COHERENT X-RAY DIFFRACTION

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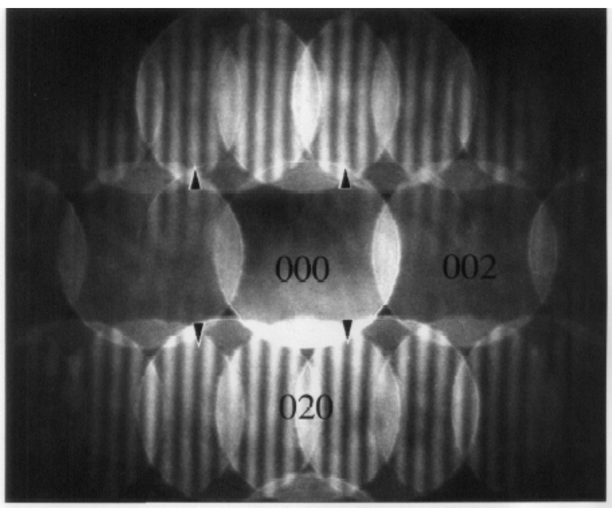
Ph.D. Project vacancies in the area of Coherent X-ray Diffraction.

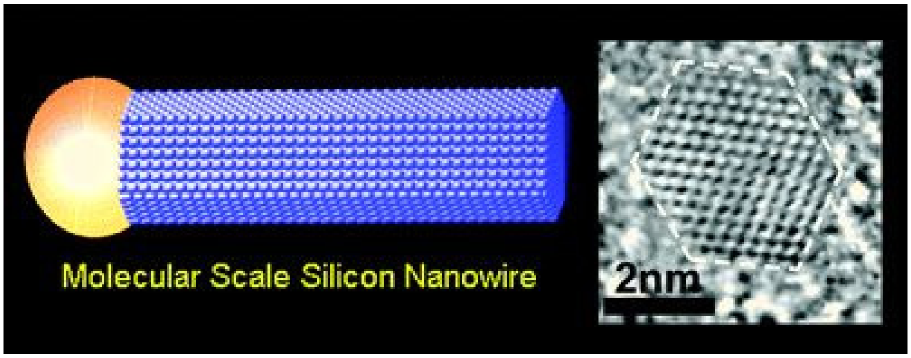
Our group is developing the methodology of using the coherence of the latest X-ray sources, synchrotron and free-electron laser. The method of Coherent X-ray Diffraction (CXD) is now ripe for exploitation. The X-ray experiments are carried out at central facilities, ESRF (Grenoble), APS (Chicago), Diamond (Oxford) and XFEL (Hamburg). Our group presently operates a beamline at APS for developing the techniques. Students joining the group should be prepared for some component of travel to use these facilities.

Project 1. X-ray Ptychography.



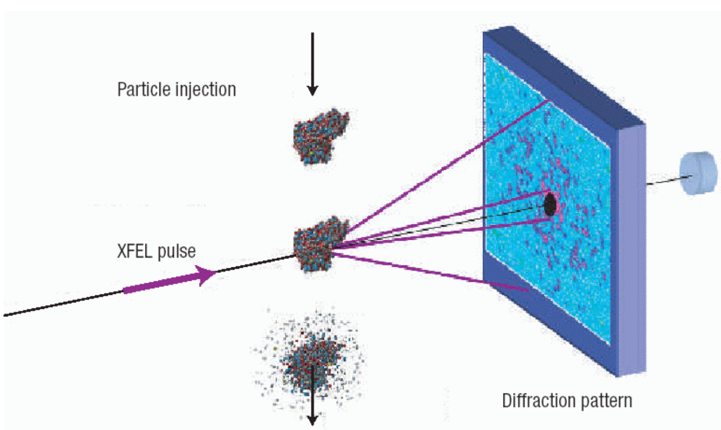
The project will develop the methodology of X-ray Ptychography, which is the simultaneous inversion of diffraction patterns measured from overlapping regions of a sample. This will be used to investigate domain-wall structures in alloys and oxides, but the scope will expand to include other nanoscale materials and biological samples. The resulting sets of overlapping diffraction patterns will be inverted using a ptychography algorithm, which exists already but will require further development.

Project 2. Structure of nanowires



CXD methods will be used to study individual Silicon Nanowires (SiNWs) to look for evidence of strain fields. The diameters of these, in the range 20-80nm, are considerably smaller than the 500-1000nm crystals of Au and Pb previously studied. The scattering cross section of Si is also considerably smaller. It is therefore essential to focus the beam. This is possible using Kirkpatrick-Baez (KB) mirror optics, which are available at the APS 34-ID-C beamline, but this must be achieved without spoiling the coherence. The lateral coherence lengths inherent to the 3rd generation undulator sources, like the APS, are in the range of 10 microns, which is rather wasteful to study nanometre-sized objects. Focusing of a fully coherent beam down to one micron, achievable with the KB optics that preserve the coherence in the same way as a lens, can improve the flux by several thousand times. The diffraction from a small object being more spread out means that the additional divergence, a consequence of Liouville's theorem, can still be tolerated. Nanowire samples will be prepared by the Vapour-Liquid-Solid (VLS) method using a eutectic catalyst, which will also act as a support structure. Rich patterns of strain are expected inside the wires as a consequence of the growth conditions.

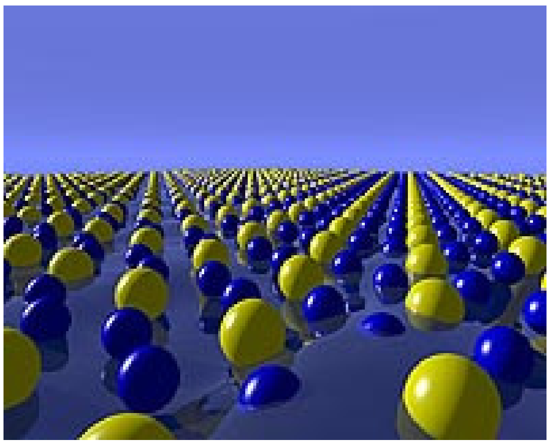
Project 3. Single molecule imaging



Hard X-ray free-electron laser X-ray sources have not yet been built, but will exist one day at Stanford and Hamburg. Such a source will be able to capture the diffraction pattern of a single molecule in a single flash of duration 10-20 femtoseconds. It is predicted that the diffraction pattern will emerge *before*

the molecule is destroyed by the radiation dose. Before the sources are available, we are developing the methods that will be used one day for this purpose:
i) massively parallel X-ray detectors
ii) inversion algorithms for phasing the diffraction
iii) x-ray optics for focusing the beam while preseving its coherence
iv) test experiments with synchrotron radiation on nanocrystals

Project 4. Au-Si Eutectic Structures



In our coherent diffraction (CXD) work to date, we have observed that drops of Au can be created by thermal dewetting of an evaporated film of the appropriate thickness, at least on an inert SiO_2 substrate, and that these can crystallise into randomly-oriented crystals.   Dewetting upon heating of Au deposits on UHV-clean Si will produce similar particles, and subsequent intermixing with the substrate should cause a eutectic phase to separate. Because it is liquid, a eutectic phase is very hard to identify, but, with the new information that it has a unique ordered surface structure over a certain temperature range, this can now be achieved by surface diffraction methods. This will be studied by tracking the texture changes as a function of time and the breakup of the powder ring into discrete Bragg spots from the individual crystals. Evidence of Au-Si intermixing will be sought by the formation of the eutectic-related surface-crystallised phase recently seen by Shpyrko et al (PRL). Interesting structures are expected to arise associated with the characteristic melting behaviour of the eutectic at 380C.