Determining Atomic Coordinates in 3D by Atomic Electron Tomography

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Scanning transmission electron microscopy is an important technique in materials science to examine the atomic structure of materials with sub-Å resolution and single-atom sensitivity [1]. Combining this imaging tool with powerful iterative 3D reconstruction algorithms for electron tomography is opening a new field called atomic electron tomography (AET) with the ability to determine the coordinates of atoms in a structure without the assumption of crystallinity [2]. This talk will cover recent develops in AET, which will be critical to our understanding of the atomic structure of complex materials systems. The details of the AET acquisition and reconstruction method, atom tracing procedure and atomic scale quantitative analysis will be presented using a recent 3D atomic resolution reconstruction of a FePt nanoparticle [3].

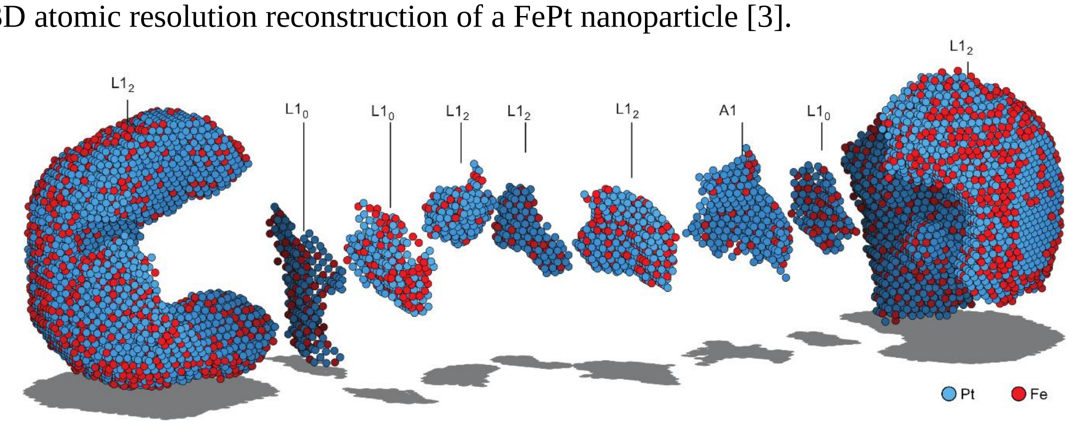

Figure 1. The nanoparticle consists of multiple FePt grains (type L1$_0$ and L1$_2$) and a Pt-rich A1 grain.

References

[1] S.J. Pennycook and P.D. Nellist. Scanning Transmission Electron Microscopy: Imaging and Analysis, Springer, NY, 2011.
[2] J. Miao, *et al.*, Atomic electron tomography: 3D structures without crystals, Science 353 (2016), aaf2157.
[3] Y. Yang, *et al.*, Deciphering chemical order/disorder and material properties at the single-atom level, Nature 542 (2017), 75–79.