

J. Synchrotron Rad. (1999). 6, 746–748

Structural transition in epitaxial Co/Cr multilayers as studied by X-ray absorption spectroscopy

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We have performed Cr and Co *K*-edge x-ray-absorption measurements to investigate the dependence of local electronic and atomic structures on the Cr-layer thickness in epitaxial Co (40Å)/Cr (t_{Cr}) ($t_{\text{Cr}} = 2, 3, 5, 7, \text{ and } 9\text{Å}$) multilayers. The Cr *K* x-ray absorption near edge structure (XANES) spectra of Co/Cr multilayers indicate an abrupt transition of the Cr layer from a bcc structure to a hcp structure when the thickness of the Cr layer is decreased down to $\sim 5\text{Å}$ or three atomic layers. The structural transition and bond-length distortion in Cr and Co layers observed in the extended x-ray absorption fine structure (EXAFS) measurements are consistent with the XANES results.

Keywords: Structural transition, XANES, EXAFS

1. Introduction

The electronic properties and atomic structure of synthetically magnetic multilayers have attracted great attention over the last decade because of their peculiar magnetic properties of technological and fundamental importance (Bland & Heinrich, 1994). According to the reflection high-energy electron diffraction (RHEED) analyses by Vavra *et al.* (1993) and Henry *et al.* (1993), the Cr layer in Co/Cr multilayers were found to exhibit an abrupt transition from the bcc structure to the close-packed structure (fcc or hcp) at a Cr-layer thickness of $\sim 5\text{Å}$ because the interfacial energy can stabilize the thermodynamically less favored densest atomic arrangement. However, they obtained different local atomic structures around Cr when the Cr layer is very thin. Vavra *et al.* found that the pseudomorphic grown Cr are strained coherently into the hcp structure of the underlying Co, while Henry *et al.* reported that no pseudomorphism occurs at the Cr/Co interface but it is more likely that interdiffusion resulted in forming a close-packed CoCr alloy. In this work we focus on the dependence of the local electronic and atomic structures on the Cr-layer thickness.

2. Experimental

X-ray absorption spectra of Co/Cr multilayers were measured using a double-crystal Si(111) monochromator at the wiggler beamline with an electron-beam energy of 1.5 GeV and a maximum stored current of 200 mA at the Synchrotron Radiation Research Center (SRRC), Hsinchu, Taiwan. The absorption spectra of Co/Cr multilayers and the CoCr alloy at the Cr and Co *K*-edges were measured using the fluorescence mode at room temperature. The spectra of the reference compounds, Cr and Co foils, were obtained in transmission mode. Samples of $24\times[\text{Co}(40\text{Å})/\text{Cr}(2\text{Å})]$ and $20\times[\text{Co}(40\text{Å})/\text{Cr}(t_{\text{Cr}})]$ multilayers with $t_{\text{Cr}} = 3, 5, 7, \text{ and } 9\text{Å}$ deposited in the alternating Co/Cr multilayers. The details of the preparation of a similar Co/Cr multilayer have been described elsewhere (Huang *et al.*, 1995).

3. Results and discussion

Figures 1 and 2 show, respectively, the Cr and Co *K*-edge XANES spectra obtained for the Co/Cr multilayers, reference CoCr alloy, and Cr and Co foils. For all the spectra, the zero energy was selected at the inflection point of the threshold in the spectra. The normalized EXAFS oscillations $\chi(k)$ are weighted by k^3 for both Cr and Co *K*-edges and the corresponding Fourier transforms of the $k^3\chi$ data for the Co/Cr multilayers and referencing samples are shown in Figs. 3 and 4, respectively.

