, using both diffuse and Bragg scattering combined with modelling
- 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
- X-ray and neutron scattering applications to thin films and multilayers

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 a highly effective way to maximise the achievements of the work on Structural Physics in the UK, and to maintain the health of the subject through training and nurturing of new talent. It will also enable the work of the Structural Physics community to have a greater impact within high-technology industries (electronic, ceramics) and into other disciplines such as Earth Sciences.

The participating groups in this proposal, with their areas of expertise and facilities, are listed in Appendix 1 (under Track record of applicants). Each has a substantial track record in various aspects of Structural Physics, as testified by the funding of the work (Appendix 2 under Track record of applicants). Some groups participate in the Physical Crystallography Group jointly organised within the Institute of Physics and the British Crystallographic Association. Others are involved in the Mineral Physics group of the Mineralogical Society. A number of groups are part of the Collaborative Research Group involved with the building of the new General Materials Diffractometer (GEM) at ISIS (funded by EPSRC). Appendix 3 below gives some case study examples of the work carried out in the Structural Physics community, and Appendix 4 below gives some representative publications which highlight the quality and breadth of the work.

2. Benefits from supporting a network on the theme of Structural Physics

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. The network will 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.

3. 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. The network will stimulate members of the network to form collaborations with other laboratories with specialised equipment and allow effient exploitation of these resources.

4. Parallel to the developments in experimental work are exciting new developments in computational methods and theory. Examples are the ability to perform detailed electronic structure calculations on ceramics, new theories of phase transitions in silicates, and theories and simulations of inhomogenous structures. For theory and computer simulations to have maximum effect it is essential that there is close coordination with the experimentalists in the community, which the network will provide.

5. 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. The network will provide the necessary experience for the development of these programmes, and will provide the forum for the collaboration involved in these larger programmes.

6. A lot of the work of the network has considerable relevance for high-technology industries, such as that on the optical (particularly non-linear), piezoelectric and pyroelectric properties of ceramics, materials for solid-state battery technology, silicate ceramics, inhomogenous semiconductors and superconductors. The network will act as a focus for industries to tap into the expertise that exists within the Structural Physics community.

7. A network will provide the means for training and nurturing new talent, by the provision of workshops and by supporting visits to other laboratories. In addition, the network will facilitate the transfer of skills between established laboratories.

8. A network will raise the profile of the Structural Physics community within the overall Physics community and the research funding organisations.

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

5. The network will provide a forum for industrial partners to learn first-hand 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. Members of the network proposal already have a wide range of individual links with industrial partners, including 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), BNFL (Cambridge). Of note is the CLRC Daresbury Research and Technology Services, which provides facilities for industrial use and has a wide range of industrial contacts.

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

7. 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.

8. The network will significantly optimise use of CLRC facilities for experiments in Structural Physics, by spreading expertise in the use of these facilities, and by stimulating developments of these facilities towards the needs of the Structural Physics community (e.g. sample environment).

9. 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.

10. The network will stimulate applications of Structural Physics to the Earth Sciences through the use of the techniques, and in turn will be able to learn from the insights given through the study of complex mineral behaviour.

4. Network activities (costed)

(The costs summarised here are given in more detail in the EPS(RP) form).

The primary focus of the network will be two meetings each year that all groups will participate in. One will 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. The proceedings of these meetings will be published as special collections in *Journal of Physics: Condensed Matter*, which will ensure wide dissemination (the editor of the journal has welcomed this opportunity). Industrial contacts will be encouraged to attend these meetings 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 £4,275)

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. 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 are requesting the purchase of a portable Macintosh to allow administration of the network to be readily ported from Cambridge to the locations of meetings. (Cost £2204)

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

We expect that the support for the Structural Physics network will eventually transfer to a trust established through industries buying into the network in order to maintain direct access to the Structural Physics community. Cambridge Earth Sciences has an "Industrial Associates" scheme that involves industries (mostly oil industries) paying an annual subscription (of order £8000) in return for an annual presentation of the work of the department.

5. Support for existing research programmes within the proposed network

The members of the network hold a large number of current research grants and contracts, a few of which are listed in Appendix 2 (Track record of applicants). These include some high-profile projects, such as support for a collaborative research group to build and operate a high-resolution diffraction instrument at the ESRF, development of high-pressure research at CLRC facilities, and NMR facilities at Warwick. Members of this proposal are members of the ISIS GEM collaborative research group.

6. Exploitation of results

1. The network will consolidate the position of the UK as the world leader in Structural Physics. We will use this to increase the size and diversity of the community.

2. The network will actively seek to promote the results of its work to its industrial partners through the means described in sections 4 and 7. The industrial partners will better be able to use the expertise and knowledge base of the whole Structural Physics community.

3. The network will actively seek to promote the results of its work to the Earth Sciences community through the participation of the Cambridge group in the network.

7. Dissemination of results

1. Research results will be disseminated by publication of the proceedings of our twice-yearly workshops as special collections in *Journal of Physics: Condensed Matter*. Reprints of the proceedings will be sent to industrial partners.

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. Several of the participating groups have arrangements in place already 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 3: Example case studies

1. *Phase transition in silica polymorph cristobalite*

There is a structural phase transition in silica that is important because of the presence of cristobalite in silica ceramics and in geology. The phase transition has elicited a lot of work because the high-temperature phase is clearly disordered — the average structure given by diffraction is not consistent with chemical considerations of bonding. The phase transition has been studied within the Rigid Unit Mode theory, and a plausible model for the disorder as arising from the action of a large number of low-frequency modes with large amplitude has been proposed. This has been tested using inelastic neutron scattering, total neutron scattering measurements to determine the local structure over the 1–10 Å range, and high-resolution neutron powder diffraction, all at ISIS. The theory has been supported by molecular dynamics simulations and electronic structure calculations. Similar phase transitions in other silica polymorphs have been studied by NMR. This work has involved the groups at Cambridge, ISIS and Warwick.

2. *High pressure research*

The high-pressure programme at ISIS and the SRS at Daresbury have introduced many new techniques into high-pressure structural research, giving results of unprecedented accuracy at higher pressures. Highlights of this work include studies of simple compounds at high pressures (semiconductors, geological materials), molecular solids (such as ammonium, methane) that are of significance for planetary research, ice, hydrogen-bonded materials, boron compounds. These results have revised many older viewpoints and settled controversies. The work will now develop into simultaneous high pressures and high/low temperatures, and will be developed for single crystal work. The ability to collect two-dimensional data using image plates enable information of microstructure to be extracted. The work will also encompass magnetic structures and dynamical measurements. High-pressure research is of considerable interest to the Earth Sciences, and the new insights given will enhance design of materials.

Appendix 4: Selected publications

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

Observation of a cinnabar phase in GaAs at high pressure. McMahon, MI,. Physical Review Letters, 1997, 78, 3679-3700

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

Interpretation of the diffraction profile resulting from strain relaxation in epilayers. Kidd, P, Fewster PF, Andrew, NL. J. Phys. D: Appl. Phys. 1995, 28, A133-A138

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

Ab initio total energy of uncharged 2:1 clays and their interation with water. Bridgeman, CH, Buckingham, AD, Skipper, NT and Payne, MC. Molecular Physics, 1996, 89, 879–888

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