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

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Abstract. The spin-resolved electronic structure of thin Cr overlayers on top of the Fe(110) surface was investigated by means of spin- and angle-resolved photoelectron spectroscopy. The initial fast drop of photoelectron spin-polarization at the Fermi level, followed by weak oscillatory behavior with the period of about 2 ML, can give an evidence for the first time spectroscopic observation of the short period oscillations in (110)-oriented thin Cr films.

PACS. 73.20.-r Electron states at surfaces and interfaces – 75.30.Fv Spin-density waves – 79.60.-i Photoemission and photoelectron spectra

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 mainly due to the fact that magnetic properties of such objects often deviate strongly from the properties of the bulk material. This can lead to a 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 and a long period of oscillatory coupling [3] are present between the Fe layers, depending on the Cr layer thickness. Experiments on Fe/Cr/Fe(001) trilayers [4,5] show a 2 monolayer (ML) period modulated by long (∼18 Å) period oscillations. 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) [9]. The averages over the Fermi surface show that this behavior is only weakly dependent on the interface orientation [10]. 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 surface and Cr one (Fig. 1).

A long-period oscillations were also found in all calculations that include the Cr Fermi surface, whether they be Ruderman-Kittel-Kasoya-Yosida calculations [11], or calculations based on the local-density approximation [12–15]. 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 [16].

The vast majority of chromium thin films and multilayers studied to date have been oriented in a ⟨100⟩ direction. In such structure one has a case of transverse spin-density wave (SDW) and its wave vector **q** generally lies normal to the film plane. Many interesting results have been reported that stem from SDW quantization along the film normal [17–19]. Similar lattice constants and surface energies [20] promise a layer by layer growth of Cr on Fe close to systems which can be handled by theory. This simple growth mode was indeed observed for Cr films on perfect Fe(100) whisker surfaces [21] although investigations show that at the open (100) Fe/Cr interface an interface diffusion involving two monolayers may occur even at room temperature deposition [22,23]. The layer by layer growth mode leads to the observation of a short oscillation period of 2 ML of the bilinear coupling term in addition to the long oscillation period of 9 ML which still can be observed for a worse growth.

A much little 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 [24] in contrast to the observations for (100)-oriented interface. 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].

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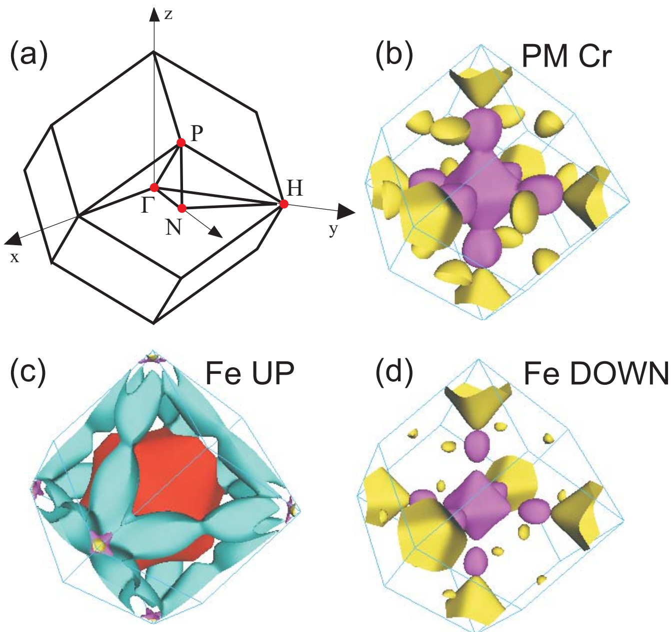

Fig. 1. Upper panel shows the first Brillouin zone together with high-symmetry points of the *bcc* structure (a) and Fermi surface of *bcc* Cr crystal (b). The *bcc* Fe spin-up (c) and spin-down (d) Fermi surfaces are shown in the lower panel. Images are taken from the Fermi Surface Database [9].

This fact was also successfully interpreted by coupling strength which comes from the extremal vector centered at the ellipsoid N of the Fermi surface of Cr (Fig. 1) [25]. In this theoretical work [25] as well as in the earlier work on exchange coupling in magnetic heterostructures [26] the short-period oscillations with a period of 4.7 Å in Cr were also predicted. Some indication of such short-period oscillations can be found in the experimental work on determination of bilinear coupling constant in Fe/Cr/Fe(110) trilayers [27]: 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 (110)-oriented 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 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.

Spin-resolved photoelectron spectra (He Iα, $h\nu$ = 21.22 eV) were recorded at 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 [28]. The angular resolution was 2° and energy resolution was set to 100 meV. Effective Shermann function was determined to be 0.1. The light incident angle was 30° with respect to the sample surface. Spin-resolved measurements were performed in magnetic remanence after having applied a magnetic field pulse of about 500 Oe along the in-plane $\langle 1\bar{1}0\rangle$ 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 [29,30]. The base pressure during the experiment was 7×10^{-11} mbars rising to 3×10^{-10} mbars during metal evaporation. Thin Fe(110) films with a thickness of 40 Å and Cr layers on top of the Fe film with different thicknesses 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 (XPS)] 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 low-energy electron diffraction (LEED). The cleanness of the films was routinely monitored by LEED and XPS of core levels as well as by means of UPS of the valence band.

