Structural Rearrangements in the Magnetic Trilayer System: Fe/Pd/Fe on GaAs(001)-(4×6)

P. S. Budnik, R. A. Gordon, E. D. Crozier
Simon Fraser University, Burnaby, British Columbia, Canada

Introduction

The small lateral dimensions of spintronic devices and high-density memory bits require the employment of magnetic ultrathin metallic film structures. In magnetic trilayer systems of the form F/M/F, the magnetic moments in the ferromagnetic film F are locked together by exchange coupling through the nonmagnetic spacer layer M. The magnetic behavior of these systems — the magnetic anisotropy and interlayer coupling — strongly depends on the thickness of the layers, nature of the interface between the layers, strain in the layers, and extent of any interdiffusion or reaction between the layers and substrate. Understanding the structure is critical for correctly interpreting the magnetic behavior. The molecular beam epitaxy facility, MBE-1, was developed for use on the Pacific Northwest Consortium Collaborative Access Team (PNC-CAT) undulator beamline to permit *in situ* epitaxial growth of metal films and to allow their structural characterization by synchrotron radiation techniques.

In an earlier study [1], we used polarization-dependent x-ray absorption fine structure (XAFS) in the total reflection mode to characterize the epitaxial growth of Fe on GaAs(001)-(4×6). The small lattice mismatch of 1.4% between bcc iron (a = 2.866 Å) and GaAs ($a/2$ = 2.827 Å) has made it a model system for growing ferromagnetic materials on semiconductors. It has been found that room temperature growth of Fe on the Ga-terminated 4×6 reconstructed surface of GaAs(001), prepared by mild sputtering and annealing in ultrahigh vacuum (UHV), can prevent magnetic-dead layer formation [2, 3]. Quantitative analysis of our *in situ* XAFS data [1] indicated a body-centered tetragonal (bct) structure with c/a of ~1.03 starting at ~5 ML (monolayers) and persisting to 15 ML, the thickest film studied. This differs from a low-energy electron diffraction (LEED) study [4] that concluded that the Fe layers have a bcc structure. In an *ex situ* study [1] of 10 ML of Fe epitaxially grown on GaAs(001)-(4×6) and capped with 20 ML of Au, we concluded that Fe retains its free-surface bct structure with c/a of 1.03.

Here, we present *in situ* results of a polarization-dependent XAFS study both above and below the critical angle for total reflection from Fe/Pd/Fe trilayers epitaxially grown on GaAs(001)-(4×6). Palladium was chosen as the spacer layer for three reasons. First, Pd is easily influenced magnetically by ferromagnetic species such as iron. Second, Pd has been grown on single-crystal Fe(001) [5], and iron has been grown on single-crystal Pd(001) [6] but with different structural conclusions. Third, the lattice mismatch between the naturally occurring fcc structure of Pd and in-plane lattice of bct Fe grown on GaAs(001)-(4×6) is smaller than it is for single-crystal bcc Fe(001). Thus Pd in the GaAs trilayer system will have a different elastic strain, different structure, and consequently a different magnetic response than when single-crystal substrates of Fe(001) or Pd(001) are used.

Methods and Materials

Samples on GaAs(001)-(4×6) were prepared *in situ* by molecular beam epitaxy (MBE) on epiready GaAs (American Xtal Technology) wafers. Wafer sections were sputtered by using an Ar^+ beam (0.5 keV) at room temperature with continuous azimuthal rotation of the GaAs crystal. The sections were subsequently annealed under UHV conditions (~5×10^{-10} Torr) until (4×6) reconstruction was observed by reflection high-energy electron diffraction (RHEED). Layer deposition was monitored by RHEED, with the number of oscillations of specular (anti-Bragg) spot intensity giving the layer thickness in ML.

Trilayers were grown with different deposition rates and with different layer thicknesses. In the first sample, 30 ML of Fe was deposited. Ar^+ sputtering was then used to remove the less than 1 ML of As that is known to float from the GaAs to the surface during Fe deposition [1]. The sample was annealed, and another 8.5 ML of Fe was deposited at the anneal temperature. Subsequent Pd and Fe overlayers were deposited at room temperature. The Fe and Pd deposition rates were 0.42 and 0.29 ML/min, respectively. In Figs. 1 and 2, this sample is identified with the leading term 30 or 38.5 ML Fe. For the second sample, similar sputtering and annealing processes were followed, but the Fe and Pd deposition rates were 1 and 0.16 ML/min, respectively. Again, the Pd and Fe overlayer growths were made at room temperature. This sample is identified with the leading term 24 ML Fe. The final trilayer systems that were grown were GaAs(001)/38.5Fe/7Pd/10Fe and GaAs(001)/24Fe/8Pd/10Fe. After XAFS measurements, the trilayers were capped with Au to prevent oxidation before *ex situ* magnetic characterization.

