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# Magnetic structure of nonideal Fe/Cr interface

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**Abstract**

Different kinds of space defects on the background of ideal smooth interface in Fe/Cr multilayers, such as steps, embedded clusters, pinholes, random interface roughness, are investigated within model Hamiltonian approach. Calculations of magnetic structure are performed in the periodic Anderson model (PAM) in mean field approximation by recursion method in the real space.

The distribution of magnetic moments obtained for two sets of interfaces (with different roughness) shows strong sensitivity of magnetic structure to the interface roughness and interdiffusion. Application of the theory for interpretation of Mössbauer spectra of Fe/Cr multilayers is discussed. Spectra obtained for three perpendicular orientations of the sample relatively to the incident beam allowed to avoid the problem of nonrandom distribution of magnetic moment direction in the multilayers.

Information about the angular dependence of hyperfine fields on the Fe atoms in Fe/Cr superlattices obtained by means of Mössbauer spectroscopy technique is discussed within the framework of the theory of noncollinear magnetic structure.


*Keywords:* Roughness; Interdiffusion; Electronic structure; Mössbauer spectroscopy

Fe/Cr interface magnetism is one of the challenging topics of modern science of low-dimensional structures. It attracts a number of experimental tools and theoretical approaches [1], but up to now the electronic and magnetic structure at the interface region remains partly unknown. One of the reasons is connected with the formation of defects such as embedded clusters, steps, and pinholes near the interface in the layered system. The space structure of this region appears to be very complex and it crucially influences the physical properties. For example, Heinrich et al. [2] have shown that bilinear exchange coupling of Fe/Cr multilayers can be changed by factor of 5 by varying the substrate temperature during the growth of the first atomic layer. So, the development of the theory for description of different kinds of space defects near the interface is very important for the adequate interpretation of the experiments in Fe/Cr systems.

In this paper we discuss the results of calculation of nonideal Fe/Cr interface and its application to the explanation of Mössbauer spectra of such a system.

Note that taking into account complex space defects for the description of real interface magnetic structure forbid the use of ab initio-like theories due to huge increasing of numerical calculation which is out of possibility of modern computers. In this case tight binding models like PAM or Hubbard model (HM)

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remain so far the main tool for the description of non-ideal rough interface under experimental investigation.

On the basis of such theories the different kinds of defects were investigated. Calculation of magnetic moments on the stepped vicinal Cr surface and Fe/Cr stepped interface [3,4] revealed reasonable agreement of the magnetic moment distribution obtained in PAM and HM. Computation of magnetic moments perturbation of Fe atoms due to Cr impurities [4] and Fe clusters embedded into the Cr matrix (both in the bulk and near the surface or interface) [5] have revealed important role of defects of magnetic structure for interpretation of hyperfine fields (hff) distribution given by Mössbauer spectroscopy. In particular, the deviation from additivity in the perturbation of magnetic moment of Fe atoms by Cr impurities and dependence of magnetic moments of Fe clusters in the Cr matrix on the distance from the surface and interface, that are usually not considered in the spectra treatment, are discussed.

In [6] within PAM the distribution of magnetic moments in Fe/Cr/Fe sandwiches with pinhole defects has been studied. The distribution of the Fe moments inside pinholes appears to be similar to the ones in Fe clusters embedded into a Cr matrix. Such defects also should be taken into account especially for interpretation of experiments on the Fe/Cr superlattices with short period.

However, all mentioned papers give only magnetic structure around special kinds of defects and cannot be compared with experimental distributions of obtained on samples with a number of different defects.

Modelling of the magnetic properties of the Fe/Cr interface [7] on the basis of the special "epitaxy algorithm" within the framework of PAM allows to obtain the distribution of magnetic moments for the random structure with different kinds of defects. Self-consistent calculation of magnetic moments gave reasonable explanation of Turtur's and Bayreuther experiment [8]. However, for this purpose it was not necessary to calculate the distribution of magnetic moments, because only total magnetic moment of the sample was measured. On the contrary, for interpretation of Mössbauer data it is necessary to find the number of atoms with given magnitude of magnetic moments, because it is the distribution that can be compared with one for hff. Below we will represent such a data for two variants of modelling of epitaxy process.

