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Lattice Strain in Magnetic Ultrathin Films

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ABSTRACT A clear understanding of the mechanisms of interfacial magnetic anisotropy rests on the structural characterisation of magnetic multilayers which, typically, consist of two ferromagnetically coupled (F) layers separated by a non-magnetic spacer layer. Fe/Cu/Fe trilayers are of special interest since the coupling between the F layers of Fe changes from F to antiferromagnetic depending on the thickness of the Cu spacer layer. Here, a magnetic multilayer system, grown by molecular beam epitaxy (MBE), was modified by inserting Cr in the Cu: Ag(001)/8.7 Fe/3 Cu/6 Cr/3 Cu/5 Fe/10 Au where the integers refer to monolayers. Polarized K-edge XAFS spectra (E parallel to the substrate) were obtained from fluorescence measurements in the total reflection geometry. The multiple scattering paths were analysed for the Cr edge. The initial Cu grew pseudomorphically in a BCC structure on Fe/Ag(001). The Cr proved to be tetragonally distorted from its BCC structure. The overlayers of Fe on Cu are contracted by 1.27% within the plane and conserve the *c* lattice parameter of Fe, though the atomic volume is contracted by 2.8%. The Cu adopts a BCT, rather than keeping its bulk FCC, structure and the corresponding decrease in its atomic volume from the FCC is only 0.3%.

INTRODUCTION

In its bulk BCC form Cr is a weak antiferromagnet ($0.5\mu_B$) [1]. Large augmentations of magnetism (up to $2.49\mu_B$) are expected for small clusters of atoms and ultrathin films possessing a reduced coordination [1,2]. Thin films (<3ML) of Cr grown epitaxially on Ag(001) and Cu(001) have been demonstrated to be substantially different than BCC, with the initial mode of growth characterized by the formation of islands (Volmer-Weber growth.) At low temperatures (<300°C) the growth of Cr on Fe(001) is shown by STM measurements to be rough and limited by diffusion kinetics [3] and the structure can be directly linked to the subsequent magnetic properties of the film. In this study of Cr grown in a non-magnetic Cu spacer, we use XAFS to obtain the film structure in order to characterize the local environment in the Cr and neighbouring layers which will provide a structural basis for understanding the magnetism of the multilayer system.

EXPERIMENT

The following sample was deposited on an Ag(001) single crystal substrate with miscut within 0.1° : Ag(001)/5.7 Fe/3 Fe/3 Cu/6 Cr/3 Cu/5 Fe/10 Au, where the integers refer to full monolayers (ML) of material. The layers were grown by MBE at room temperature (RT) except where otherwise stated. The growth was monitored by reflection high energy electron diffraction (RHEED) and a quartz crystal thickness monitor. The intensity of the RHEED specular spot was followed as the growth took place, and shows distinct cusps [4] indicating layer-by-layer growth in the case of Cu and Fe, and semi layer-by-layer growth (the 2nd layer starts to grow before the first is terminated, as in Volmer-Weber growth of islands) in the case of Cr. In this manner, 5.7ML of Fe were grown at RT, followed by 3.0ML of Fe at 150°C , insuring a surface which is flat across each terrace. 3ML of Cu were deposited on this surface, followed by 6ML of Cr, and 3ML of Cu to finish the non-magnetic spacer layer. The top magnetic layer was comprised of 5ML of Fe. The structure was then passivated with 10ML Au in order to perform ex-situ XAFS on the sample.

K-edge spectra were taken on beamline IV-1 at SSRL using a Si(111) double crystal monochromator with an entrance slit of 1mm. Harmonic reduction was achieved by detuning the monochromator by 25% 200 eV above the edge being studied. The sample was mounted in the total reflection geometry using a sample positioner described elsewhere [5] with the polarization of the radiation parallel to the (001) surface of the substrate. The critical angle (φ_c) was determined for each edge by measuring the reflectivity and fluorescence as a function of incident angle, at a fixed energy 200eV above the edge. Bragg peaks, due to reflections from the substrate, were eliminated by covering appropriate regions of the fluorescence detector with lead tape. The data were acquired with the sample surface at a fixed angle of $0.75\varphi_c$ with respect to the beam. Up to fifty scans were measured at each edge, and the data analysis was carried out on the averaged scans.

RESULTS AND DISCUSSIONS

The x-ray absorption near-edge structures (XANES), obtained in fluorescence mode, of the Cr K-edge in the MBE sample and its normal BCC phase in a foil are plotted in fig. 1(a). In figure 1(b) the XANES of the Fe edge is compared to normal BCC Fe (foil), whereas in fig. 1(c) Cu edge is compared with normal FCC Cu (foil).

