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Structure of Cr overlayers on Fe surfaces: a new approach for the interpretation of spin-resolved photoemission and magnetic dichroism spectra

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Abstract

Results of investigations of Cr overlayers on Fe surfaces by magnetic linear dichroism in the angular distribution and spin-resolved core level photoemission are analysed within the framework of a new model approach. It includes a special algorithm for modelling epitaxial growth of overlayers with different roughness together with self-consistent calculations of the magnetic moment distribution within a Periodic Anderson Model. On this basis the value of the magnetic dichroism and the spin polarisation in photoemission as functions of the Cr coverage can be modelled also for rough surfaces. The comparison of experimental spectra and theoretical coverage dependencies obtained for the different surface roughnesses leads to conclusions about the microscopic structure of Cr overlayers.

Keywords: Magnetic dichroism; Core-level photoemission; Surface and interface roughness

The number of contradictory conclusions about the magnetic structure of Cr overlayers on Fe substrates reflects the complexity of this system and its sensitivity to surface roughness, which depends on the details of sample preparation. Spin-polarised electron spectroscopy and magnetic dichroism in angle-resolved core level photoemission prove to be very efficient tools for investigation of such a system because they represent a combination of a chemical and a magnetic probe [1–5]. The surface sensitivity of photoemission makes it necessary to develop a theory for the description of emission from rough surfaces for the interpretation of experimental spectra. This paper proposes such a theory, which includes a self-consistent calculation of the magnetic moments, that takes into account interface roughness and interdiffusion and a description of photoemission from rough surfaces. The analysis proceeds in three steps: first, a rough surface or interface is generated by an epitaxy algorithm; second, the magnetic moments are calculated using an Anderson periodic model; and third, the magnetic signature of the photoemission signal is expressed in terms of a weighted averages of the individual magnetic moments. The weighting of the moments is important because of the finite escape depths of the photoelectrons. In addition we suggest that for rough surfaces the concept of surface atoms itself needs revision.

We suppose that electron polarisation in a core-level photoemission experiment and the magnetic linear dichroism is proportional to the value of the localised magnetic moments. For an ideally smooth surface, all the atoms in one atomic layer have the same magnetic moment, such that the resulting spin polarisation can be written as

$$I = M_1^S + \alpha M_2^S + \alpha^2 M_3^S + \cdots,$$

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where M_i^S is the local magnetic moment of S type atoms (S = Fe or Cr) from ith layer, and α takes into account the attenuation of the photoelectron signal arising from non-surface layers due to the finite mean free path. In a simple approach, α can be expressed through a universal escape depth λ, which depends on the kinetic energy of the photoelectrons, and a characteristic length L, which is proportional to the lattice constant and determined by geometry of experiment:

$$\alpha = \exp(-L/\lambda).$$

For rough interfaces, where a given atomic layer may contain Fe and Cr atoms with different magnetic moments as well as empty sites, we obtain for the normalised difference between the number of electrons with spin up and spin down projection emitted from the surface ($I = (I_+ - I_-)/(I_+ + I_-)$) the following expression:

$$I = \frac{\sum_{i=1}^{\infty} M_i^S \prod_{j=1}^{i-1} \left[1 + (\alpha - 1)\frac{N_j}{N}\right]}{\sum_{i=1}^{\infty} N_i^S \prod_{j=1}^{i-1} \left[1 + (\alpha - 1)\frac{N_j}{N}\right]},$$

where M_i^S and N_i^S are the total magnetic moment and d-electron number on S type atoms in the i-layer; N_j/N is the fraction of the filled sites in layer j.

To model rough surfaces and interfaces, we use an 'epitaxy' algorithm [6], which fills the sites of the ideal bcc lattice inside a prism of $8 \times 8 \times 20$ atoms (Fe or Cr) using a special random procedure. Outside the prism we chose periodic boundary conditions. Variation of the parameters in the algorithm allows one to create samples with different interface roughness. For determination of the average, the sample construction was repeated 20 times, and for each of these configurations the d-electron number and the magnetic moment on every site were calculated within Periodic Anderson Model [6]. A distribution of the magnetic moments is determined self-consistently in the mean-field approximation by taking into account the d–d interaction in the first coordinate sphere of the atoms. Parameters of the model were chosen so as to reproduce the bulk Fe and Cr moments and the d-electron numbers.

