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Interface alloying in the metallic magnetic heterostructures with BCC lattice

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Abstract

Analysis of STM images of Fe grown on Cr and Cr grown on Fe with the exploitation of the differences of the Fe and the Cr surface state energies demonstrates strong intermixing during the epitaxial growth. We suggest a theoretical approach for modelling the epitaxial growth with subsequent self-consistent calculations of electronic and magnetic structure. On the basis of these calculations together with the experimental data obtained by complementary experimental methods, the structure of the interface on the atomic scale and the correlation between the chemical and magnetic roughness are investigated. We show that interface alloying is not symmetrical from both sides of the interface and suggest a scenario of the epitaxial growth that leads to this asymmetry. © 2001 Published by Elsevier Science B.V.

Keywords: Magnetization; Thin films; Superlattices; Epitaxy

Metallic magnetic superlattices with BCC structures present a wide class of low-dimensional magnetic systems, demonstrating a number of new phenomena important for fundamental magnetism and for applications. Interdiffusion and interface roughness strongly affect all macroscopic properties of these systems. Accordingly, the control of the epitaxial growth and the investigation of the interface structure are important problems. Scanning tunneling microscopy (STM) is a very powerful tool allowing to determine the position of individual atoms and, consequently, to perform direct measurement of the surface structure during the epitaxial growth. Generally, STM information is not element specific but for metallic BCC-systems, even in the case of close lattice constants, imaging at the bias voltages near the corresponding surface states can differentiate elements and it also provides microscopic information about alloying and the chemical structure of overlayers.

The results of STM investigations of alloying at the interfaces Fe/Cr (Fe on Cr [1]) and Cr/Fe (Cr on Fe [2]) differ very quite essentially although both studies confirmed strong intermixing at the interfaces. Davis et al. [1] show that layer-by-layer growth at 300°C leads to the formation of a Cr–Fe alloy that is observed as a distribution of single atomic Cr impurities dispersed in the Fe substrate in the submonolayer-coverage regime. In the low-coverage regime where the individual Cr atoms can be resolved, the spatial correlation can be evaluated from the experimental data. Suppression of nearest-neighbor occupation is indicative of an effective repulsive interaction between the Cr impurities. According to Choi [2], the surface-alloy formation can also occur at the low Fe coverage on the Cr(1 0 0) surface. The Fe was deposited at room temperature and subsequently, the sample was annealed at temperatures between 200°C and 300°C. In contrast to the case when Cr diffuse into the Fe matrix and form a disordered isomorphic alloy, observed Fe atomic rows indicate an ordered alloy formation for Fe grown on a Cr(1 0 0) substrate. Our own STM study of the structure of Cr on Fe(0 0 1)-films grown on an Ag(0 0 1)-substrate also confirmed the intermixing at Fe/Cr interface. The difference between Fe/Cr and Cr/Fe interfaces was also detected by means of Mössbauer spectroscopy [3]. Conversion electron Mössbauer spectra (CEMS) of Fe/Cr(0 0 1) superlattices with 2 monolayers thick ^{57}Fe

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probe layers placed at Fe/Cr and Cr/Fe interfaces, respectively, gave the different distribution of the hyperfine fields (hff). In particular, for the Fe-on-Cr interface (as compared with Cr-on-Fe), a larger contribution of the bulk hff (33 T) was obtained, whereas the satellite peaks with lower field were more narrow and gave less contribution to the total spectra. The amplitude of the low field peak (20 T) often was associated with atoms at the ideally smooth interface [4], but our calculations did not confirm this assumption [5]. Correlation between the amplitude of 20 T peak and giant magnetoresistance effect (GMR) leads to the conclusion about the role of interface and bulk scattering for GMR in Fe/Cr systems [4]. This conclusion and assumption, that alloying at the interfaces is driven by the melting points of bulk Fe and Cr [6], have to be revized in accordance with our calculations of Fe/Cr superlattices with rough interfaces.

For the interpretation of experimental data within the terms of local atomic environment and atomic magnetic moments at each site, we developed the theoretical approach, which includes the modelling of the alloyed interfaces and subsequent calculation of magnetic structure within a periodic Anderson model [7,5]. Interface alloying was introduced into the system by several random algorithms. For Fe/Cr systems with bcc structure, which will be discussed in the following, these algorithms place atoms into the sites of ideal BCC lattice inside the prism. Out of the prism we used periodic boundary conditions. The simplest routine, which leads to intermixing at the interface, is the algorithm of ballistic deposition. This algorithm adds single atoms to the top level of the prism in a random procedure and lets them descend through empty sites until further descending is blocked by occupied sites. The bottom layer initially is blocked. The procedure of ballistic deposition