The Cr resembles the BCC Cr in the main features of the XANES, though they are somewhat attenuated in the thin film. Fe shows the main edge features present in the bulk. In the case of Cu it is quite obvious that the structure is not FCC as it is in the bulk, but resembles BCC.

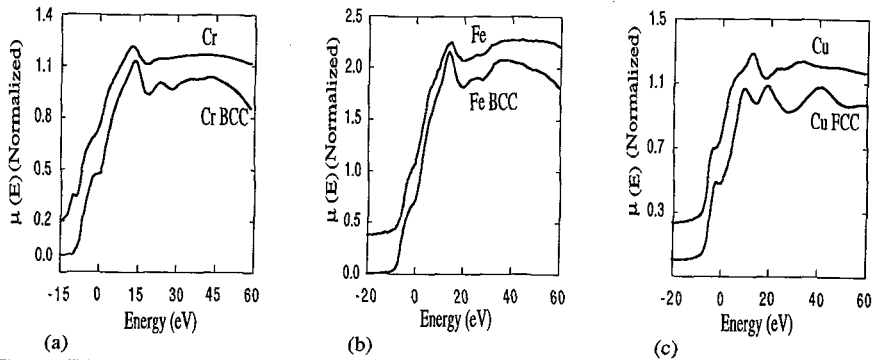


Figure 1. The XANES of Cr and Cr BCC (a), Fe and Fe BCC (b), Cu and Cu FCC (c).

The XAFS interference function $\chi(k)$ was obtained from the measured fluorescence using the background removal program AUTOBK [6]. The normalized raw XAFS spectra for the Cr, Fe and Cu edges are shown in fig. 2(a). The corresponding radial structure functions are shown in fig. 2(b). A BCC Fe foil, taken in transmission, has been included as a guide. In all the $\chi(k)$, two peaks are clearly visible in the region between 4.0 and 6.0 \AA^{-1} , as in the case of BCC Fe, showing the films to be approximately BCC.

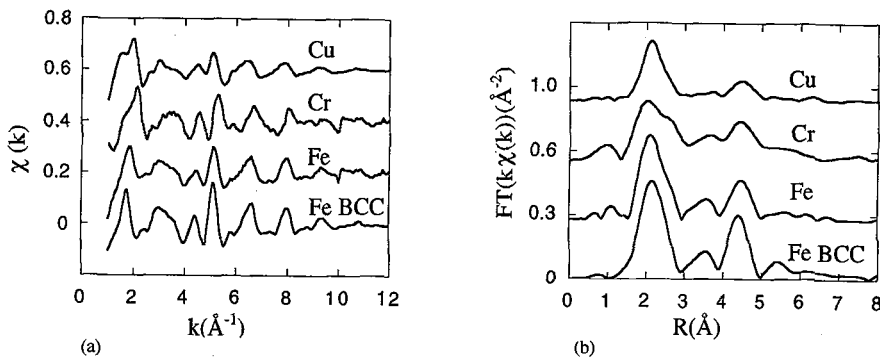


Figure 2. (a) XAFS interference function for BCC Fe, Fe, Cr and Cu (the various edges of the sample).

(b) Magnitude of the Fourier transform of $k\chi(k)$. A 10% Gaussian window was imposed over the range from 2 to 11.5 \AA^{-1} .

R-space curve fitting results were obtained using the non-linear least squares program EXAFIT [7]. The reference amplitude function $S(k)|f_j(k)|e^{-2R_j/\lambda}e^{-2\sigma_j^2k^2}$ was calculated using FEFF6 [8], and scaled by S_0^2 which was set at the value found for the bulk elements. The ΔE_0 were fixed to be equal for all shells having the same scatterers [9]. The $k\chi(k)$ (2.2 to 15.0 \AA^{-1}) of the Cu was Fourier transformed using a 10% Hanning window and the curve fitting was applied to both the real and imaginary parts of the FT within the range from 1.73 to 2.58 \AA . For Fe the k space range was 2.13 to 14.0 \AA^{-1} , and in R space from 1.76 to 2.86 \AA . The respective ranges for the Cr were from 1.54 to 10.15 \AA^{-1} , and 1.61 to 2.84 \AA . ΔE_0 was found either by fitting the first peak of the FT of the corresponding bulk element, or by fitting the unknown data while allowing all parameters of the first two shells to vary. The asymmetry due to deviations from a Gaussian distribution of positions was investigated in the curve fitting, found to be close to the theoretical values for the bulk [10], and was fixed at the bulk value. Four parameters were then allowed to vary in the fitting: R_1 , R_2 and their corresponding mean-squared relative displacements σ_1^2 , and σ_2^2 . The uncertainties in the results were obtained by finding the change in a parameter which is required to double the residual sum of squares. Allowing N_2/N_1 to vary in the range from 0.75 to 1.0 gave essentially the same R_1 values.

