Isotropic Debye-Waller factor measurements for Cu, $SrTiO_3$ and GaAs using digital electron diffraction

Hubert, A.[1], Beanland, R.[1] and Roemer, R.[1]

[1] University of Warwick, United Kingdom

As we heat or cool crystals, atoms vibrate relative to their nominal equilibrium positions. This property can be probed by the change in intensity of scattering events with temperature. The effect on scattering strength may be given by an envelope function describing the probability density of an atom's time-averaged position, whose Fourier transform is commonly known as the Debye-Waller factor (DWF).

In electron diffraction, as in other forms of diffraction, increased thermal vibrations produce diffuse scattering between Bragg diffracted beams. However, they also have a strong and distinctive effect on elastically scattered electrons that is not just a simple attenuation of diffracted intensity. We present a study of three materials using Digital Large Angle Convergent Beam Electron Diffraction (D-LACBED), using computer control to capture thousands of individual diffraction patterns. These are combined to give data covering a relatively large range of incidence angles, from a region of crystal a few tens of nm in size. We show that refinement of isotropic DWFs to match simulation with experiment can be performed efficiently and quickly, even in the simplistic independent atom model (IAM), i.e. using neutral spherical atoms. Furthermore, the results are comparable to X-ray, neutron and Mossbauer scattering experiments [1].

Significant residual differences between simulation and experiment are present. These are due to anisotropy, anharmonicity, charge transfer and bonding. It seems likely that these contributions could also be quantified by refinement of suitable models against D-LACBED data. Since electron diffraction is inherently more sensitive to these effects and can be obtained from nanoscale regions, there is great potential for new and exciting work in this area.

1. Shukla RC, Sternin E (1996) Philos Mag B 74:1 - 11

Acknowledgement: This work has been financially supported by the EPSRC

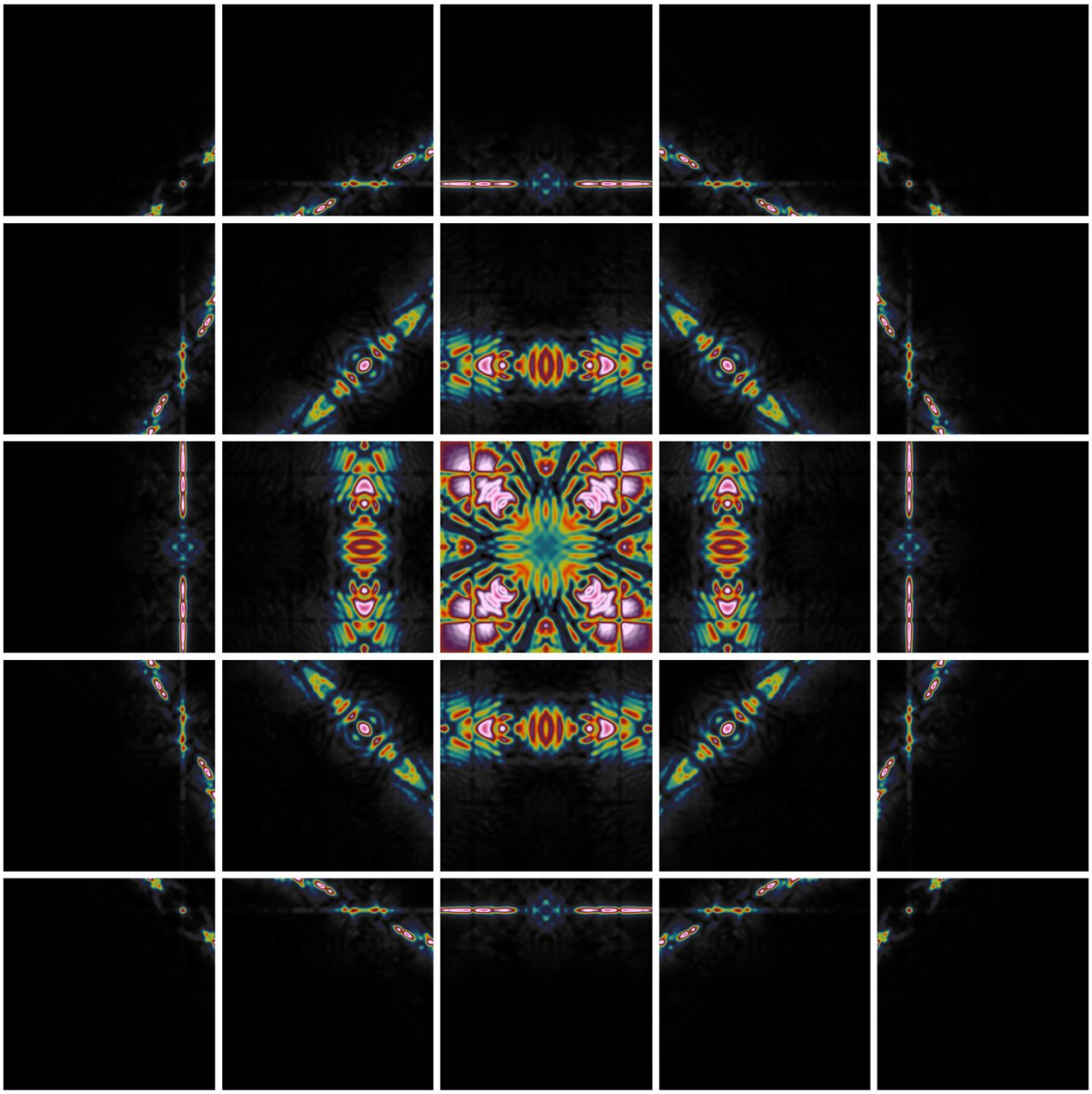

Fig 1. Simulated D-LACBED pattern of Cu in the [001] direction