

Phase Structure due to Refraction in Coherent X-ray Diffraction

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We have recently succeeded in obtaining full three dimensional complex density maps of a lead nanocrystal, prepared in UHV in our beamline at APS. Quantitative maps of the deformation of the crystal from its equilibrium lattice spacing have been obtained by iterative phasing and hence inversion of the coherent X-ray diffraction pattern [1]. Generally, the interpretation of the phase in such maps offers novel opportunities for mapping strain fields in nanocrystals. However the interpretation of the phase map requires careful consideration of the effects of refraction, which are considered in this presentation. The refraction effect can be calculated completely without adjustable parameters. Once corrected for refraction our image shows a distinct expansion of the surface layers at a temperature just below the melting point. Over most of the surface of the crystal there is a clear outward displacement, which decays exponentially into the bulk. The displacement is suppressed on the (111) facet itself and stronger on the surrounding regions, indicating an orientational variation in surface stress.

[1] M. A. Pfeifer et al, Nature **442** 63-66 (2006)