Evidence for the short-period oscillations in spin-resolved photoemission of thin Cr(110) films

Yu S Dedkov
Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany
E-mail: dedkov@physik.phy.tu-dresden.de

Abstract. The spin-resolved photoelectron spectroscopy study of the Cr/Fe(110) interface are presented. The system was investigated at room temperature for different thicknesses of Cr overlayer. As a result, we observe the initial fast drop, followed by a weak oscillatory behavior, of the photoelectron spin-polarization ($P$) at the Fermi level, $E_F$. The observed period of weak oscillations of $P$ give an evidence for the first time observation of short-period oscillations in Cr(110) oriented thin films.

In the last decade, the magnetism of ultrathin films and nanostructures has been a field of intense research (for review, see, for example [1,2]). This is mainly due to the fact that the magnetic properties of such objects often deviate strongly from the properties of the bulk material. This can lead to new physical phenomena as, e.g., oscillating exchange coupling of ferromagnetic films across non ferromagnetic spacer layers. The Fe/Cr system is one of the most intensively studied magnetic multilayer systems. A short (2 ML) and a long period (~18 Å) of oscillatory coupling [3-5] are present between the Fe layers, depending on the Cr layer thickness. Multilayers are known to exhibit just long period oscillations, which are similar for epitaxial Fe/Cr(100), (211) [6], and (110)-textured polycrystalline films [7], although highly strained Fe/Cr(110) [8] shows some differences. The common long-period for all three orientations suggests that there may be a common origin for coupling in all three cases. In some sense it can be assigned to the fact that at the Cr/Fe interface, for minority electrons, the reflection is weak for most of the electrons, because the Fe minority Fermi surface is very similar to that of Cr (Fig. 1). For the majority electrons, the reflection is much more complicated, and depends more strongly on interface orientation since there is a big difference in between Fe majority electrons Fermi surfaces and Cr one (Fig. 1).

A long-period oscillations was also found in all calculations that include the Cr Fermi surface, whether they be Ruderman-Kittel-Kasoya-Yosida calculations [9], or calculations based on the local-density approximation [10-13]. In spite of all this work, the origin of the long period in Fe/Cr is still not well understood, especially its apparent independence on growth orientation [14].

The vast majority of chromium thin films and multilayers studied to date have been oriented in a $<100>$ direction. Similar lattice constants and surface energies [15] promise a layer by layer growth of Cr on Fe close to systems which can be handled by theory. A much less attention was paid to the (Cr/Fe) system with (110) orientation that is somewhat surprising since at Cr/Fe(110) interface no interdiffusion occurs at room temperature [16] in contrast to the observations for (100)-oriented interface [17,18]. As was mentioned above the long oscillation period with the nearly same value of about 18 Å was found for (Cr/Fe) systems with (110) orientation [7]. This fact was also successfully
interpreted by coupling strength which comes from the extremal vector centred at the ellipsoid N of
the Fermi surface of Cr (Fig. 1) [19]. In this theoretical work [19] on exchange coupling in magnetic
heterostructures the short-period oscillations with a period of 4.7 Å in Cr was also predicted. Some
indication of such short-period oscillation can be found in the recent experimental work on
determination of bilinear coupling constant in Fe/Cr/Fe(110) trilayers [20]: Independent on
the temperature the bilinear coupling constant $J_1$ shows a sharp transition from a ferromagnetic coupling
for $d_{Cr} < d_0 = 2.5$ ML to an antiferromagnetic coupling at $d_{Cr} > d_0$, followed by a minimum value at
$d_{Cr} = d_1 = 3.4$ ML.

The aim of the present work is an attempt to find such short-period oscillations in thin Cr films by
spectroscopic methods. Here we present, for the first time, the high quality spin-resolved
photoelectron spectroscopy study of the Cr/Fe(110) interface. The system was studied at room
temperature for different thicknesses of Cr overlayer. As a result, we observe initial fast drop followed
by a weak oscillatory behaviour of the photoelectron spin-polarization ($P$) at the Fermi level, $E_F$. The
observed period of weak oscillations of $P$ give an evidence for the first time observation of short-
period oscillations in Cr(110) oriented thin films.

Spin-resolved photoelectron spectra (He I $\alpha$, $h\nu = 21.22$ eV) were recorded at a room temperature
(RT) in angle-resolved mode in normal photoelectron-emission geometry with a 180° hemispherical
energy analyzer SPECS PHOIBOS 150 combined with a 25 kV mini-Mott detector for spin analysis
(from SPECS). The angle resolution was 2° and energy resolution was set to 100 meV. Effective
Shermann function was set to 0.1. The light incident angle was 30° with respect to the sample surface.
Spin-resolved measurements were performed in normal emission geometry in magnetic remanence
after having applied a magnetic field pulse of about 500 Oe along the in-plane easy magnetization axis
of the Fe(110) substrate. The experimental setup asymmetry was accounted for in the standard way by
measuring spin-resolved spectra for two opposite directions of applied magnetic field [21,22]. The
base pressure during the experiment was $8 \times 10^{-11}$ mbars rising to $3 \times 10^{-10}$ mbars during metal
evaporation. Thin Fe(110) films with a thickness of $40$ Å and Cr layers on top of Fe film with different
thickness were grown epitaxially on W(110) at RT by deposition of high-purity Fe and Cr metals from
carefully degassed electron-beam evaporators. The thicknesses of the films were simultaneously
measured by carefully calibrated (by means of x-ray photoelectron spectroscopy) quartz microbalance.
The absolute error of the layer thickness given below is approximately 5%. Subsequent annealing at
400°C led to a well-ordered Fe(110) surface as indicated by LEED. The cleanness of the films was
routinely monitored by LEED and XPS of core levels as well as UPS of the valence band.