The part of the Cr *K*-edge XANES spectra of the Co/Cr multilayers, reference CoCr alloy, and Cr foil and of the off-set Co *K*-edge XANES spectra of the Co foil between labels b_1 and b_2 as shown in Fig. 1 can be attributed to the dipole $1s$ -to- $4p$ transitions above the Fermi level. The two small bumps in the region from about 0 to 10 eV above the edge (labeled as a_1 and a_2) are primarily due to the Cr and Co $1s$ -to- $3d$ quadrupolar transition. Two-peak features b_1 and b_2 in the Cr *K*-edge XANES of the Co/Cr multilayers with a Cr-layer thickness, t_{Cr} , less than 5Å closely resemble that of the Co foil having a hcp structure. In contrast, a single peak feature presents in the Cr *K*-edge spectra of the Co/Cr multilayers with $t_{\text{Cr}} > 5\text{Å}$, which resembles the single sharp feature b^* located at the region between peaks b_1 and b_2 in the spectrum of the Cr foil with a bcc structure. The general trend of the first derivatives of the XANES spectra of the Co/Cr multilayers, CoCr alloy, and Cr and Co foils are shown in the inset of Fig. 1, which are much easier to see the change from the single peak b^* to the peaks b_1 and b_2 (labeled by vertical arrows) with the decrease of the Cr-layer thickness in Co/Cr multilayers. This general behavior clearly indicates that the local structural transition occurs at $t_{\text{Cr}} \sim 5\text{Å}$ in Co/Cr multilayers. It also implies that pseudomorphic Cr films can be grown on Co and strained coherently into the hcp structure in thin layers ($t_{\text{Cr}} < 5\text{Å}$). In contrast, the Cr layer prefers to be bulk-like when its thickness is greater than 5Å . The intensity of bumps a_1 and a_2 in the Cr *K*-edge XANES spectra remain nearly constant. The Co *K*-edge XANES spectra of the Co/Cr multilayers (i.e. the off-set Cr *K*-edge XANES spectra for the Cr foil) as shown in Fig. 2 show relatively sharp two-peak features b_1 and b_2 for $t_{\text{Cr}} < 5\text{Å}$, which closely resemble that of the Co foil. The two-peak features b_1 and b_2 change to a single feature similar to feature b^* at $t_{\text{Cr}} \sim 5\text{Å}$, and then become

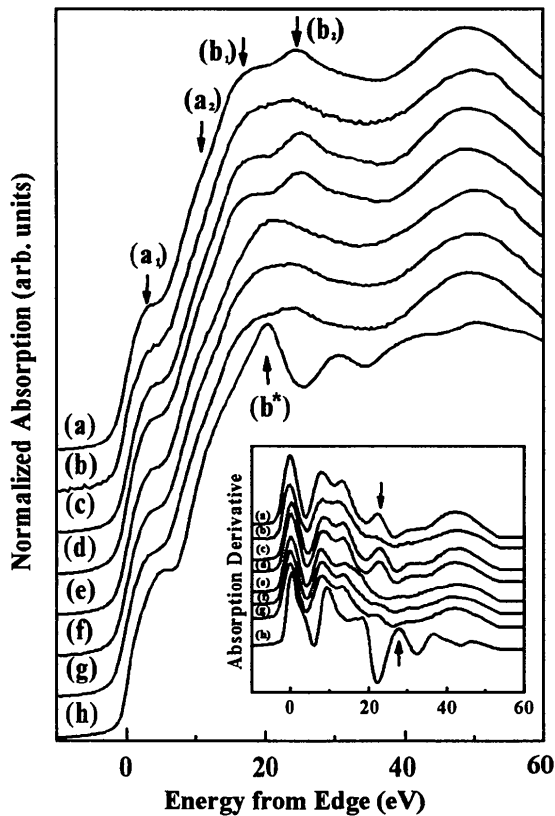


Figure 1

Normalized Cr K near-edge absorption spectra for epitaxial Co (40Å)/Cr (t_{Cr}) ($t_{Cr} = 2, 3, 5, 7,$ and 9Å) multilayers. (a) Co foil (off-set Co K -edge); (b) CoCr alloy; (c) $t_{Cr} = 2\text{Å}$; (d) $t_{Cr} = 3\text{Å}$; (e) $t_{Cr} = 5\text{Å}$; (f) $t_{Cr} = 7\text{Å}$; (g) $t_{Cr} = 9\text{Å}$; (h) Cr foil.

broader with the increase of t_{Cr} up to 9Å . The first derivatives of the Co K -edge XANES spectra of the Co/Cr multilayers, CoCr alloy, and Co and Cr foils are also shown in the inset of Fig. 2. The Co K -edge XANES spectra exhibit that the Co local structure is clearly dependent on the Cr-layer thickness.