The coverage dependencies of the polarisation on Cr atoms as calculated for a smooth interface (2–3 layers containing both Fe and Cr atoms) and for a rough interface (Fe and Cr intermixed in 10–11 layers) are depicted in Figs. 1 and 2. In both cases, the Cr polarisation is negative for low Cr coverage [1–5]. This is related to the antiferromagnetic coupling between the Cr submonolayer and the Fe substrate. The polarisation may oscillate [3,4] or decrease monotonically with coverage [2,5], depending on the surface roughness and interdiffusion in the interface region. In the case of an oscillatory behavior, the oscillations are more pronounced for small α. The maximal positive polarisation, when the sign of

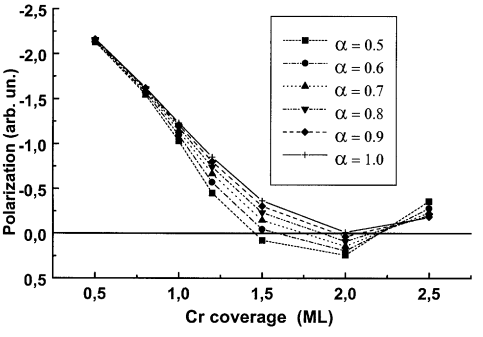

Fig. 1. Coverage dependence of polarisation on Cr atoms for a Cr overlayer on Fe with 'smooth' interface generated by algorithm 'epitaxy' (interface region is 2–3 layers). Different symbols correspond to various values of the parameter α.

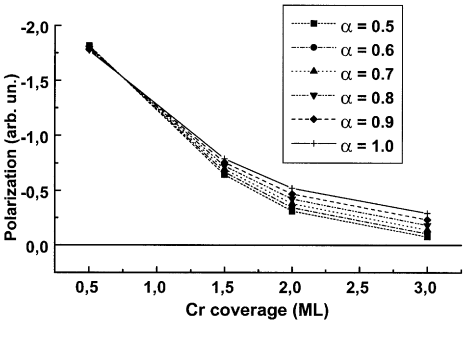

Fig. 2. Coverage dependence of polarisation on Cr atoms for Cr overlayer on Fe with 'smooth' interface generated by 'epitaxy' (interface region is 10–11 layers). Different symbols correspond to various values of the parameter α.

the polarisation coincides with that of the Fe atoms, occurs at Cr coverage 2 ML. For ideally smooth surfaces such behaviour is quite natural. The first Cr monolayer on Fe has a surface-enhanced moment opposite to the Fe moments. When another 'ideally smooth' Cr layer is deposited, it will have a surface-enhanced moment opposite to that of the previous layer. Furthermore, it will reduce the value of the magnetic moment of the previous layer, because the atoms in that layer cease to be at the surface. That is why with every monolayer one can expect a change of the sign of polarisation. Roughness will erode such an oscillation, but as is seen in Fig. 1, it does not destroy the oscillation for relatively smooth surfaces. For rough interfaces, this signature of the antiferromagnetic structure is fully destroyed, as is seen in Fig. 2.

Comparison of the experimental [4] and theoretical curves suggests some conclusions about the microscopic structure of the Cr overlayer. Theory predicts a monotonic change of the spin polarisation up to 2 ML Cr coverage, and even a change of sign of polarisation near this point for smooth surfaces. The dichroism

experiment, in contrast, shows an oscillation and a maximum instead of a minimum for 2 ML coverage [4]. This contradiction can be explained if one supposes a non-uniform growth of the second layer. If the growth of the overlayer passes through that stage when the formation of the second Cr ML is suppressed, then instead of uniform coverage we obtain a superposition of 1 and 3 ML coverages and an increase of the absolute value of dichroism on Cr atoms results. Further deposition of Cr leads to the filling of the space around islands, which decreases the absolute value of dichroism. The physical reason for the three-dimensional growth can be connected with electron confinement in the Cr islands on Fe and with an oscillation of the energy of these electrons with thickness of islands [7], in a similar manner to the quantum well model for exchange coupling oscillation [8]. The same mechanism may be responsible for the non-Poisson island growth reported in Refs. [2,5].

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