Figures 2 and 3 show the experimental spin-resolved photoemission spectra and corresponding spin polarization as a function of binding energy, respectively, of the Cr/Fe(110) system measured in normal emission geometry for different thicknesses of the Cr overlayer (marked on the figure foe each spectra). In these figures 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 [31,32]. 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 in the spin-resolved spectra of Fe that can be explained by predominant spin-dependent scattering of photoelectrons penetrating through Cr layer [33]. Further spin-resolved spectra can not be simply described by the spin-selective scattering of photoelectrons 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. As was pointed earlier [34] the energy position of this feature can be used as a measure of the magnetic moment of the surface Cr layer. Alternatively to the (100)-oriented interface, in the present case the small BE of this

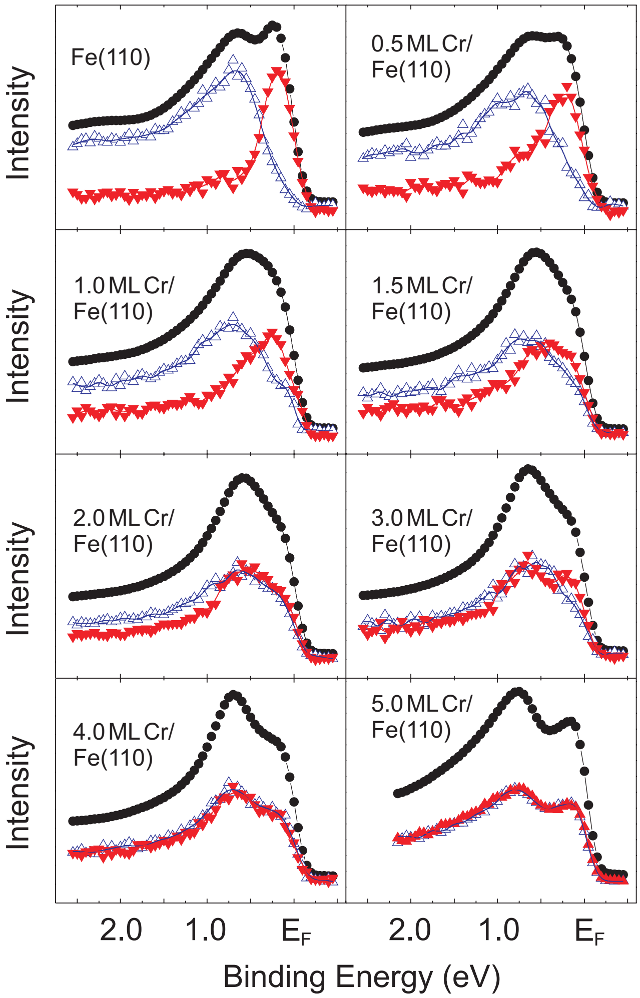

Fig. 2. Spin-resolved photoelectron spectra of the Cr/Fe(110) system obtained at photon energy of $h\nu = 21.22\,\text{eV}$ for different thicknesses of Cr overlayer (marked on the figure). All spectra were obtained in normal emission geometry. Solid circles, empty triangles up, and solid triangles down shows total intensity, spin-up, and spin-down intensities, respectively.

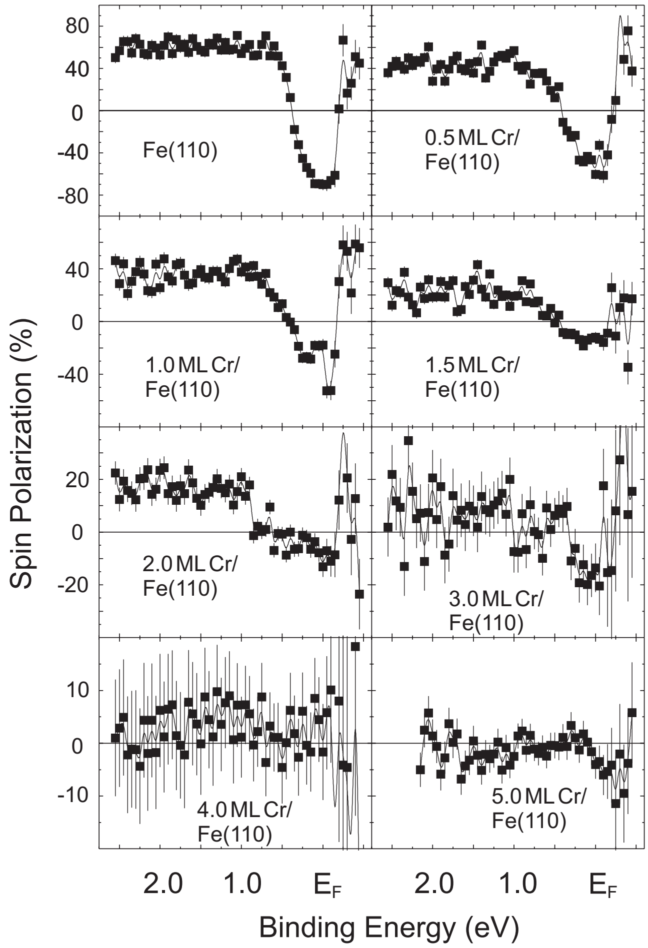

Fig. 3. Spin polarization as a function of binding energy for the corresponding spin-resolved photoelectron spectra in Figure 2.