Figs. 3 & 4 show the Fourier transform of the Cr and Co K -edge Fourier transforms (FT) of the $k^3\chi$ data for the Co/Cr multilayers, CoCr alloy, and Cr and Co foils. The first peak in the FT spectra as shown in Fig. 3 appears to be roughly in the same location though not equivalent in magnitude and the corresponding full widths at the half maximum. However, the peaks at a distance larger than $\sim 3\text{Å}$ appear to differ significantly and can be attributed to differences in the average environment in further away shells in both cases of Cr with $t_{Cr} > 5\text{Å}$ and $t_{Cr} < 5\text{Å}$ in Co/Cr multilayers. Obviously, the local atomic structure of thick Cr layers ($t_{Cr} > 5\text{Å}$) in the Co/Cr multilayers closely resembles that of the Cr foil and yields a peak at $\sim 4.5\text{Å}$, which is typical of the bcc structure (Pizzini *et al.*, 1992&1993). Besides, it also shows that the local atomic structure of thin Cr layers ($t_{Cr} < 5\text{Å}$) in the Co/Cr multilayers and CoCr alloy, is quite similar to that of the Co foil with a

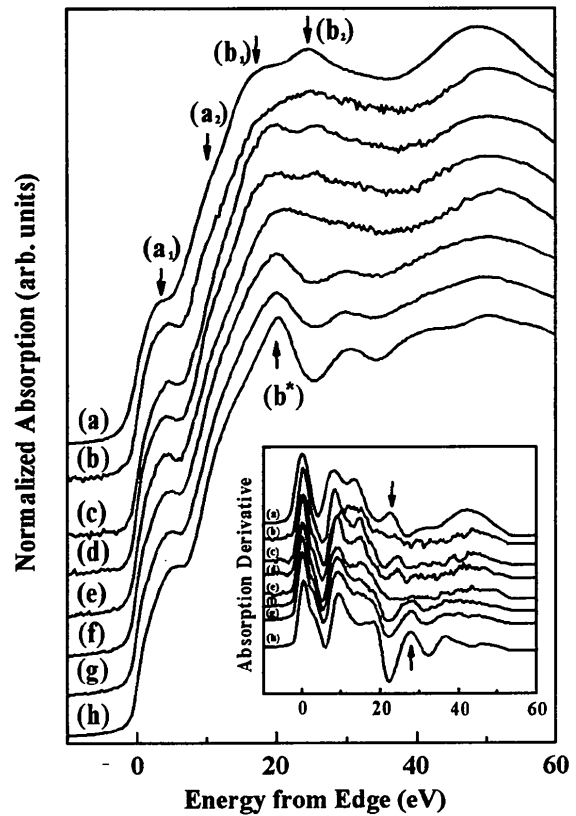


Figure 2

Normalized Co K near-edge absorption spectra for epitaxial Co (40Å)/Cr (t_{Cr}) ($t_{Cr} = 2, 3, 5, 7,$ and 9Å) multilayers. (a) Co foil; (b) CoCr alloy; (c) $t_{Cr} = 2\text{Å}$; (d) $t_{Cr} = 3\text{Å}$; (e) $t_{Cr} = 5\text{Å}$; (f) $t_{Cr} = 7\text{Å}$; (g) $t_{Cr} = 9\text{Å}$; (h) Cr foil (off-set Cr K -edge).

hcp structure and gives rise to the characteristic of the two neighbor shells in the region between $3.8\text{--}5.0\text{Å}$ in the FT spectra as shown in Fig. 3. These splitting two neighbor shells in the region between $3.8\text{--}5.0\text{Å}$ of the hcp structure were also found in the FT spectra of the Co K -edge for the Co/Cr multilayers, CoCr alloy and Co foil as shown in Fig. 4. In the same figure, the splitting two neighbor shells are nearly at the same position for the Co/Cr multilayers, CoCr alloy and Co foil but the amplitude is obviously smaller for thick Cr layers than thin Cr layers in the Co/Cr multilayers. This property can be primarily attributed to the decrease of the structural order due to severe bond-length distortion in the Co layer caused by the thick Cr layer. FT data show that with $t_{Cr} \leq 5\text{Å}$, the Cr-layer stacking faults present, which stabilizes the hcp structure of the Co layer. This agrees with the results of XANES and further confirms that the epitaxially grown $t_{Cr} \leq 5\text{Å}$ Cr layer stacking in the Co/Cr multilayers is constrained to be Co-metal-like as reported by earlier RHEED studies (Henry *et al.*, 1993 & Vavra *et al.*, 1993).

