DF 3: SYCM - Crystallography in Materials Science (Joint Session with KR)

Time: Monday 15:00–17:45 Location: HSZ 02

Invited Talk DF 3.1 Mon 15:00 HSZ 02

Complexity on Compression: The Crystallography of High-Density Matter — •Malcolm McMahon — School of Physics and Astronomy, The University of Edinburgh, Edinburgh, UK.

The crystal structure of iron was determined at *normal* conditions as long ago as 1917. But what is the structure of iron within *Super-Earth* exoplanets where core conditions approach 10 million atmospheres (1 TPa) and 10,000 K, and where carbon exists as either diamond, or as an exotic metallic form.

Until the early 1990s, the consensus was that at high pressures, all materials would become metallic, and assume high-symmetry, close-packed crystal structures. But the advent of modern crystallographic methods on synchrotron sources in the early 1990s revealed completely different behavior: even the simplest materials underwent phase transition to complex, frequently incommensurate, forms, while metals became semiconductors or insulators. This complexity is thought to arise from the constraints placed on the electronic wave functions due to the Pauli exclusion principle, the need to orthogonalise the wave functions of both core and valence electrons, and the reduction in the available interstitial space at high compression

In this talk I will present results from recent diffraction studies of elemental metallic systems showing some of the extreme complexity observed at high pressures. I will also look at the new opportunities in extreme conditions crystallography offered by x-ray lasers such as the LCLS in the Stanford, and XFEL in Hamburg.

Invited Talk DF 3.2 Mon 15:30 HSZ 02

X-Ray Microscopy with Coherent Radiation: Beyond the Spatial Resolution of Conventional X-Ray Microscopy — •Christian G. Schroer — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany

Hard x-ray microscopy has greatly benefited from the high brilliance of modern synchrotron radiation sources and x-ray free-electron lasers (XFELs). Today, the spatial resolution of conventional x-ray microscopes is limited by the x-ray optics to a few tens of nanometers. Scanning coherent diffraction microscopy, also known as ptychography, can overcome this limitation. In ptychography, the sample is scanned through a confined coherent beam, recording at each location of the scan a far-field diffraction pattern. From these data, the complex transmission function (projected complex refractive index) of the sample and the illuminating complex wave field can be reconstructed with a spatial resolution that clearly exceeds the lateral size of the illuminating beam. The spatial resolution in a ptychogram is shown to depend on the shape (structure factor) of a feature and can vary for different features in the object. In addition, the resolution and contrast depend on the coherent fluence on the sample. For an optimal ptychographic x-ray microscope, this implies a source with highest possible brilliance and an x-ray optic with a large numerical aperture to generate the optimal probe beam. Ptychography closes the gap between real space imaging and reciprocal space structure determination and merges these two fields.

[1] A. Schropp, et al., Appl. Phys. Lett. **100**, 253112 (2012).

Invited Talk DF 3.3 Mon 16:00 HSZ 02

Modulated martensite: A scale bridging Lego game for crystallographers and physicists — •Sebastian Fähler — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, 01062 Dresden, Germany — Technische Universität Chemnitz, Faculty of Natural Sciences, Institute of Physics, D-09107 Chemnitz, Germany

Among various materials exhibiting reversible phase transformations structures with low crystal symmetry, so-called modulated phases, exhibit the best ferroelectric, magnetocaloric or magnetic shape memory properties. Here it is describe how modulated martensite can be built in a kind of Lego game from simple tetragonal building blocks. It's complex crystallographic (micro-) structure is determined by the boundary conditions during the nucleation process. Though this building principle can be describe in terms of continuum mechanics, it is consistent with first principle calculations. Supported by SPP 1239 and SPP 1599.

15 min break

Invited Talk DF 3.4 Mon 16:45 HSZ 02

Switching of magnetic domains reveals evidence for spatially inhomogeneous superconductivity — •Michel Kenzelmann — Paul Scherrer Institut

The interplay of magnetic and charge fluctuations can lead to novel quantum phases with exceptional electronic properties. Magnetic order in such quantum phases can fundamentally affect the underlying symmetry and generate new physical properties. Importantly, it has been predicted that spin-density wave (SDW) order in a singlet d-wave superconductor is coupled to triplet superconductivity. We performed neutron diffraction studies of the Q-phase SDW [1] in $CeCoIn_5$, and we make two important observations [2]. We observe a complete and extremely sharp SDW domain switching that is unexplained by current microscopic theories for $CeCoIn_5$. Using representational theory, we interpret our experimental results as evidence for the presence of p-wave superconductivity that coexists with d-wave superconductivity and SDW order. The triplet component is of p-wave symmetry, similar to that found in the A-phase of superfluid ^{3}He, and is modulated as a Cooper pair density wave. Our findings identify the Q-phase as a unique quantum phase where d-wave and modulated p-wave superconductivity are coupled to SDW order, and which emerges in a magneto-superconducting quantum critical point [2].

[1] M. Kenzelmann et al, Science 321, 1652 (2008). [2] S. Gerber et al, submitted to Nature Physics (2013).

Invited Talk DF 3.5 Mon 17:15 HSZ 02

The key role of magnetic neutron diffraction in materials science — •Laurent C. Chapon — Institut Laue-Langevin, Grenoble, France

Since the 1950s, neutron scattering, and more specifically diffraction, has been a tool of choice for studying magnetism at the atomic scale. From the very first experimental proof of antiferromagnetism, a phenomenon predicted by Louis Néel, to unveiling how complex multiferroic materials work, the technique has always offered information of crucial importance to build the physical models that are required to explain macroscopic properties of materials. I will review briefly the historical development of magnetic neutron scattering and present key neutron diffraction experiments in recent areas of interest for condensed matter physicists, in particular highlighting the use of the technique for multiferroics and frustrated magnetic systems.