feature at very low Cr coverages seen in Figure 2 can be explained by strong covalent $d-d$ bonding in addition to metallic cohesion between Fe and Cr at the Cr/Fe(110) interface [35]. The magnetic moment at such interface is reduced, since neighboring Fe and Cr atoms tend to align their magnetic moments antiparallel to each other. Upon further Cr deposition, the bonding of the surface Cr atoms with Fe underlayer becomes weak 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 the 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 extracted from Figure 3 as a probe of possible different period oscillations in Cr(110) film. This dependence as a function of Cr overlayer thickness is shown in Figure 4. The first monotonic decreasing of spin polarization at E_F from $70 \pm 5\%$ to nearly 0% for Cr thicknesses of $0\,\text{ML} < d_{Cr} < 2.5\,\text{ML}$ 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 of the spin-down character in the vicinity of the Fermi level. The corresponding spin-resolved spectrum is shown in Figure 2 (third spectra in the right panel). The nearly same behavior was observed for the thickness of Cr overlayer of about 5 ML where again slight increasing of spin-polarization was detected. Also, spin-resolved spectrum for 3 ML of Cr overlayer demonstrate 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. [25] for different orientations of the interface: (100), (110), and (211). In case of the (110)-oriented interface, as in the widely studied

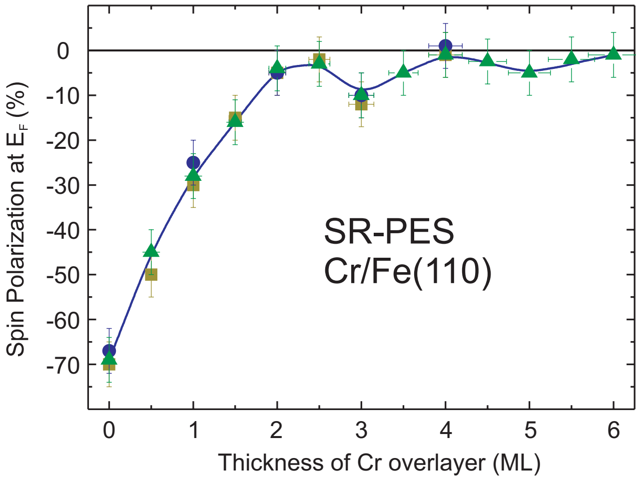

Fig. 4. Spin polarization at E_F as a function of thickness of Cr overlayer in Cr/Fe(110) system. Different symbols correspond to three different series of measurements. The solid line is eye-guide to experimental points.

(100) case, one can find extremal vectors that span the lens (please, see the notation in work [25]) and vectors at the N ellipsoids (see Fig. 1). As was found, the most important contribution to the coupling is made by N ellipsoid vectors responsible for long-period oscillations. In this case, similar to (100)-oriented interface, the majority electrons are strongly confined in the Cr 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 [25] the prediction on the existing of possible short-period oscillations was made. It was shown that there are a non-negligible coupling strength for (110) orientation with periods of 5.86 Å (∼2.9 ML) and 4.7 Å (∼2.35 ML) that have coupling strength of 0.86 mJ/m^2 and 2.02 mJ/m^2, respectively. The first one corresponds to the $\mathbf{k}_{||} = (0, 0)$ vector and observed experimental oscillations measured in normal emission geometry can be assigned to it. 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 peaces of the Fermi surface and in case of (110) oriented film there are two possible candidates for such periodic behavior. The first one is the nesting vector between Γ electron and H hole octahedrons and the second possible candidate might be the nesting vector between Γ electron octahedron and N hole pocket (Fig. 1). The role of each vector have to be clarified in additional calculations of the electronic structure of the Cr/Fe(110) system. To the best of our knowledge, this is a first time experimental evidence for the observation of the short period oscillations in photoemission of (110) oriented Cr thin film which is supported by theoretical calculations [25,26].

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 behavior of P for thicker film, that gives an evidence for the observation of short-period oscillations in photoemission of thin (110)-oriented Cr film on top of Fe(110). Observed effects are supported by theoretical calculations that take into account different nesting conditions in electronic structure of Cr. Our studies demonstrates that spin- and angle-resolved photoemission is a powerful instrument for studies of **k**- and spin-space origins of different oscillation periodicities in the interlayer magnetic coupling. This can be broadly used in studies of the electronic structure of magnetic multilayers.

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