Fig. 2(a) shows the experimental spin-resolved photoemission spectra obtained in normal emission
geometry of the Cr/Fe(110) system for different thicknesses of the Cr overlayer (shown on the left-
Figure 2. (a) Spin-resolved photoelectron spectra of the Cr/Fe(110) system obtained at photon energy of $h\nu = 21.22$ eV for different thicknesses of Cr overlayer. Solid circles, empty triangles up, and solid triangles down show total intensity, spin-up, and spin-down intensities, respectively. (b) Spin polarization at $E_F$ as a function of thickness of Cr overlayer in Cr/Fe(110) system. Different symbols correspond to three different series of measurements.

hand side of each spectra). In this figure 1 ML of Cr has a thickness of 2 Å. The spin-resolved spectra of the valence band of the pure Fe(110) film show the emission from the $\Sigma_1^\downarrow \otimes \Sigma_3^\downarrow$ states near 0.25 eV of binding energy (BE) and from the $\Sigma_1^\uparrow \otimes \Sigma_4^\uparrow$ states near 0.7 eV of BE. The value of the spin polarization and the shape of the spectra are in good agreement with previous measurements [23,24]. Deposition of thin Cr overlayers leads to the changing in the shape of spin-polarized spectra as well as in the spin polarization at the Fermi level. Firstly, the shape of energy split spin-resolved features changes with Cr deposition. The initial small thicknesses of Cr overlayer (less than 1 ML) lead to fast decreasing of intensity of spin-down component of iron spin-resolved spectra that can be explained by predominant spin-dependent scattering of photoelectrons penetrating through Cr layer [25]. In further spin-resolved spectra we can not simply describe the decreasing of spin polarization since polarized Cr valence band states are developed in the same energy range. In the non spin-resolved spectra there are two spectral features in the valence band of Cr: the first feature is located close to $E_F$ and second one monotonically changes its binding energy from 0.54 eV to 0.84 eV when Cr thickness is changed from 1 ML to 6 ML, respectively. The energy position of this feature can be used as a measure of the magnetic moment of the surface Cr layer. The small BE of this feature at very low Cr coverages [Fig. 2(a)] can be explained by slight intermixing at room temperature of Fe and Cr at the Cr/Fe(110) interface. The magnetic moment at the intermixed interface is reduced, since neighbouring Fe and Cr atoms tend to align their magnetic moments antiparallel to each other. Upon further Cr deposition, the relative concentration of Fe in the surface region decreases and the surface magnetic moment increases. More interesting is that at particular thicknesses of Cr overlayer of about 3 ML and 5 ML (not shown here) we observe the quantum-well like changes of the intensity of the spin-down component.

Since detection of possible spin-polarized quantum-well states in Cr/Fe system is very difficult task, in further considerations we chose the monitoring of the spin polarization at $E_F$ as a probe of possible different period oscillations in Cr(110) film. This dependence as a function of Cr overlayer thickness is shown in Fig. 2(b). The first monotonic decreasing of spin polarization at $E_F$ from 70$\pm$5% to nearly 0% for Cr thicknesses of 0 ML $< d_{Cr} < 2.5$ ML is changed to the significant value of about 12$\pm$5% for Cr thickness of about 3 ML. Such drastic change in the value of spin polarization at $E_F$ can
be assigned to the increasing of spin-down photoelectron intensity for these thicknesses of Cr overlayer due to the presence of possible quantum-well state in the vicinity of the Fermi level. The corresponding spin-resolved spectrum is shown in Fig. 2(a) (right spectra in the lower panel). The nearly same behaviour was observed for the thickness of Cr overlayer of about 5 ML where again slight increasing of spin-polarization was detected. Also, both spin-resolved spectra (for 3 and 5 ML) demonstrate two distinct features in spin-down channel which can be assigned to spin-resolved quantum well states in Cr overlayer. These states are predominantly $d$ character.

