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Convergent beam electron diffraction of ordered $L1_0$ nanoparticles

Rumyana V. Petrova*, Richard R. Vanfleet**, Daniel R. Richardson**, Bo Yao*, and Kevin R. Coffey*

* Advanced Materials Processing and Analysis Center (AMPAC), University of Central Florida, Orlando, FL 32816-2455
** Department of Physics and Astronomy, Brigham Young University, Provo, UT 84602

We have determined the long-range order parameter of individual [001] oriented FePt $L1_0$ nanoparticles. Measurement of convergent beam electron diffraction intensities of single particles in scanning transmission electron microscopy (STEM) mode, and comparison of the measured intensities to multislice simulations of diffracted beam intensities allow determination of the order parameter of the particle.

FePt films were prepared by co-sputtering high purity Fe and Pt targets onto SiO2/Si substrates using ultra high vacuum dc magnetron sputtering. Ex-situ anneals between 500°C and 800°C in one atmosphere of a flowing reducing gas, argon with 3% hydrogen, were used to stabilize the isolated cluster morphology and to induce ordering. The composition of the Fe-Pt deposit was measured by Rutherford backscattering spectrometry (RBS) and determined to be 50 ±0.5 atomic % Fe.

The CBED patterns were simulated with a multislice approach [1] for [001] oriented particles under conditions matching the experiment. The multislice approach specifically includes important dynamical scattering effects. Thermal effects were included using the frozen phonon method with root-mean-square deviations from the atomic positions of 0.007 nm for Fe and 0.0063 nm for Pt (estimated from the international table for X-ray crystallography [2]). The order parameter is included by statistically weighting each site in the structure with the correct fraction of the atomic species found on those sites. An example simulated CBED pattern is shown in Fig 2. In Fig. 3 we show the simulated I_{110}/I_{220} intensity ratio as a function of changing order parameter (S) for several thicknesses close to the observed particle thickness. Also in Fig 3 are two examples of experimental intensity ratios and the corresponding range of order parameter.

Single particle diffraction data was acquired in the STEM mode of the TEM. A convergent beam of 4 mrad convergence semi-angle was focused on the specimen, and CBED patterns were collected from the ordered particles. The 4 mrad angle was chosen to give minimal overlap between the diffracted disks. Fig 4 shows an [001] oriented particle CBED pattern after subtraction of an off-particle background pattern.

Dynamical scattering effects are seen in the oscillatory nature and flattening of the curves in Fig 3. This introduces uncertainties in the measurements of order parameter. With those uncertainties taken into account, the order parameter for the two cases shown is determined to be S = 0.4±0.1 and S=0.62±0.24 [3].

References

[1] E.J.Kirkland: *Advanced Computing in Electron Microscopy*, Plenum Press, New York, 1998.
[2] International Tables for X-ray Crystallography Vol. III, Editors C. MacGillavary, G Rieck, Kynoch Press, Birmingham, 1962.
[3] This work was supported by the U.S. National Science Foundation grant ECS-0304005

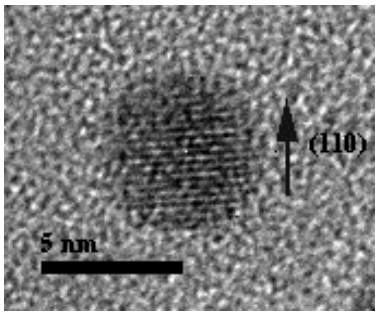

Fig. 1. High resolution image of an $L1_0$ FePt ordered particle

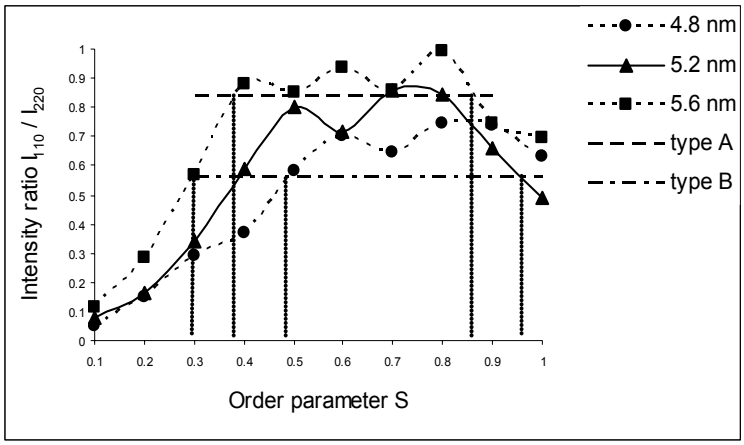

Fig. 3. Order parameter dependence on the intensity ratio, determined by the multislice simulation is shown with the curves for three thicknesses. The horizontal lines (type A and B) correspond to experimentally obtained intensity ratios, and the vertical lines mark the range of the *S* values

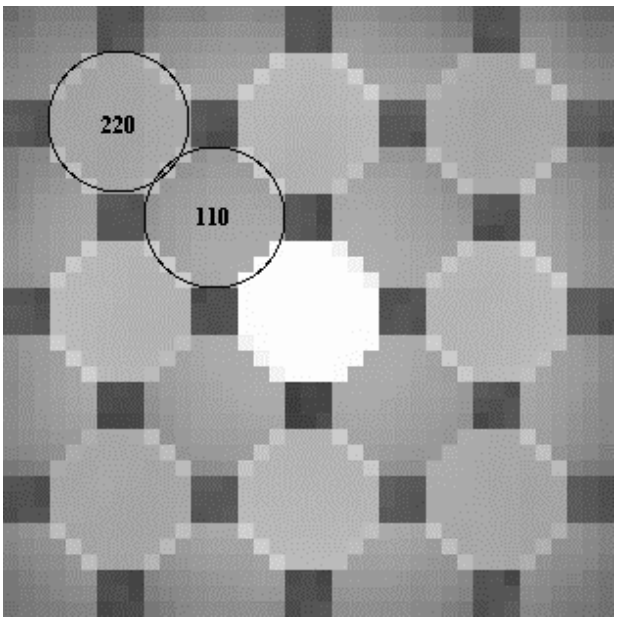

Fig. 2. Simulated CBED pattern for [001] FePt, thickness 5.2 nm and order parameter 0.7. The central bright disk is the direct beam, and the dark circles mark the locations of (110) and (220) diffraction peaks

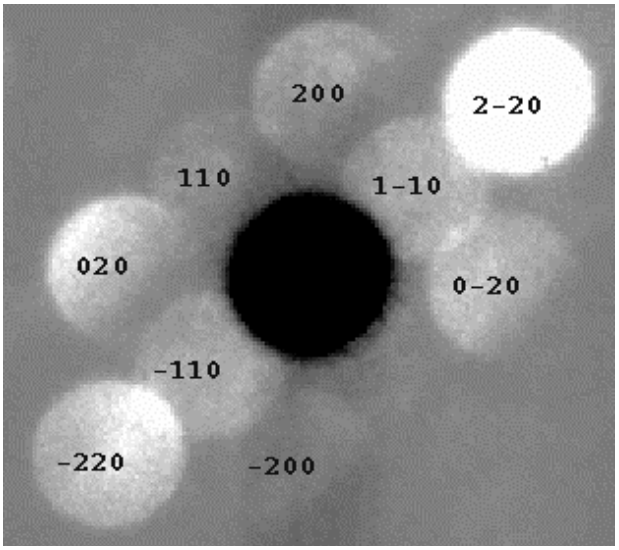

Fig. 4. Experimental, corrected for background CBED pattern of a [001] $L1_0$ FePt oriented nanoparticle

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