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Long-Range Order Parameter Determination by Convergent Beam Electron Diffraction

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The $L1_0$ phase of Fe-Pt has been identified as a leading candidate for ultrahigh-density magnetic storage media because of its high magnetocrystalline anisotropy, K_u [1]. The K_u of this alloy has been known to be strongly dependent on the long-range order parameter *S*, where K_u decreases with *S* [2]. *S* can be determined by a number of methods. The most readily available technique is x-ray diffraction. Experimentally, *S* is determined by measuring the total integrated peak intensities of the superlattice and fundamental reflections according to kinematical scattering theory [3]. However, the amount of x-ray scattering from thin films can be very small and difficult to measure with laboratory diffractometers. In contrast, electron scattering can be more amenable for diffraction studies of small volumes, though the strong interaction of electrons with the thin film results in multiple scattering events. As a result, the traditional methodology of taking the ratio of integrated intensities no longer applies and *S* determination becomes more complex. In this study, the multislice simulation approach was used to simulate electron transmission in crystalline thin films including dynamical scattering [4] to determine *S* which was then compared to x-ray measurements of *S* on the same films.

An 11.7 nm $Fe_{50}Pt_{50}$ thin film was dc magnetron sputter-deposited from commercially pure Fe and Pt targets onto an MgO <001> substrate heated to a temperature of 500 °C. Post-deposition, the film was annealed at 600°C for 30 minutes in an $Ar/4\%H_2$ atmosphere. The composition of the film was determined by Rutherford backscattering spectrometry (RBS). Convergent-beam electron diffraction (CBED) patterns were experimentally collected using scanning transmission electron microscopy (STEM) in a FEI Tecnai F20 operated at 200 keV. A convergent beam of 4 mrad convergence semi-angle was focused on the specimen to obtain the CBED patterns. This angle was chosen to give the minimal overlap between the diffracted disks. In this experiment, CBED patterns with [001] beam incidence were recorded using a 1k charge-coupled device (CCD) camera using an integration time of 0.5 s.

To correctly account for multi-scattering events of the electrons, a multislice simulation needs to be used to predict the CBED intensities for given order parameters and thicknesses. In this study, the ratio of the (110) superlattice to the (220) fundamental reflection (I_{110}/I_{220}) was used. The input parameters for the multislice simulations were matched to the experimental conditions (*e.g.* convergence semi-angle of 4 mrad; spherical aberration coefficient C_s of 1.35 mm; temperature of 94K; and specimen thickness). Fig. 1a is a simulated CBED pattern for [001] zone axis, order parameter of 0.4, and a film thickness of 11.7 nm. Fig. 2 is the simulated results for the measured film thickness and for thicknesses associated with the estimated error of the measurements.

Fig. 1b is experimental data from the 11.7 nm film. The intensity ratio after background subtraction is 0.60 ±0.05. From Fig. 2, the order parameter from the simulated results was between 0.4 and 0.5. To verify the results obtained by CBED, the order parameter has been determined by traditional diffraction methods using the National Synchrotron Light Source at Brookhaven National Laboratory. The *S* value as determined by this method was 0.47.

It is worth noting that the shape of the curves in Fig. 2 is dependent not only upon the order parameter and thickness but the orientation of the film. Changing the zone axis can have significant effects on the shape of the curves. The effect of order parameter, thickness, and composition on the determination of *S* by CBED will be addressed in this presentation.

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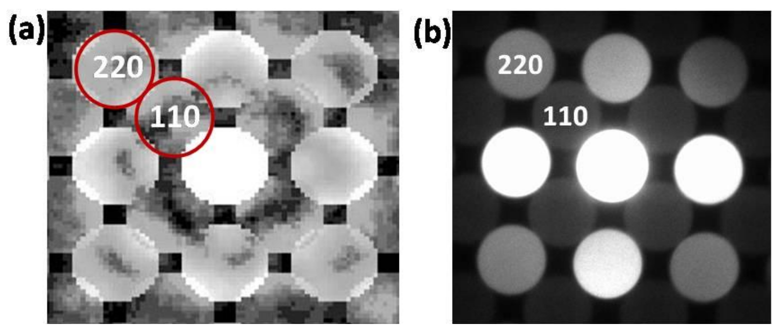

FIG. 1. (a) Simulated CBED pattern of an 11.7 nm $Fe_{50}Pt_{50}$ thin film with an *S* value of 0.4 at 94K. The central bright disk is the direct beam, and the circles mark the locations of the (110) and (220) diffraction peaks. **(b)** Experimental results of the 11.7 nm $Fe_{50}Pt_{50}$film at 94K.

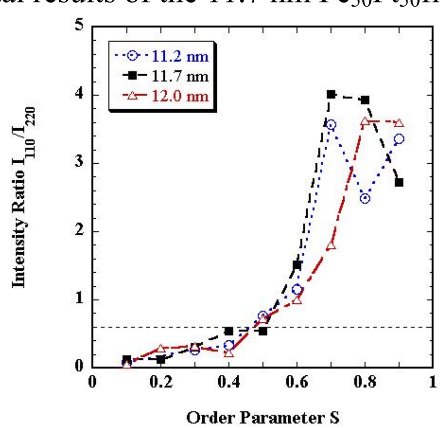

FIG. 2. Simulated intensity ratio as a function of order parameter. The horizontal line corresponds to the experimentally obtained intensity ratio.

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