For analysis of spin-resolved spectra we have used the theoretical calculations for Cr/Fe interface which are reviewed in the work of Tsetseris et al. [19] for different orientations of the interface: (100), (110), and (211). In case of the (110)-oriented interface as in the widely studied (100) case, one can find extremal vectors that span the lens (please, see the notation in work [19]) and vectors at the $N$ ellipsoids. As was found, the most important contribution to the coupling is made by $N$ ellipsoid vectors. In this case similar to (100)-oriented interface the majority electrons are strongly confined in the spacer, whereas the minority electrons are only partially reflected at the interface (see Fig. 1 for similarity between Cr and Fe spin-down electrons Fermi surfaces). Therefore, the origin of the long-period oscillations, observed earlier [7] was again attributed to an $N$ ellipsoid spanning vector. In the same theoretical work [19] the prediction on possible short-period oscillations was made. It was predicted that there is a non-negligible coupling strength for (110) orientation with a period of 4.7 Å (~2.35 ML). Also, similar prediction was made in the work [26] where the large geometrical weight was found for the period of about 4.5 Å (~2.25 ML) of Cr mid-layer in (110)-oriented Fe/Cr/Fe sandwich. These considerations suggest that the maximum of the geometrical weight have to be for parallel planes of the Fermi surface and in case of (110) oriented film there are two possible candidates for such periodic behaviour. The first one is the nesting vector between $\Gamma$ electron and $H$ hole octahedrons and the second possible candidate might be the nesting vector between $\Gamma$ electron octahedron and $N$ hole pocket. The role of each vector have to be clarified in additional calculations of Cr/Fe(110) system. To the best of our knowledge, this is a first time experimental observation of the short period oscillations in (110) oriented Cr thin film which is supported by theoretical calculations.

In conclusion, we perform careful spin-resolved measurements of electronic structure of thin Cr overlayers on top of Fe(110). Observed, for small thicknesses of Cr layer, the fast decreasing of spin-polarization at the Fermi level is explained by predominant spin-flip scattering of spin-down photoelectrons penetrating through Cr overlayer. It is changed to the weak oscillatory behaviour of $P$ for thicker film, that gives an evidence for observation of short-period oscillations in thin (110)-oriented Cr film on top of Fe(110). Observed effects were supported by theoretical calculations which take into account different nesting conditions in electronic structure of Cr.

References
[1] F.J. Himpsel, J.E. Ortega, G.J. Mankey, and R.F. Willis, Adv. Phys. 47, 511 (1998).
[2] J. I. Martin, J. Nogués, Kai Liu, J. L. Vicent, and I. K. Schuller, J. Magn. Magn. Mater. 256, 449 (2003).
[3] J. Unguris, R. J. Celotta, and D. T. Pierce, Phys. Rev. Lett. 67, 140 (1991).
[4] C. M. Schmidt, D. E. Bürgler, D.M. Schaller, F. Meisinger, and H.-J. Güntherodt, Phys. Rev. B 60, 4158 (1999).
[5] B. Heinrich, J. F. Cochran, T. Monchesky, and R. Urban, Phys. Rev. B 59, 14520 (1999).
[6] E. E. Fullerton, M. J. Conover, J. E. Mattson, C. H. Sowers, and S. D. Bader, Phys. Rev. B 48, 15755 (1993).
[7] S. S. P. Parkin, N. More, and K. P. Roche, Phys. Rev. Lett. 64, 2304 (1990).
[8] H. J. Elmers, G. Liu, H. Fritzche, and U. Gradmann, Phys. Rev. B 52, R696 (1995).
[9] Y. Wang, P. M. Levy, and J. L. Fry, Phys. Rev. Lett. 65, 2732 (1990).
[10] M. van Schilfgaarde and F. Herman, Phys. Rev. Lett. 71, 1923 (1993).
[11] M. van Schilfgaarde, F. Herman, S. S. P. Parkin, and J. Kurdnovský, Phys. Rev. Lett. 74, 4063 (1995).
[12] S. Mirbt, H. L. Skriver, M. Alden, and B. Johansson, Solid State Commun. 88, 331 (1993).
[13] S. Mirbt, A. M. N. Niklasson, B. Johansson, and H. L. Skriver, Phys. Rev. B 54, 6382 (1996).
[14] M.D. Stiles, J. Magn. Magn. Mater. 200, 322 (1999).
[15] E. Bauer and J. H. van der Merwe, Phys. Rev. B 33, 3657 (1986).
[16] J. Zukrowski, G. Liu, H. Fritzsche, and U. Gradmann, J. Magn. Magn. Mater. 145, 57 (1995).
[17] D. Venus and B. Heinrich, Phys. Rev. B 53, R1733 (1996).
[18] A. Davies, J. A. Stroscio, D. T. Pierce, and R. J. Celotta, Phys. Rev. Lett. 76, 4175 (1996).
[19] L. Tsetseris, B. Lee, and Y.-C. Chang, Phys. Rev. B 55, 11586 (1997).
[20] J. Schwabenhausen, T. Dürkop, and H.-J. Elmers, Phys. Rev. B 55, 15119 (1997).
[21] J. Kessler, Polarized Electrons, 2nd ed. (Springer-Verlag, Berlin, 1985).
[22] P. D. Johnson et al., Rev. Sci. Instrum. 63, 1902 (1992).
[23] R. Kurzawa, K.-P. Kämper, W. Schmitt, and G. Güntherodt, Solid State Commun. 60, 777 (1986).
[24] Yu. S. Dedkov, M. Fonin, U. Rüdiger, and G. Güntherodt, Appl. Phys. A 82, 489 (2006).
[25] H. C. Siegmann, Surf. Sci. 307-309, 1076 (1994).
[26] M. D. Stiles, Phys. Rev. B 48, 7238 (1993).