The Pd/Fe Interface in the Epitaxial System Pd/Fe/GaAs(001)- 4 x 6

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Abstract. Magnetic properties of thin magnetic films are strongly affected by the nature of the interface between magnetic and non-magnetic layers. In spintronic devices the extent to which spins are scattered at an interface depends upon interfacial roughness, alloying, and impurities. We present a polarization-dependent XAFS study of a 1Pd/9Fe/GaAs(001)-(4x6) structure grown *in situ* in the MBE facility at the PNC/XOR, APS. To increase the interfacial roughness, the 1ML Pd was grown on the 9 ML Fe without first sputtering and annealing the Fe. An estimate of interfacial roughness, evidence for formation of Pd islands, their height, and the amount of As floating to the Pd surface from the GaAs are given.

Keywords: XAFS, MBE, surface, thin film, GaAs, PdFe
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INTRODUCTION

The nature of the interface between epitaxially grown ferromagnetic/non-ferromagnetic bilayers plays an important role in the magnetic properties of spintronic devices. The operation of a spintronic device depends upon the efficiency with which an electron carries its spin through an interface. The efficiency is affected by interdiffusion between the layers, strain in the layers, roughness of the interface, and island formation. Understanding the structure is a critical component of developing the correct interpretation of the magnetic behaviour. Polarization-dependent XAFS in the total reflection mode provides a probe of these factors in both bare and buried interfaces. We have used the *in situ* MBE facility at the PNC/XOR beamline to deposit 1 ML of Pd on 9 ML of Fe epitaxially grown on the Ga-terminated 4 x 6 reconstructed surface of GaAs(001). At 9 ML the deposition of Fe is in the layer-by-layer growth mode and yet, is sufficiently thin that Fe K-edge XAFS measurements below the critical angle for total reflection still have some sensitivity to the Pd/Fe interfacial region.

We discuss the differences in the Fe spectra collected before and after the deposition of Pd. We also discuss the evidence provided by Pd K-edge XAFS for the formation of Pd islands. In addition, we confirm previous reports that small amounts of As (~0.5ML) float to the surface of the Fe during Fe deposition.

METHODS AND MATERIALS

The sample on GaAs(001)-(4x6) was prepared *in situ* by MBE on epiready n-type GaAs (American Xtal Technology) wafers using methods described elsewhere [1,2]. Layer deposition was monitored by reflection high-energy electron diffraction (RHEED) with the number of oscillations of specular (anti-Bragg) spot intensity giving the layer thickness in ML. In growing the Fe/Pd sample, a total of 9 ML of Fe were epitaxially deposited. Unlike previously [3], the Fe was not Ar+ sputtered to remove As which is known to float to the top of Fe during growth. Nor was the sample subsequently thermally annealed to reduce surface roughness.

In the growth of Pd on bct Fe, the Pd fcc lattice can be considered as a bct structure with in-plane lattice parameter being smaller than the underlying Fe in-plane lattice. The Pd fcc lattice rotates 45º with respect to the Fe bct lattice and expands in-plane in an attempt to match Fe. This causes contraction in the out-of-plane direction at the same time.

XAFS measurements were made at the Fe and Pd K edges using the PNC-CAT undulator beamline, ID-20 [4]. X-rays were incident in the total-reflection geometry with the electric vector (near) perpendicular,

$E_\perp$, to the substrate. To minimize distortion of the spectra due to anomalous dispersion effects in the sample and adjacent media, the angle of incidence was set to approximately 2/3 of the critical angle φ_c, at 250eV above the respective K-edges [5]. Fe K-edge measurements were also made at ~$2\varphi_c$ after deposition of 1ML Pd in order to examine the effect of the overlayer of Pd on the structure of the underlying Fe.

RESULTS

The collected data was averaged in E-space (typically, 20 scans per measurement). The background was removed using the AUTOBK[6] program. The resulting $E_\perp$ χ(k) for Fe (before and after Pd deposition) and Pd K-edges are shown (Fig. 1).

