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Atomic Electron Tomography: Adding a New Dimension to See Single Atoms in Materials

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To understand material properties and functionality at the fundamental level, one must know the 3D positions of atoms with high precision. For crystalline materials, crystallography has provided this information since the pioneering work of Max von Laue, William Henry Bragg, and William Lawrence Bragg over a century ago. However, perfect crystals are rare in nature. Real materials often contain crystal defects, surface reconstructions, nanoscale heterogeneities, and disorders, which strongly influence material properties and performance. Here, we present atomic electron tomography (AET) for 3D structure determination of crystal defects and disordered materials at the single-atom level (1). Using powerful Fourier-based iterative algorithms (2,3), we first demonstrated electron tomography at 2.4-Å resolution without assuming crystallinity in 2012 (4). We then applied AET to image the 3D structure of grain boundaries and stacking faults and the 3D core structure of edge and screw dislocations at atomic resolution (5). Furthermore, in combination of AET and atom tracing algorithms, we localized the coordinates of individual atoms and point defects in materials with a 3D precision of ~19 pm, allowing direct measurements of 3D atomic displacements and the full strain tensor (6). More recently, we determined the 3D coordinates of 6,569 Fe and 16,627 Pt atoms in an FePt nanoparticle, and correlated chemical order/disorder and crystal defects with material properties at the individual atomic level (7). We identified rich structural variety with unprecedented 3D detail including atomic composition, grain boundaries, anti-phase boundaries, anti-site point defects and swap defects. We showed that the experimentally measured coordinates and chemical species with 22 pm precision can be used as direct input for density functional theory calculations of material properties such as atomic spin and orbital magnetic moments and local magnetocrystalline anisotropy (7). Looking forward, AET will not only advance our ability in 3D atomic structure determination of crystal defects and disordered materials, but also transform our understanding of materials properties and functionality at the single atomic level [8].

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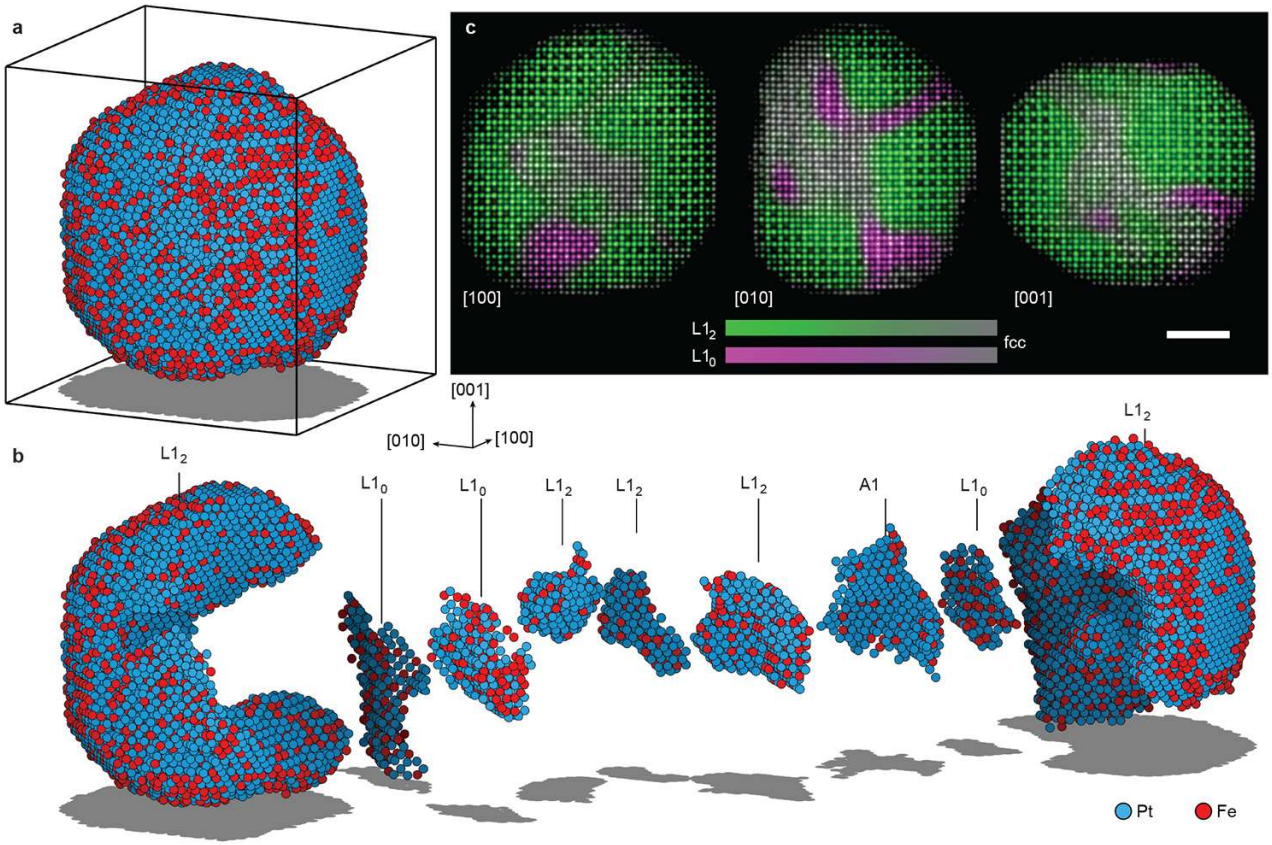

Figure 1. 3D determination of atomic coordinates and chemical order/disorder of an FePt nanoparticle. (a) Overview of the 3D positions of individual atomic species with Fe atoms in red and Pt atoms in blue. (b) The nanoparticle consists of two large L12 grains, three small L12 grains, three small L10 grains and a Pt-rich A1 grain. (c) Multislice images obtained from the experimental 3D atomic model along the [100], [010] and [001] directions, where several 'L10 grains' (magenta) appearing in the 2D images are deceptive structural information. Scale bar, 2 nm.

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