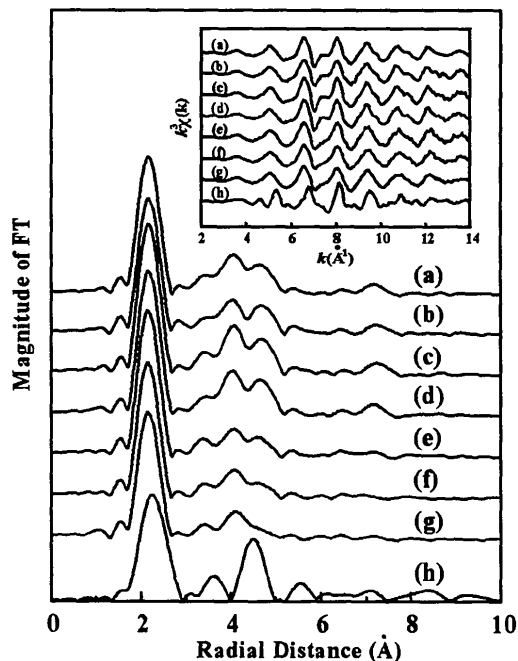


Figure 3

Fourier transform amplitudes of the EXAFS $k^3\chi$ data at the Cr K -edge for Co/Cr multilayers. (a) Co foil; (b) CoCr alloy; (c) $t_{\text{Cr}} = 2\text{\AA}$; (d) $t_{\text{Cr}} = 3\text{\AA}$; (e) $t_{\text{Cr}} = 5\text{\AA}$; (f) $t_{\text{Cr}} = 7\text{\AA}$; (g) $t_{\text{Cr}} = 9\text{\AA}$; (h) Cr foil. The inset represents the Cr K -edge EXAFS oscillations $k^3\chi$ data.

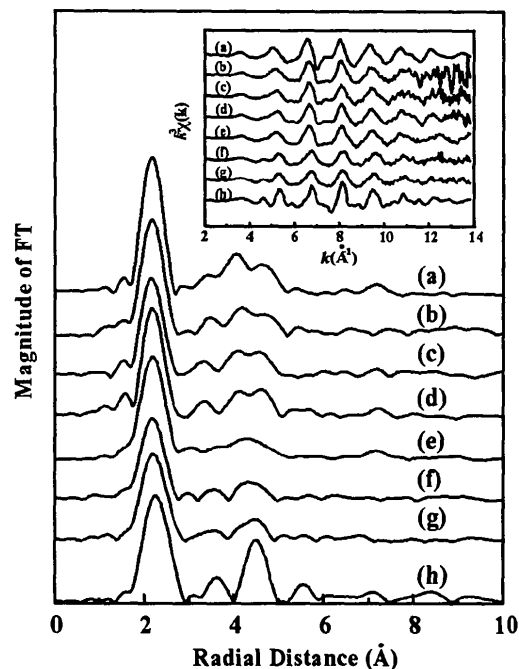


Figure 4

Fourier transform amplitudes of the EXAFS $k^3\chi$ data at the Co K -edge for Co/Cr multilayers. (a) Co foil; (b) CoCr alloy; (c) $t_{\text{Cr}} = 2\text{\AA}$; (d) $t_{\text{Cr}} = 3\text{\AA}$; (e) $t_{\text{Cr}} = 5\text{\AA}$; (f) $t_{\text{Cr}} = 7\text{\AA}$; (g) $t_{\text{Cr}} = 9\text{\AA}$; (h) Cr foil. The inset represents the Co K -edge EXAFS oscillations $k^3\chi$ data.

Acknowledgments

One of the authors (W. F. P.) would like to thank the National Science Council of the R.O.C. for supporting this research under contract No. NSC 88-2112-M-032-009. SRRC is also appreciated for use of their wiggler beamline to perform this study.

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(Received 10 August 1998; accepted 26 November 1998)