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Authors

O'Keefe, Michael A.
Allard, Lawrence F.
Downing, Kenneth H.

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Atomic-Resolution Tomography

Michael A. O'Keefe*, Lawrence F. Allard** and Kenneth H. Downing***

**Materials Sciences Division, LBNL 2-200, 1 Cyclotron Road, Berkeley, CA 94720, USA*

***Metals and Ceramics Division, ORNL, Oak Ridge, TN 37831-6064, USA*

****Life Sciences Division, LBNL Donner, 1 Cyclotron Road, Berkeley, CA 94720, USA*

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Atomic Resolution Tomography

Michael A. O'Keefe*, Lawrence F. Allard** and Kenneth H. Downing***

*Materials Sciences Division, LBNL 2-200, 1 Cyclotron Road, Berkeley, CA 94720, USA

**Metals and Ceramics Division, ORNL, Oak Ridge, TN 37831-6064, USA

***Life Sciences Division, LBNL Donner, 1 Cyclotron Road, Berkeley, CA 94720, USA

High-resolution electron-beam tomography is a promising technique to produce the three-dimensional structure of nanoparticles (and other suitable specimens) at atomic resolution.

Conventional tomography has been used to produce reconstructed 3D images of nanoparticles¹, but accurate three-dimensional reconstruction from two-dimensional projections requires that intensity in the series of 2-D images be a monotonic function of the specimen structure (usually density, but in our case atomic potential). This condition is not satisfied in electron microscopy when specimens with strong periodicity are tilted close to zone-axis orientation and produce "anomalous" image contrast because of a strong dynamic diffraction component. Attempts at atomic-resolution reconstruction from tilt series containing zone-axis images (with contrast enhanced by strong dynamical scattering) are distorted when these strong images overwhelm those obtained in other "random" orientations where the atoms do not line up in neat columns.

On the other hand, it has been shown that 3-D atomic resolution reconstruction is possible using only zone-axis images from specimens that are thin in the beam direction or that consist predominantly of light atoms. Downing et al.² used images obtained in five zone-axis projections ([100], [010], [001], [101] and [310]), but needed to prepare three different specimens to achieve the five directions (so it wasn't really tomography).

It is feasible to combine ultra-high (sub-Ångstrom) resolution zone-axis images with off-zone images by first using linear reconstruction of the off-zone images whilst excluding images obtained within a small range of tilts (of the order of 60 milliradian) of any zone-axis orientation. The (partial) reconstruction can then be used as a model for forward calculation (image simulation) in zone-axis directions and the structure refined iteratively to achieve satisfactory fits with the experimental zone-axis data.

Another path to atomic-resolution tomography combines "zone-axis tomography" with high-resolution dark-field hollow-cone imaging. Electron diffraction theory indicates that dynamic (multiple) scattering is much reduced under highly-convergent illumination. DFHC TEM is the analog of HAADF STEM, and imaging theory shows that image resolution can be enhanced under these conditions. Image data obtained in this mode will provide the initial reconstruction, with zone-axis images used for refinement.³

¹ "3D electron microscopy in the physical sciences: the development of Z-contrast and EFTEM tomography" P.A. Midgley and M. Weyland, *Ultramicroscopy* **96** (2003) 413-431.

² "Resolution of oxygen atoms in staurolite by three-dimensional transmission electron microscopy", Kenneth H. Downing, Hu Meisheng, Hans-Rudolf Wenk and Michael A. O'Keefe, *Nature* **348** (1990) 525-528.

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