From R_1 and R_2 we calculate the a and c lattice constants. We find that all three films have a tetragonal distortion. In Fe c assumes the bulk value ($2.86 \pm 0.01 \text{ \AA}$) but a is shortened by 0.036 \AA (1.3%, $c/a=1.010$). Both Cr and Cu have c longer than in their normal phases. The c/a ratios are found to be 1.020 and 1.024 respectively. The tetragonal distortion is particularly evident as the bump on the high-R side of the first peak of Cr (fig. 2b). This bump has as its source the polarization dependence of the single and triangular multiple scattering paths. The polarization dependence was included for all the BCT films via FEFF6 with the E vector in the $\langle 110 \rangle$ direction. This direction coincides with the a axis of the substrate, the $\langle 110 \rangle$ axis of the films, since the first layers of BCC Fe grow with a 45° rotation with respect to the underlying Ag(001) substrate. The coordination numbers N_1 and N_2 listed in Table 1 are lower than found in the bulk, but are within 10% of those calculated for films 3, 5 and 6ML thick [2].

Polarization dependent XAFS has shown that Co deposited on Cu(001) is tetragonally distorted [11]. The local structure of the overlayer first deduced by fitting the first peak of the FT was confirmed by FEFF simulations of the higher shells out to 5 \AA . The well-defined FT peaks beyond the nearest neighbours in fig 2.b indicate that our epitaxial films also have appreciable medium range order. FEFF6 simulations of 6ML of Cr in between two 3ML layers of Cu (out to 6 \AA) confirmed the BCT structure. We find for 6ML Cr that the peak at 4.5 \AA is enhanced by the presence of its overlayer of 3ML Cu and is not consistent with the formation of a Cu-Cr alloy. In summary, it was useful to fit the first peak of FT to a polarization independent model in order to determine the rough structure of the growths, and then to optimize the results with a fully polarization dependent simulation of the films.

Table 1 Results of fitting the 5ML Fe, 3ML Cu, and 6ML Cr edges of the XAFS spectrum.

	Fe	Cu	Cr
$R_1 (\pm 0.01 \text{ \AA})$	2.46 \AA	2.48 \AA	2.50 \AA
$R_2 (\pm 0.01 \text{ \AA})$	2.83 \AA	2.84 \AA	2.86 \AA
$\sigma_1^2 (\pm 1.6 \times 10^{-3})$	5.0×10^{-3}	8.0×10^{-3}	5.6×10^{-3}
$\sigma_2^2 (\pm 1.6 \times 10^{-3})$	8.0×10^{-3}	17.0×10^{-3}	6.5×10^{-3}
$N_1 \pm 0.5$	6	7.0	6.1
$N_2 \pm 0.5$	5.4	6.5	5.7

Fixed parameters are $\Delta E_0 = -0.4 \text{ eV}$ for Cu, -6.0 eV for Fe, and 2.0 eV for Cr. The values of c are 2.86 \AA for Fe, 2.91 \AA for Cu and 2.92 \AA for Cr.

The surface of the underlying film acts as a template forcing the deposited layer to expand (contract) to lattice match it. To zeroth order, perpendicular to the template the lattice contracts (expands) to keep the atomic volume equal to its bulk value. For the different layers of our sample the tetragonal strain is small. For the overlayer of Cu the tetragonal distortion is induced by the underlying Cr, which forces the Cu to grow in a BCT structure, as opposed to its bulk FCC one. Nonetheless, the atomic volume of the Cu (number of atoms in unit cell/volume of unit cell) remains almost constant, decreasing by only 0.3%. The corresponding decrease in Cr is 0.4%, and the atomic volume of the Fe has diminished by 2.8%. The tetragonal distortion is seen to diminish: as subsequent multilayers are grown on the Cr it decreases from 1.020 to 1.010. These structural parameters include the effects of the strains induced at each interface which dictate the magnetic properties of the system.

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