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RECENT DEVELOPMENTS USING THE PARIS-EDINBURGH CELL FOR NEUTRON DIFFRACTION AT HIGH PRESSURE AND HIGH TEMPERATURE

Y. Le Godec[1] M.T. Dove[2] S.A.T. Redfern[2] W.G. Marshall[3] M.G. Tucker[2] G. Syfosse[1] S. Klotz[1]
[1]Laboratoire De Physique Des Milieux Condenses Universite Pierre Et Marie Curie Tour 13-23, 2eme Etage, B77, 4 Place Jussieu PARIS PARIS 75252 FRANCE [2]Department of Earth Sciences, University of Cambridge [3]ISIS Facility, Rutherford Appleton

Neutron diffraction is a powerful tool of high pressure research and in many ways can be considered to be complementary to X-rays for crystallographic experiments. The special features of neutron diffraction include its sensitivity to hydrogen (deuterium) and other common light atoms, its contrast for atoms having similar atomic weights, and its sensitivity to magnetic order. However, despite these advantages, neutron diffraction has been much less used than X-ray scattering for high pressure studies because until recently, large sample volumes were required and the maximal attainable pressures were limited to ~2 GPa. These limitations were overcome in 1992 with the advent of the Paris-Edinburgh cell which allows structural studies by neutron diffraction at pressure up to 30 GPa. In this talk, I will give an introduction to high pressure neutron diffraction techniques with a strong emphasis on recent developments, in particular the new design of a cell assembly with internal heating which enables neutron diffraction to be performed at simultaneous high temperatures and pressures (8 GPa, 2000 K). A novel non-invasive neutron radiographic method to measure the temperature of the sample in the high-P/T cell will be also presented. I will illustrate the potential of these methods for fundamental Solid State Physics, Planetology and Earth Sciences by presenting some structural studies on a variety of materials under pressure. Finally, future developments and improvements will be reviewed.

Keywords: NEUTRON DIFFRACTION HIGH PRESSURE HIGH TEMPERATURE

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PHONON DENSITY OF STATES IN IRON-BASED MATERIALS AT HIGH PRESSURES

V. V. Struzhkin
Geophysical Laboratory, Carnegie Institution of Washington, Washington DC USA

Elastic properties of iron and magnesiowustite at high pressures are very important for geophysical science, however, they are not easily accessible in high-pressure experiments.

We will explain in detail how nuclear resonant inelastic X-ray scattering can provide experimental information regarding phonon density of states and elastic properties at pressures close to the Earth's outer core conditions. Specifically, experimental data for Fe to 153 GPa, Fe-Ni(7.5at%) to 110 GPa, and FeO-FeMgO to 120 GPa will be presented.

This work was done in collaboration with H. K. Mao and R. J. Hemley (Geophysical Laboratory, Washington, DC), W. Sturhahn and E. Alp (Advanced Photon Source, Argonne, IL), W. Mao (University of Chicago), E. Huang (Institute of Earth Sciences, Taiwan), and G. Shen (GSECARS and University of Chicago, Argonne, IL).

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LATEST DEVELOPMENTS IN LASER HEATING OF DIAMOND ANVIL CELLS AT VERY HIGH PRESSURE

D. Andrault[1] E. Schultz[2] M. Mezouar[3] G. Fiquet[4]
Institut De Physique Du Globe De Paris Laboratoire Des Geomateriaux 4 Place Jussieu PARIS 75252 FRANCE

The last decade has seen the development of very bright third generation X-ray synchrotron sources that have significantly improved X-ray diffraction experiments at high-pressure and high-temperature. In the same time, focusing optics as well as detectors have been improved in such a way that X-ray diffraction experiments can be routinely carried out on samples in laser-heated diamond anvil-cell, i.e. under extreme static pressure and temperature conditions. It is now possible to obtain from a laser heated (LH) sample in a diamond anvil cell (DAC) very high quality powder patterns, needed for accurate *in situ* phase boundary and PVT equation of state determinations, as well as for structural refinements. The set-up for *in situ* X-ray investigation at simultaneous high pressure and temperature is complex, since perfect alignment of X-ray path, infrared-laser hot spot, and optical temperature measurement is required. It provides, however, the most accurate information on the structural behavior with step by step increases of pressure and temperature. In addition, a range of experiments can also be realized at room-temperature after laser-annealing of DAC samples, which has been shown very efficient in releasing stresses build on compression, and/or overcoming phase transitions kinetic barriers.

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TEACHING MACROMOLECULAR CRYSTALLOGRAPHY: INTEGRATING THEORY WITH 'HANDS-ON' EXPERIENCE

W. Furey
Veterans Affairs Medical Center Biocrystallography Laboratory, Bldg 6 University Drive C PO Box 12055 PITTSBURGH PA 15240 USA

Effective teaching of macromolecular crystallography can be a daunting task, particularly when it must be done in a short time and to people with diverse backgrounds. For more than a decade now a two-week course dealing with the subject has been offered annually at Cold Spring Harbor Laboratories. It is an intensive, thorough, and constantly evolving course that provides the necessary background and experience to pursue independent protein structure determination. In the course students attend theoretical lectures, and alternately carry out laboratory 'practicals' experiencing how things are actually done both in the wet lab and computationally. The students start with a protein sample, grow crystals, collect synchrotron data, solve for heavy atom/anomalous scatterer sites, phase the data, compute and fit electron density maps, and refine the structure. The course has been extremely successful as it is always highly oversubscribed, and many alumni have since established productive research groups involving structure determination. In order for the course to be so successful careful attention must be paid to many areas, both scientific and logistic. These areas include: (1) applicant selection; (2) well equipped laboratories, lecture hall, cafeteria, and housing, all in close proximity; (3) unrestricted access to labs and enthusiastic support by host personnel; (4) a cohesive set of 'core' instructors; (5) appropriate guest instructors and speakers; (6) numerous reference books and handouts; (7) local stockpile of 'essentials,' and a way to make it 'fun.' How the course works and the topics covered will be described in detail.

Keywords: TEACHING PROTEIN CRYSTALLOGRAPHY