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Atomic Electron Tomography: Probing 3D Structure and Material Properties at the Single-Atom Level

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Perfect crystals are rare in nature. Many of the real materials contain crystal defects and chemical order/disorder including grain boundaries, dislocations, interfaces, surface reconstructions and point defects that disrupt the periodicity of the atomic arrangement and determine their properties and performance [1-3]. One prominent example is intermetallic compounds involving two or more atomic species, in which chemical order/disorder determines their mechanical, catalytic, optical, electronic and magnetic properties [4-6]. For instance, as-synthesized at room temperature, FePt nanoparticles and thin films with a near-1:1 composition have a chemically disordered fcc structure (A1 phase) [5,7,8]. When annealed at high temperatures, they undergo a transformation from an A1 phase to an ordered face-centered tetragonal ($L1_0$) phase. Due to the chemical ordering and strong spin-orbit coupling [8], $L1_0$ FePt exhibits extremely large magnetocrystalline anisotropy energy (MAE) and is among the most promising candidates for next-generation magnetic storage media [7]. However, although this material system has attracted considerable attention, a fundamental understanding of 3D chemical order/disorder, crystal defects and its magnetic properties at the individual atomic level remains elusive.

Using atomic electron tomography (AET) [1,9-14], we determine the 3D coordinates of 6,569 iron and 16,627 platinum atoms in an FePt nanoparticle to correlate the 3D atomic structure with material properties at the single-atom level [15]. We identify rich structural variety and chemical order/disorder including 3D atomic composition, grain boundaries, anti-phase boundaries, anti-site point defects and swap defects. We show for the first time that experimentally measured 3D atomic coordinates and chemical species with 22 pm precision can be used as direct input for first-principles calculations of material properties such as atomic magnetic moments and local magnetocrystalline anisotropy. This work not only opens the door to determining 3D atomic arrangements and chemical order/disorder of a wide range of nanostructured materials with high precision, but also will transform our understanding of structure-property relationships at a fundamental level [16].

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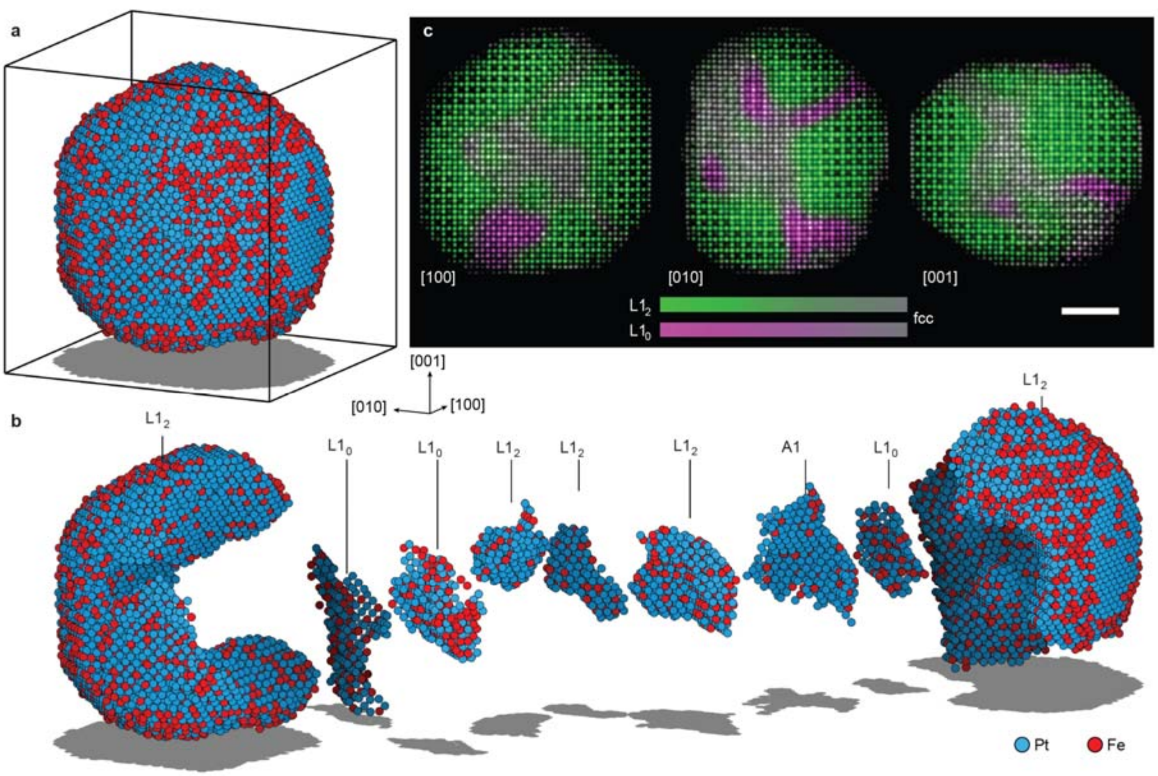

Figure 1. **3D determination of atomic coordinates, chemical species and grain structure of an FePt nanoparticle**. **a**, Overview of the 3D positions of individual atomic species with Fe atoms in red and Pt atoms in blue. **b**, The nanoparticle consists of two large $L1_2$ grains, three small $L1_2$ grains, three small $L1_0$ 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 ‘$L1_0$ grains’ (magenta) appearing in the 2D images are deceptive structural information. Scale bar, 2 nm. [Ref. 15]

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