Proposal for Physics Network on the theme of Structural Physics

Track record of applicants

The UK Structural Physics Community

The UK Structural Physics community has a strong international lead in this area of Physics research. The community has pioneered experimental techniques, theoretical approaches and computer simulation methods that have led the way for the rest of the world, and the science that has emerged has broken a large amount of new ground. The participants in this network proposal are listed in Appendix 1 below with their areas of expertise and facilities. The importance of the work of the Structural Physics community is highlighted by the list of representative currents grants that fund the work of individual members given in Appendix 2 below. The range of interests of the Structural Physics community is highlighted in the small sample of publications listed in Appendix 4 of the main Case for Support, and it should be noted that a large faction of these are in flagship journals such as Physical Review Letters.

The UK Structural Physics community also has a good track record in forging links with various industries, a point that is noted in more detail in the main Case for Support.

The track record of the Principal Investigator

Dr Dove has been a lecturer in Mineral Physics in the Department of Earth Sciences in the University of Cambridge. His work has been mainly concerned with experimental and theoretical studies of phase transitions in silicates. The experimental work has mostly been performed using the ISIS neutron scattering facility, and has encompassed diffraction, inelastic scattering, and diffuse scattering measurements. The theoretical and computational work recently has focused on the Rigid Unit Mode model, developed in collaboration with Prof Volker Heine (Cavendish Laboratory, Cambridge), which provides a theoretical framework for understanding the origin of displacive phase transitions in silicates, the atomistic basis for the actual value of the transition temperature, the nature of high-temperature phases, the thermodynamics of phase transitions etc., and more recently the model has been used to understand negative thermal expansion, catalytic behaviour of zeolites, and the low-energy excitations of silica glasses. A few publications are listed below.

Dr Dove's international rating is indicated by a good number of invitations to speak at international conferences. Over the past 1–2 years he has been invited to lecture at a NATO workshop on glasses, to give talks at the APS Spring meeting, the CMMP winter meeting, the Gordon conference in disordered materials, and two CECAM workshops, just to note some examples of flagship meetings. He was a participant in the two workshops to develop the case for the proposed European Spallation Source.

The final report of Dr Dove's grant from NERC to support the development of the Rigid Unit Mode was awarded an α5 rating, as was the final report following a recent EPSRC award to support the Cambridge DAP facility of which Dr Dove was the principal applicant.

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

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

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 diffraction, kinetics

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

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

Edinburgh Physics (Ackland, Nelmes): High-pressure structures and phase transitions, high-pressure techniques using both neutron and X-ray diffraction, structure–property relations, electronic structure calculations, computer simulations, development of empirical potentials

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

Kent Physics (Nield, Smith, Strange, van Eck): NMR, Diffuse neutron scattering, computer modelling, structures of disordered materials, oxides, nanocrystals, ferroelectrics, ice, intermetallic alloys.

QMW Physics (Kidd) High-resolution X-ray diffraction, strain and plastic relaxation in single crystal epitaxial layers

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

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

Philips (Fewster): Diffraction from imperfect materials, layered structures, semiconductors

UCL Physics (Skipper): 2-dimensional structures and intercalation compounds, X-ray and neutron diffraction, computer modelling

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

Appendix 2: Some representative examples of support for research programmes

Cambridge: NERC grant for Cation ordering in pyroxenes, amphiboles and micas (£141,983, GR3/10606). EPSRC grant for support of computational science in Cambridge, which included a component of our work (£1.7M).

Cambridge/ISIS: EPSRC grant for Low energy excitations in glasses (£135k + neutron tickets).

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).

Keele/ISIS: EPSRC support for building a detector for critical scattering measurements at ISIS (£72k + neutron tickets)

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).

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

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

QMW: EPSRC support for reciprocal space mapping of multilayer structures (£26,067 GR/L48089), Coherency strain and microstructure for strong materials (£111,301 GR/L35737), Thermophotovoltaic devices in metamorphic InGaAs/GaAs (£86,690 GR/L14756)

UCL: EPSRC grant for Neutron diffraction studies of solvation in layered materials: Graphite-metal-amine intercalates (£182,875, GR/L33962). EPSRC grant for SPM Imaging of solid-liquid interfaces (£25,560, GR/L42476). NERC grant for Neutron diffraction studies of clay-fluid interactions at elevated pressures and temperatures (£157,803, GR3/11138).

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)