XAFS measurements were carried out at different stages in the growth of the samples in the total reflection

mode with an angle of incidence of ~2/3 of the critical angles φ_c for the Fe and Pd K edges, as well as ~$2\varphi_c$. To obtain both in-plane and out-of-plane structural information, polarization-dependent measurements were made with the electric field vector perpendicular and parallel to the surface of the sample.

Results

Inspection of the $\boldsymbol{E}_{||}$ and $\boldsymbol{E}_{\perp}$ EXAFS interference functions of the first layers of Fe for both the 38.5- and 24-ML samples indicates that the Fe films are anisotropic. For example, note that in Fig. 1, when $\boldsymbol{E}_{||}$, the $\chi(k)$'s resemble the $\chi(k)$ of bulk Fe, whereas when $\boldsymbol{E}_{\perp}$, the $\chi(k)$'s are distinctively different, particularly when k is in the range of 3 to 6 Å^{-1}.

Fitting the first two shells gives values for the in-plane and out-of-plane lattice parameters a and c of 2.84 Å and 2.91 Å for the 38.5-ML Fe sample and 2.84 Å and 2.92 Å for the 24-ML Fe sample, respectively. The c/a ratio of 1.03 is unchanged from that found for thinner Fe films [1]. Measurements at angles $\varphi_{in} > \varphi_c$ indicate that depositing 4 ML of Pd does not alter the structure of the underlying Fe. Likewise, the Fe underlayer is unaffected by the overlayer combination 8Pd/10Fe (Fig. 2, $\varphi_{in} > \varphi_c$).

The structure of the Pd, however, depends on its deposition rate, and this affects the Fe overlayers. Preliminary analysis of the Fe overlayers, in which the

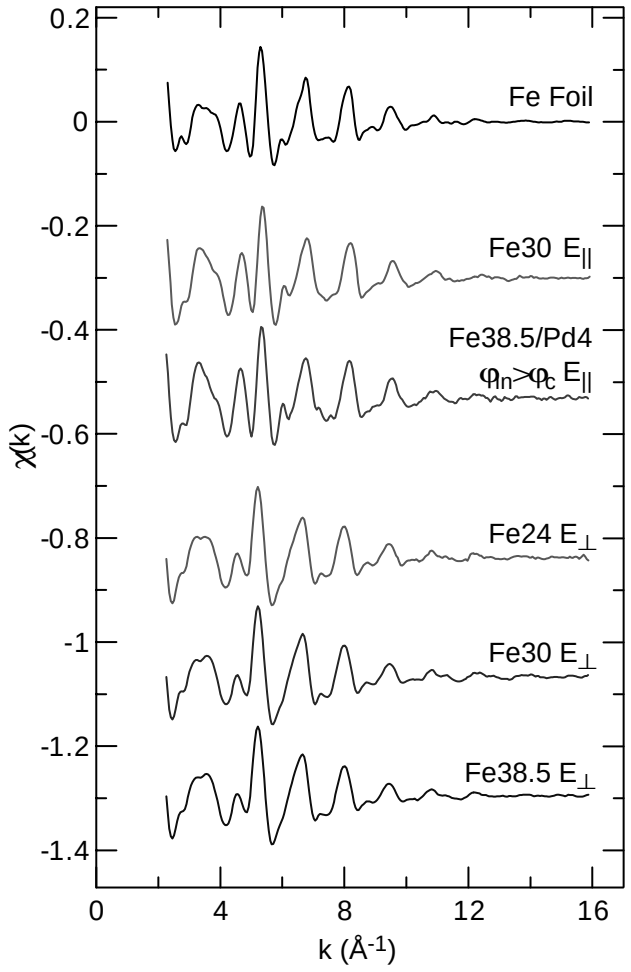

FIG. 1. Fe K-edge EXAFS interference functions for the first layers of Fe. 30 ML is an intermediate stage of growth for 38.5 ML of Fe. The $\chi(k)$'s are displaced for clarity, and the $\chi(k)$ of Fe foil is given for reference.