Detailed description of epitaxy algorithm was done in [6,7]. The prism of $8 \times 8 \times 18$ was filled with atoms Fe and Cr using random procedure. The base of this prism in our calculation comprises $8 \times 8$ elementary cells; its height is 18 levels. Outside of the prism the structure is repeated periodically. Two variants of algorithms A and B give the surfaces and interfaces with different roughness. A-algorithm gives relatively smooth interface without pores. The width of the interface region, where there are both atoms Fe and Cr do not exceed four layers. B-algorithm produces more irregular interfaces with some hollows and interface mixing of Fe and Cr atoms in the 7–10 layers. Self-consistent calculations of magnetic moments were performed for sets of 20 interfaces constructed by A or B variant of epitaxy algorithm when at first $64 \times 6$ atoms of Fe were distributed in the prism and after that $64 \times \xi$ atoms of Cr were "sputtered" on Fe substrate. Covering parameter $\xi$ in our calculation was taken from 0 to 2.5 with a step of 0.5. As a result we obtain the structure where low layers (12–18) are filled preferably by Fe atoms. After that follows "Cr" slab with thickness depending on the covering parameter $\xi$. Upper layers (with small number 1, 2 ...) are empty.

In Fig. 1 the distribution of magnetic moments on Fe atoms in the interface regions for A-type interfaces is depicted. 11, 12, and 13 layers are interface regions where there are both Fe and Cr atoms. All the sites lower than 13 layer are fully filled by Fe and all the sites in the layer higher than 11 are filled by Cr atoms or empty. The number of Fe atoms at every interface layer is shown in Fig. 1. The figure demonstrates the dynamics of change of magnetic moments on Fe atoms with Cr covering.

For $\xi = 0$ near the surface one can find the enhancement of magnetic moment up to 2.5–2.6 $\mu_B$ per site. Small Cr covering ($\xi = 0.5$) leads to the decrease of the moments. However, this decreasing differs for each layer. For Fe atoms in 13-layer most atoms have the moment which corresponds to bulk Fe, and only part of the atoms which have Cr among

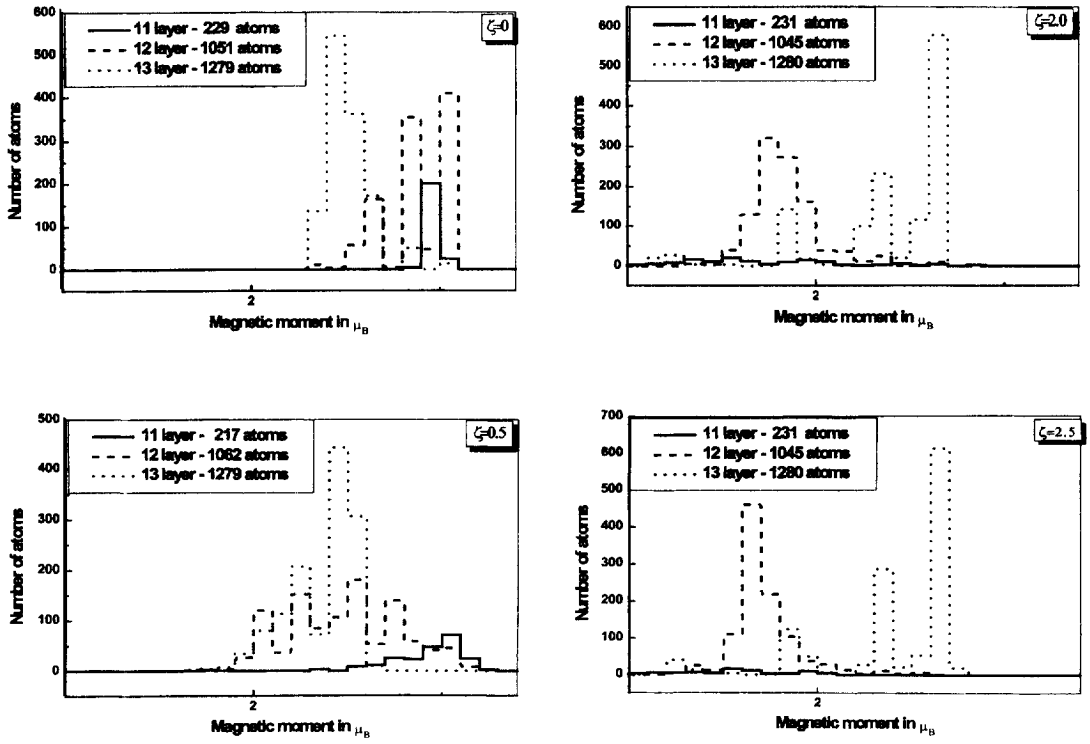


Fig. 1. Distribution of the magnetic moments on Fe atoms near Cr/Fe interface for Cr overlayer on Fe. $\xi$ is the Cr-covering parameter. Random interface is produced by A-algorithm "epitaxy". In the box of figure the number of Fe atoms in every interface layer are shown.

their nearest neighbours decrease their moment. For 12-layer, small Cr covering leads to the very wide distribution of the moments, because in this layer stay surface atoms with enhanced moment, which do not have Cr neighbours, as well as atoms with several Cr neighbours with reduced moments. Most of Fe atoms of the 11-layer conserve their large moments because Cr transfer through this layer and they stay at the surface on the top of the sample.

