Atomic Resolution Electron Tomography for 3D Imaging of Dislocations in Nanoparticles

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Dislocations and their interactions strongly influence many of the properties of materials, ranging from the strength of metals and alloys to the efficiency of light-emitting diodes and laser diodes. Although various experimental methods have been used to image dislocations in materials since 1956, a 3D technique for visualizing dislocations at atomic resolution has not previously been demonstrated. Here we report the development of atomic resolution electron tomography and achieve 3D imaging of dislocation core structures of a Pt nanoparticle at atomic resolution. Compared to conventional electron tomography, our atomic resolution imaging method incorporates three novel developments. First, the conventional alignment approach used in electron tomography either relies on fiducial markers or is based on the cross-correlation between neighboring projections. To our knowledge, neither of these alignment approaches can achieve atomic level precision. To overcome this limitation, we have developed a method based on the center of mass (CM), which is able to align the projections of a tilt series at atomic level accuracy. Second, we have implemented a data acquisition and tomographic reconstruction method, termed equally sloped tomography (EST). Compared to conventional tomography that reconstructs a 3D object from a tilt series of projections with constant angular increments, EST acquires a tilt series with equal slope increments, and can achieve much better 3D reconstructions from a limited number of projections with a missing wedge. Third, to enhance the signal to noise ratio in the reconstruction, we have developed a 3D Fourier filtering method and applied it to the EST reconstructions. 

After incorporating these three novel developments, we achieve atomic resolution electron tomography and observe nearly all the atoms in a multiply-twinned Pt nanoparticle. We find the existence of atomic steps at 3D twin boundaries of the Pt nanoparticle. The 3D core structure of edge and screw dislocations are also observed at atomic resolution in the Pt nanoparticle. Figs. 1a and b show a 7.9 Å thick internal slice of the nanoparticle and a zoomed view of an edge dislocation, where red dots label the position of atoms. By computationally sectioning through the 7.9 Å thick slice, three consecutive atomic layers with 2.6 Å thick (Figs. 1c-e) are obtained. Fig. 2b shows a zoomed view of the slice where the zigzag pattern, a characteristic feature of a screw dislocation, is visible. To better visualize the screw dislocation, surface renderings of the zoomed region are displayed in Fig. 2c where the atoms in green are on the top layer and those in red in the bottom layer.
The significant impact of this technique is that 3D atomic resolution imaging not only allows scientists to observe new structural information that is not visible in conventional 2D projections, but also provides the atomic positions as the initial model in the theoretical ab-initial calculation, thus advancing our fundamental understanding of dislocations in materials.

References:


Figure 1. Observation of the 3D core structure of an edge dislocation at atomic resolution. a, A 7.9 Å thick internal slice of the nanoparticle. b, A zoomed view of an edge dislocation in (a) where red dots represent the position of the atoms. c, d and e, 2.6 Å atomic layers sectioning through the slice of (b). The Burgers vector \( \mathbf{b} \) of the edge dislocation was determined to be \( \frac{1}{2}[10 \bar{1}] \).

Figure 2. Observation of the 3D core structure of a screw dislocation at atomic resolution. a, Volume renderings of a 5.3 Å thick slice in the \( \{\bar{1}11\} \) plane, tilted to the \( [011] \) direction in order to visualize the zigzag pattern. b, Zoomed view of a screw dislocation showing the zigzag pattern. c, Surface renderings of the screw dislocation where the atoms in green are on the top layer and those in red in the bottom layer. The zigzag pattern is more clearly visualized, the Burgers vector \( \mathbf{b} \) of the screw dislocation was determined to be \( \frac{1}{2}[01 \bar{1}] \).