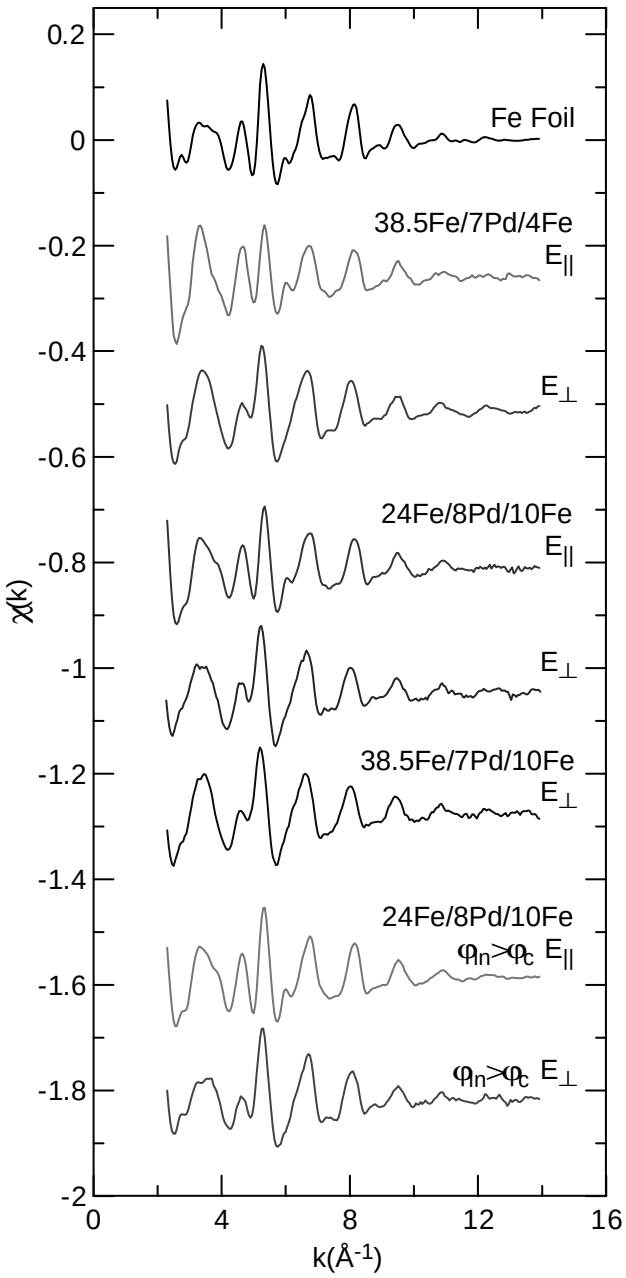

FIG. 2. Fe K-edge EXAFS interference functions for the overlayers of Fe.

presence of the Pd-Fe interface is neglected, gives c/a = 1.02 for 4-ML Fe and c/a = 1.01 for 10-ML Fe in the 24-ML sample.

A comparison of the Pd K-edge $\chi(k)$ (Fig. 3) reveals that the Pd in the 38.5-ML sample is weakly distorted from fcc, while in the 24-ML sample, the distortion is pronounced. When 10 ML of Fe is deposited on 8 ML of Pd, measurements at $\varphi_{in} > \varphi_c$ indicate that the distortion is changed from its structure before the Fe is deposited.

Discussion

Several important findings come from these results. Fe grown on GaAs(001)-(4×6) has a bct structure, independent of deposition rate. There is no indication of a structural relaxation occurring as a function of the thickness of the Fe on top of GaAs: the c/a ratio at 30 ML is 1.03, which is the same value as that found in thinner films [1]. The c/a ratio of the Fe underlayer is unaffected by the deposition of Pd overlayers. The tetragonal distortion of Pd grown on bct Fe depends on the Pd deposition rate. The structure of the Fe overlayer depends on the structure of the Pd on which the Fe is grown.

Our analysis has not covered the nature of the Pd-Fe interface, whether it is an alloy that is several monolayers in depth [6] or a 1-ML rough interface [5]. A more extensive quantitative analysis that employs advanced theoretical models of the Pd-Fe interface is currently in progress and should be able to clarify this issue. In a related study, Meyerheim [7] has made extensive surface x-ray diffraction measurements of 0.7 to 2.0 ML of Fe grown on Pd(001) and then annealed at 135ºC. He has been able to determine the Fe concentration profile as a function of distance from the interface and has also been able to extract the Pd interlayer distances.