When the Cr covering increases, the moments of 13-layer slightly grow. Similar behaviour for Fe atoms which have no Cr atoms in its nearest neighbours but only among second neighbours takes place for the inner atoms in clusters [5,9] and pinholes [6]. The 12-layer for the larger Cr covering has reduced magnetic moments because the most of these atoms have several neighbouring Cr atoms. As for 11-layer, one can find the change of direction of magnetic moments on some sites for higher Cr covering due to Fe–Cr exchange interaction.

For more rough interface of B-type the general behaviour of magnetic moments stays almost the same but the distribution of moments on every layer becomes much more wide.

Special interest concerns the distribution of magnetic moments of Cr atoms and its dependence on the roughness of the interface. In Figs. 2 and 3 such distribution for A-type and B-type surfaces correspondingly are shown. One can see the transition from layered antiferromagnetic structure to random structure with increasing of interface roughness. Despite the large (more than $2\mu_B$) local magnetic moment of subsurface Cr atoms the average moment of these layers appear to be almost zero. So, not only the existence of steps on the surface but also the distribution of the moments on the random rough interface can explain the contradiction between experimentally measured zero total moment and enhanced local moments of Cr overlayers on Fe substrate [9].

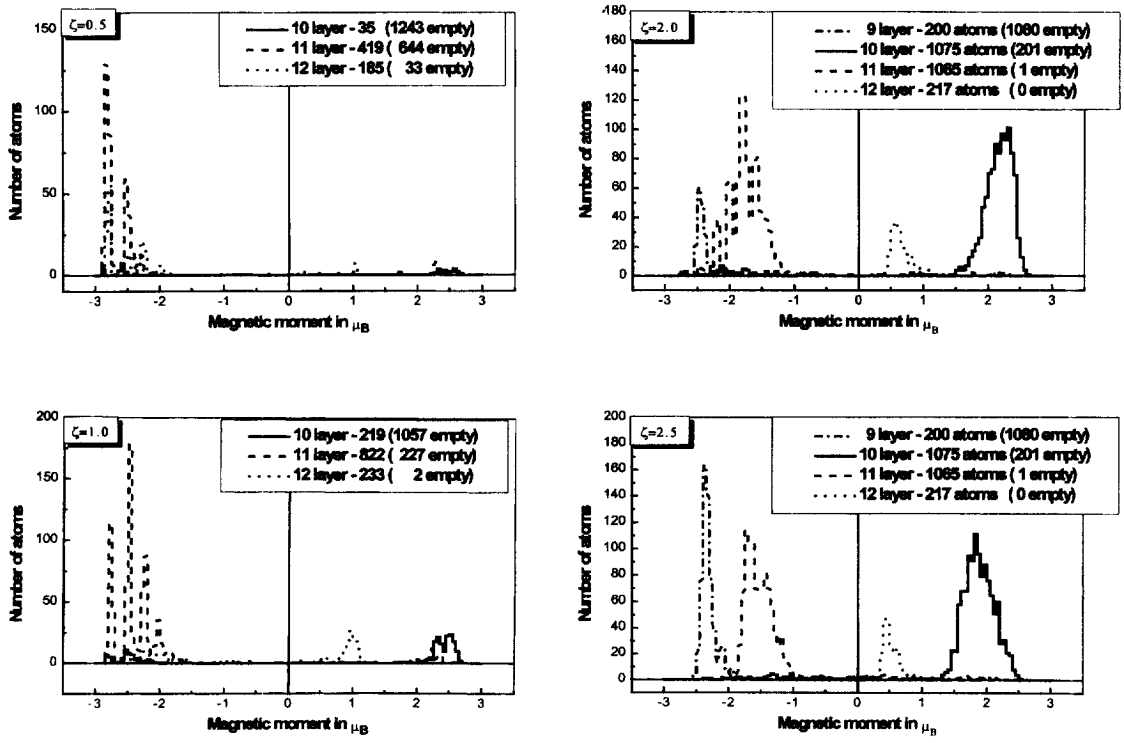


Fig. 2. Distribution of the magnetic moments on Cr atoms near interface Cr/Fe for Cr overlayer on Fe. $\xi$ is the Cr-covering parameter. Random interface is produced by A-algorithm "epitaxy". In the box of figure the number of Cr atoms in every interface layer are shown.