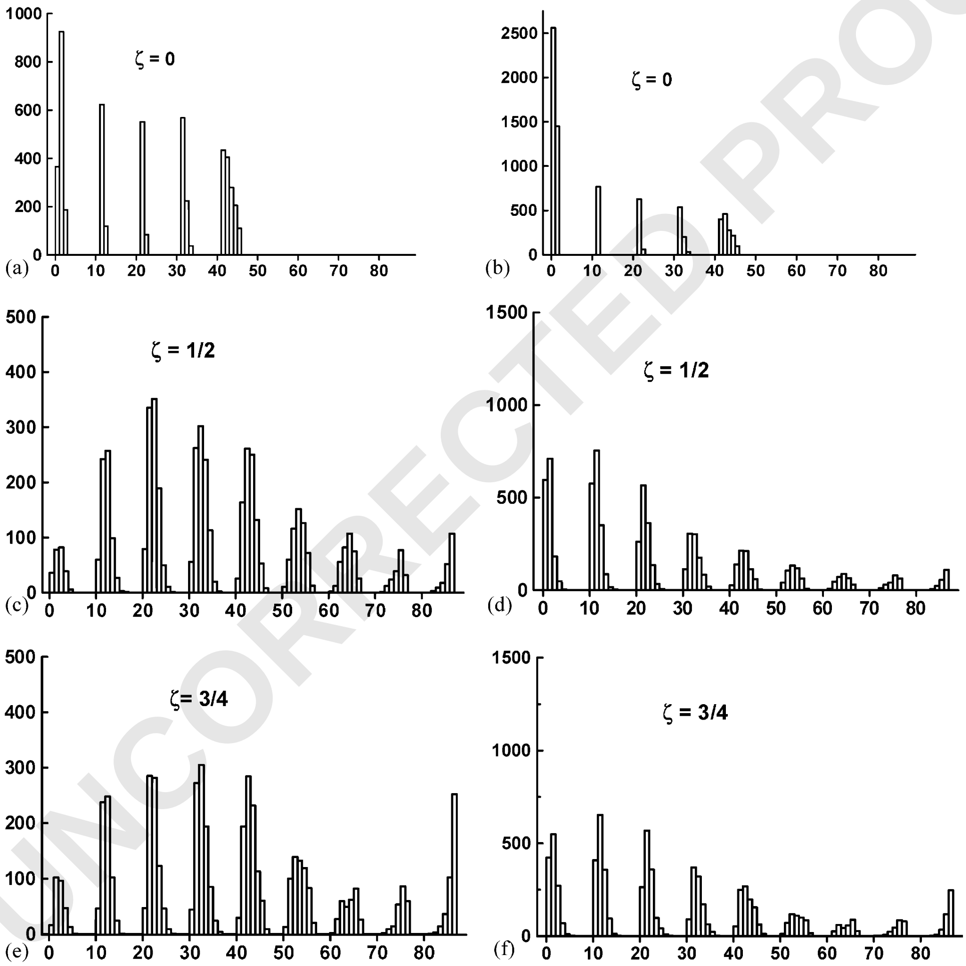

Fig. 1. Amount of Fe-atoms with adifferent number of the nearest neighbors (n_1) and second neighbors (n_2) Cr-atoms for the superlattice Fe_4/Cr_{41} (left panel) and Fe_6/Cr_{41} (right panel) and for different values of intermixing parameter ς. Bottom axis is graduated by $10n_1 + n_2$.

gives a relatively thin interface region, where only 2–3 monolayer contain atoms of different elements simultaneously. Such a scenario, however, cannot reproduce the different structures of the Fe/Cr and Cr/Fe interfaces. The second part of the algorithm presupposes the floating up of some atoms after deposition of the next layer on the surface. It assumes that site exchange of atoms and their diffusion take place only at the surface during the epitaxial growth and that there is no internal bulk diffusion. Exchange of atoms during deposition of the next layer leads to the asymmetry of the interface: atoms could flow up on several layers but did not move down due to suppression of diffusion into the internal layers below the surface. Modelling of such a scenario was organized as follows: we start from multilayers constructed by the algorithm of simple ballistic deposition. Then in every layer we chose a definite fraction (ς) of atoms using a random procedure, and layerwise, starting from the bottom, we exchanged this fraction of atoms in every pair of neighboring layers. The value of $\varsigma = N_{\text{exch}}/N_{\text{tot}}$ (where N_{exch} is the number of exchanged atoms and N_{tot} is the total number of atoms in the base layer of the prism) is the parameter of the model.

Fig. 1 shows the distribution of the Fe atoms, which have a given number of the nearest neighbors (n_1) and second neighbors (n_2) Cr-atoms for the superlattice Fe_4/Cr_{41} (a, c, e) and Fe_6/Cr_{41} (b, d, f). All structures were obtained using an algorithm with the floating of atoms during the deposition and with different parameters ς ($\varsigma = 0$ for Figs. 1a and b; $\varsigma = 0.5$ for Figs. 1c and d and $\varsigma = 0.75$ for the Figs. 1e and f). The bottom axis is graduated by the values $10n_1 + n_2$. Distributions in Fig. 1a and b with $\varsigma = 0$ correspond to the simple ballistic deposition algorithm. Increase of parameter ς leads to the more uniform distribution of Fe-atoms on the configuration, and to the filling of the state with a larger number of n_1 and n_2. Especially a large difference was found in the number of atoms with $n_1 = 8$ and $n_2 \neq 0$, i.e. for atoms inside the Cr spacer but not far from the interface. Increasing the thickness of the Fe slab leads to a larger contribution of bulk-like Fe atoms and Fe atoms with small numbers of Cr neighbors. Therefore, via the changing of the thickness of the Fe slabs and substrate temperature during the epitaxial growth or the deposition ratio (which determines the parameter ς in our model) one can manipulate the distribution of Fe atoms in the local configuration as well as the magnetic structure.

Different distributions of hff for the samples with probe ^{57}Fe layer only at Fe/Cr or Cr/Fe interface can be easily explained using the algorithm we developed. For the probe layer at Fe/Cr (Fe on Cr) interface, ^{57}Fe atoms will flow up into the Fe slab and will increase the bulk-like hff. At the Cr/Fe interface, the Fe atoms will flow up into the Cr spacer and it will increase the low-field contribution. It is such a behaviour of the hff that was observed in the experiment [3]. Note that this scenario of epitaxial growth is very general and gives a natural explanation of the change of the hff distribution on ^{119}Sn atoms in V/Cr superlattices versus the position of ^{119}Sn probe layer inside the Cr spacer [8] as well.

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