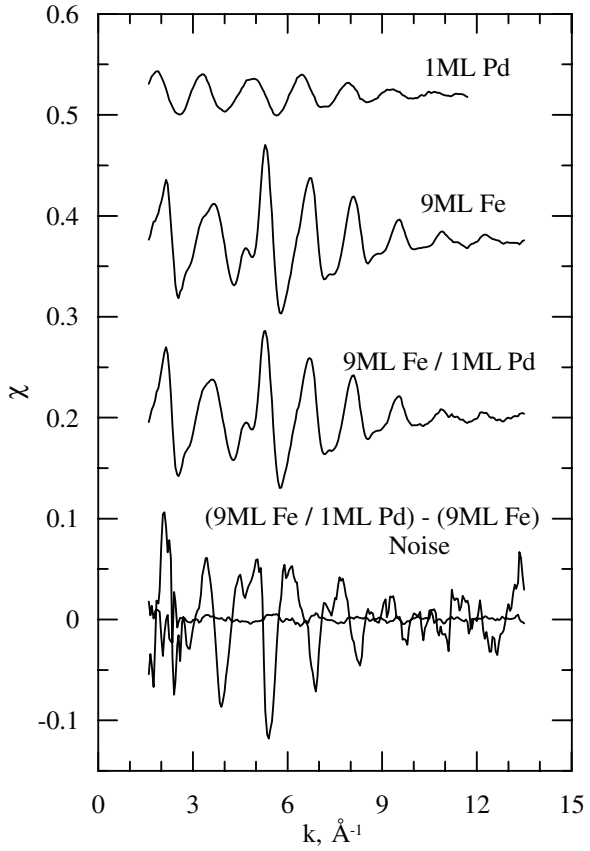

FIGURE 1. The $E_\perp$ χ(k) for Fe (before and after Pd deposition), Pd K-edges, the difference between two Fe spectra, and the noise level.

The difference between the two Fe χ(k) is shown together with the noise level included for comparison (both are multiplied tenfold). The main contribution to the difference χ(k) is caused by the dissimilarities "seen" by Fe atoms in the top few layers. This asserts

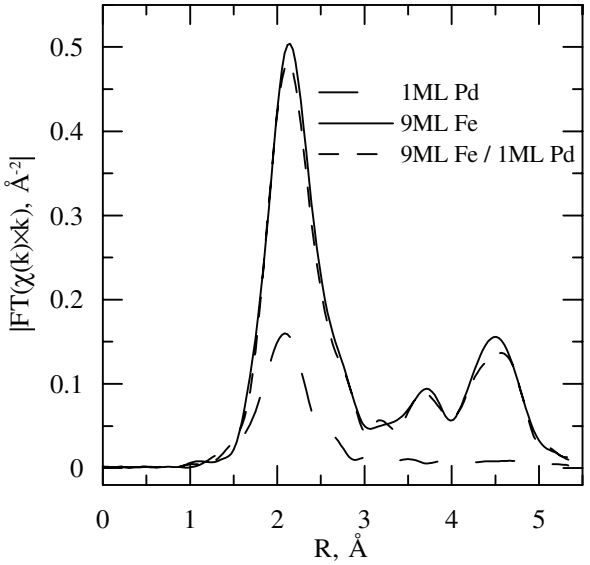

FIGURE 2. Magnitudes of the Fourier transforms for Fe (before and after Pd deposition), and Pd K-edges.

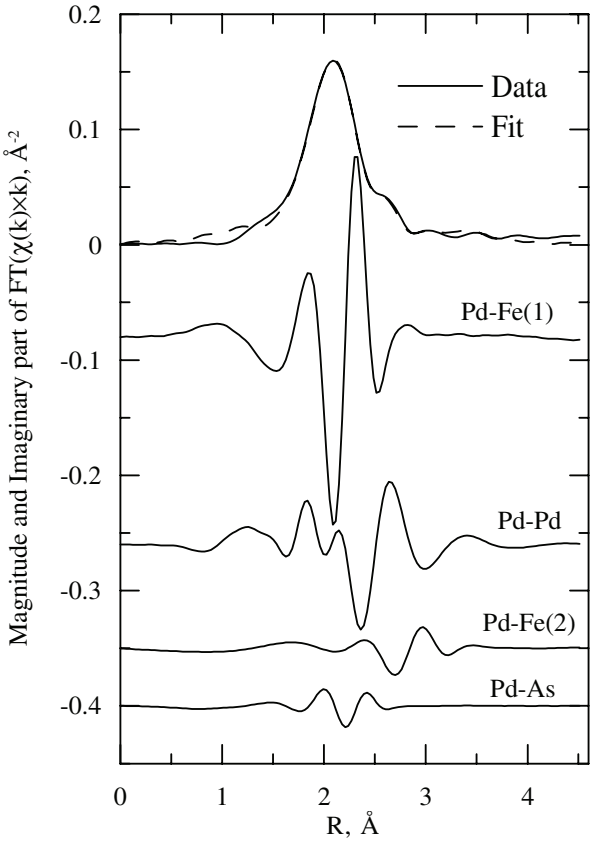

FIGURE 3. $E_\perp$ Pd K-edge fit. Imaginary parts of contributing bonds are shown with offset for clarity.