Our results for the distribution of magnetic moments in Cr overlayer on Fe can be used for interpretation of Mössbauer spectra [10,11] if as a first approach we consider that hff is proportional to the local magnetic moments on Fe atoms.

There are however two circumstances which have to be taken into account for this interpretation:

(1) If for the bulk materials assumption about proportionality between magnetic moment and hff is usual, for low-dimensional metallic systems it is true only for hff which is connected with polarisation of inner shells. Conductivity band gives direct contact contribution to the hff field which have to be taken into account separately.

(2) In the layered structures the distribution of direction of magnetic moments is not random. It leads to the dependence of Mössbauer lines amplitude on the orientation of the sample relatively to the incident beam.

A second problem can be avoided experimentally if one takes three spectra obtained for perpendicular directions of $\gamma$-radiation incidence instead of one. After composition of these three spectra one can obtain free-texture spectrum which does not depend on the distribution of direction of magnetic moments in the sample [10].

From another side these three spectra can give an additional information about the direction of magnetic moments in the sample. For its theoretical interpretation it would be useful to develop the theory for the description of noncollinear structure in the low-dimensional metallic systems. Variant of such a theory based on the PAM gives the possibility for such calculations. Note, however, that our preliminary calculations show that Fe atoms prefer to keep their moments parallel or antiparallel and only in the neighbourhood of the space defects (like step or embedded cluster touching the interface) noncollinear ordering

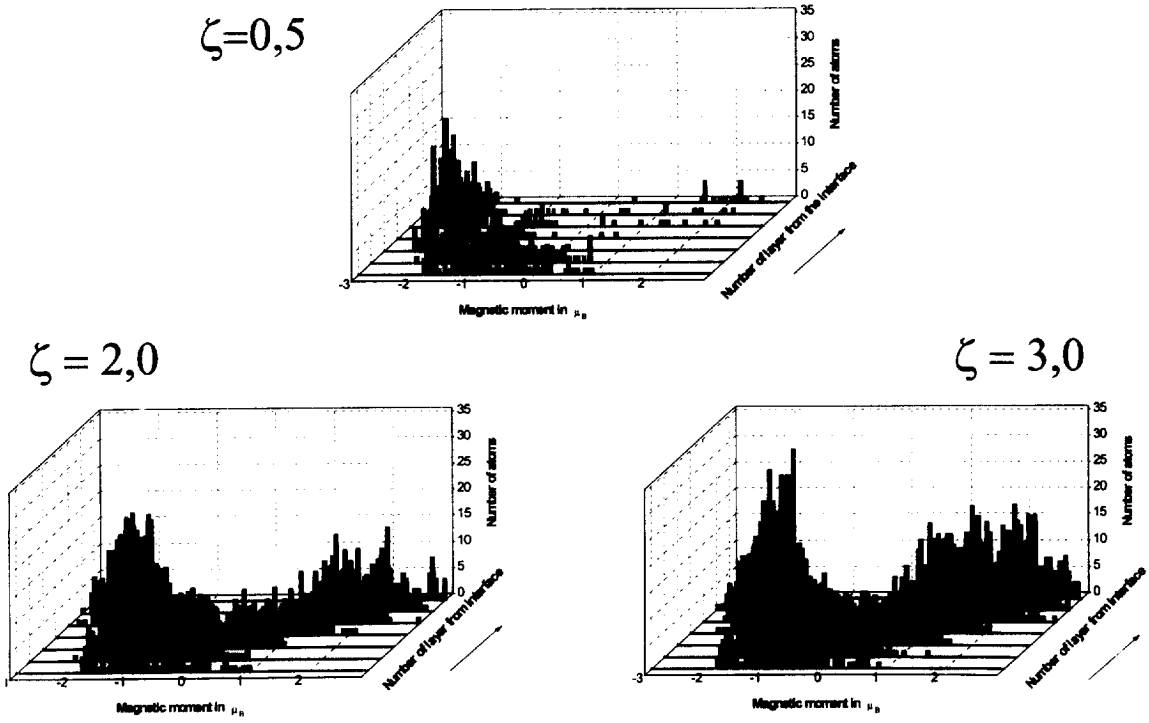


Fig. 3. Distribution of the magnetic moments on Cr atoms near interface Cr/Fe for Cr overlayer on Fe. $\xi$ is the Cr-covering parameter. Random interface is produced by B-algorithm "epitaxy".

can appear. Cr magnetic moments seem to be much more flexible and change their direction more easily.

Hff distribution obtained from these spectra can be compared with magnetic moments to clarify the influence of the interface roughness on the magnetic structure. Existence of the correlation in the position of satellites in Mössbauer spectra and maximum in the magnetic moment distribution [11] show that the contribution of 4s-band does not hide this information.

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