Acknowledgments

This work was supported by the Natural Sciences and Engineering Research Council of Canada through major facilities access and operating grants. Research at the PNC-CAT beamline was supported by the U.S. Department of Energy (DOE) under Contract No. DE-FG03-97ER45628. Use of the APS was supported by the DOE Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38.

References

[1] R. A. Gordon and E. D. Crozier et al., Phys. Rev. B **62**, 2151 (2000).
[2] M. Zolfl et al., J. Magn. Magn. Mater **175**, 16 (1997).
[3] T. L. Monchesky and B. Heinrich et al., Phys. Rev. B **60**, 10242 (1999).
[4] Y.B. Xu et al., Phys. Rev. B **58**, 890 (1998).
[5] E. E. Fullerton et al., Phys. Rev. B **51**, 6364 (1995).
[6] C. Boeglin et al., Phys. Rev. B **60**, 4220 (1999).
[7] H. Meyerheim (private communication).

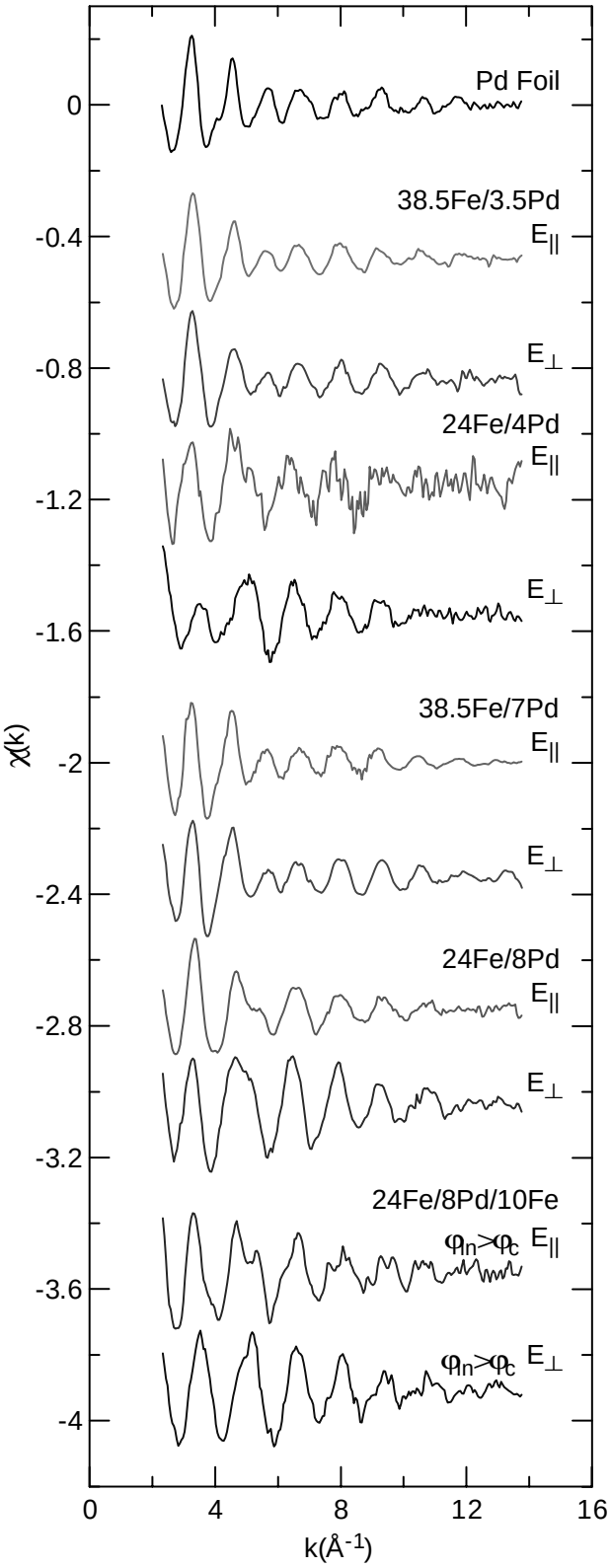

FIG. 3. Pd K-edge EXAFS interference functions. The Pd foil $\chi(k)$ is given for reference.