that glancing incident XAFS is sufficiently surface sensitive to investigate small changes in the interfacial

region. The difference $\chi(k)$ helped establish a suitable model for curve fitting. Additionally, simultaneous fits to the Pd data and the difference $\chi(k)$ were used to verify the quality of the fits in Fig.2 and Fig.3.

The magnitudes of the Fourier transforms of $k\chi(k)$ for the Fe and Pd data are shown in Fig. 2. Transforms were calculated over the k-range 1.8Å^{-1} to 11.9Å^{-1} using Kaiser-Bessel window function with sill width 2.5Å^{-1}. Fitting was performed in R-space using FEFFIT[7] program with theoretical backscattering amplitudes and phase shifts calculated with FEFF7[8].

The fitting of 1ML Pd is shown in Fig. 3. Due to the Fe surface roughness and presence of As at the surface, Pd does not form a perfect layer. This is evident from the presence of the Pd-Pd path under the fit - perfect 1ML $E_\perp$ data would not contain this path, since all Pd atoms would be in-plane.

Arsenic atoms from the Fe/GaAs interface tend to float to the top during growth of Fe and Pd. Up to 0.7ML of As has been reported to be present on top of relatively thick Fe layers. From the fit it is clear that such a small amount of As can be detected because the backscattering amplitude of As differs from both Fe and Pd.

There is a complex interplay between the Pd-Fe, Pd-As and Pd-Pd contributions to the main peak. While the Pd-Fe and Pd-Pd imaginary parts of the Fourier Transforms are in phase below 2Å, they are out of phase just below 2.5Å.

A reasonably good fit is obtained with the fit range from 0.9Å to 3.2Å. Fits to larger R are unreliable. This and large values of Debye-Waller factors indicate a significant disorder at the surface of the sample.

CONCLUSIONS

For an ideal perfectly flat 9 monolayers of Fe the theoretical first n.n. coordination number N_1 is 7.11. Experimentally N_1 = 6.7±1.0. The second n.n N_2 = 1.77 theoretically vs 1.5±0.2 experimentally. Radial distances are in agreement with a bct structure of Fe grown on GaAs-(4x6). From these values we estimate the Fe surface roughness to be ~ 2ML.

If the 1ML of Pd were perfectly flat there would be no out-of-plane Pd-Pd distance. But in the fit to the $E_\perp$ Pd data a first n.n. Pd-Pd distance is present, indicating formation of Pd islands. Absence of a detectable second n. n. Pd distance suggests that the height of the islands does not exceed 2ML. This is consistent with the measured Pd-Pd N_1 =2.3±0.3. In addition, for the second Pd-Fe distance N_2 = 0.9±0.1, which means that almost all Pd atoms have such a bond with Fe.

The presence of a Pd-As distance in the fit, with small coordination number N_1 = 0.5±0.1 indicates at least 0.5ML of As floated to the surface of Pd during the growth. There may be additional As present on those patches of the Fe surface not covered by Pd. But As was not detected in the Fe K-edge fits, so the amount of As on Fe would be small.

Pd-Fe and Pd-As radial distances are equal to 2.61±0.02Å, which is the same as for Pd-Fe in the thicker films studied previously [3]. This was expected since Fe and As have the same ionic radii. The Pd-Pd radial distance is found to be 2.81±0.02Å which is 0.02Å larger than in thicker samples.

The interfacial surface roughness affects greatly the magnetic properties of thin films such as coercivity, magnetic domain structure, and spin-transport. The investigated sample has greater surface roughness compared to samples prepared without omitting sputtering and annealing: ~2ML versus ~0.5ML. While there were no magnetic studies done on this sample, the obtained results can serve as a guide for preparing thin films with desired surface roughness.

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