Calculated magnetic properties of an $Fe_{1-x}Ni_x$ monolayer on Cu(001)

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We present a detailed investigation of the magnetic properties of a single monolayer of Fe-Ni alloy film on Cu(001) substrate by means of the spin-polarized linear muffin-tin orbitals Green's-function technique and the Korringa-Kohn-Rostoker Green's function method. The coherent-potential approximation formalism is used in both approaches. Our study shows that the FeNi film remains in a high-spin state for the whole concentration interval, which agrees with experimental data. We observe substantial deviations between the film and the bulk magnetization in Fe-rich, as well as in Ni-rich alloys. We consider the influence of main important factors on the behavior of the magnetic moment of the film: (i) the nonequilibrium lattice parameter of the alloy, (ii) the interaction between the epitaxial monolayer of FeNi with substrate, (iii) reduced dimensionality of monolayers. The possibility of a direct extrapolation of results of surface properties towards properties of bulk alloys is discussed. [S0163-1829(99)14821-5]

I. INTRODUCTION

The most prominent feature of the Fe-Ni alloy system is a nearly vanishing thermal expansion coefficient for the $Fe_{0.65}Ni_{0.35}$ alloy, an effect also known as the Invar effect discovered by Guillaume in 1897.[1] Also other properties of $Fe_{1-x}Ni_x$ alloys show unusual properties such as a martensitic bcc-fcc structural phase transition with increasing concentration of Ni and a vanishing magnetic moment of the fcc alloys near the Invar concentration accompanied by a collapse of the Curie temperature. All these peculiarities have attracted a lot of attention, and have stimulated numerous theoretical, as well as experimental investigations of this system.

The magnetic moment of the $Fe_{1-x}Ni_x$ alloys shows an anomalous behavior with substantial deviations from the Slater-Pauling curve. In the Fe-rich region the bcc structure is stable, and the magnetic moment follows the Slater-Pauling curve. However, with increasing concentration of Ni, the bcc-fcc transition occurs followed by an immediate drop of the average magnetic moment in the system to zero. Upon further addition of Ni the magnetic moment sharply increases and in the Ni-rich part of the phase diagram it is again in correspondence with the Slater-Pauling curve.

Different theoretical models for understanding the magnetic properties of Fe-Ni Invar alloys have been proposed.[2] One of those phenomenological theories, the so-called 2γ-state model, has been developed by Weiss.[3] He assumed coexistence of two different localized states, which are close in energy. These two states have different magnetic order [ferromagnetic (FM) and antiferromagnetic (AFM)], as well as different magnitudes of local magnetic moments [the high-spin (HS) and the low-spin (LS)] and different equilibrium volumes. According to Weiss theory and subsequent *ab initio* band-structure calculations[4–17] the following picture has emerged. The pure fcc Fe has two magnetic states.[10,18] The more stable one is the LS state with smaller equilibrium volume. The volume dependence of the total energy exhibits the second local minimum corresponding to the HS ferromagnetic state. In alloys, the addition of Ni leads to a decrease of the energy difference between these two states, and at certain concentration the HS state becomes more favorable. However, recent experimental and theoretical studies have shown several limitations of this model, and the importance of considering other magnetic states, such as the disordered local moment (DLM) and the noncollinear states has been emphasized.[19–22]

Thus, in order to understand better the anomalous magnetic behavior of $Fe_{1-x}Ni_x$ alloys it is necessary to investigate the Fe-rich fcc phase of this system. Unfortunately, bulk

fcc alloys become unstable with increasing concentration of Fe, and the fcc-bcc transition occurs. However, it is known that metastable structures can be stabilized on foreign substrate, and several experimental studies have been devoted to the properties of epitaxial fcc iron-nickel films grown on Cu(001) substrate over the entire Fe concentration range.[23–27] For thin films these measurements show a stability of the ferromagnetic state for the whole concentration interval,[26,28] but for films with intermediate thicknesses (about 5 monolayers) there have been indications that other magnetic phases are also present. Note, that a purpose of experimental investigations of iron-nickel epitaxial films is to analyze magnetic and structural properties of fcc $Fe_{1-x}Ni_x$ alloy layers and to attempt to explain some Invar anomalies in fcc bulk alloys based on the results obtained for thin films. However, there is a question to what extent a direct extrapolation of the experimental information obtained for a thin film towards bulk properties is valid.

Therefore, the main aim of our work is to investigate theoretically the influence of a surface as well as an interface with Cu on the magnetic properties of a single Fe-Ni monolayer on the Cu(001) surface. We have carried out first-principles calculations for this system, as well as for the bulk fcc Fe-Ni alloy over the whole concentration interval. In these calculations we use a lattice parameter equal to that of pure fcc Cu, and in doing so we are able to separate two kinds of effects originating from the Cu substrate, that is the effect of a nonequilibrium volume of the alloy film due to the necessity to match the lattice parameter of the substrate, and the effect of two-dimensional geometry itself. By comparing the results of surface and bulk calculations with each other we show how the surface influences the magnetic properties of the Fe-Ni system. In our calculations we consider only the ferromagnetic state of $Fe_{1-x}Ni_x$ alloys. This should be a reasonable approximation for a single monolayer, and also allows us to fulfil our main task; that is, to distinguish the surface and interface effects on the magnetic properties of Fe-Ni films on Cu(001).

II. METHOD OF CALCULATIONS

In order to increase reliability of our theoretical study we have employed two different computational methods. First, we have used a spin-polarized surface linear muffin-tin orbitals (LMTO) Green's function (GF) method[29–31] in conjunction with the principal layer technique.[32] The basis set included s, p, and d orbitals only. We have also included multipole contribution to the electrostatic potential in addition to monopole and dipole moments. Also bulk calculations have been carried out by means of the LMTO GF method[31,33–38] in the tight-binding (TB) representation within the coherent potential, atomic sphere, and frozen core approximations. For several bulk calculations we have used fixed spin moment method.[8,9,39] In our work we have considered only the ferromagnetic state (parallel spin alignment). The calculations of the exchange-correlation potential and energy were performed within the local density approximation using the Vosko-Wilk-Nusair parametrization of the exchange-correlation energy functional.[40]

The integration over the Brillouin zone was performed by means of the special-points technique with 505 k points in the irreducible part of the bulk Brillouin zone for fcc lattice and with 36 k points in the irreducible part of the two-dimensional Brillouin zone for the fcc (001) surface. The energy integrals were calculated in the complex plane using 16 energy points on the semicircular contour. The thickness of principal layer was equal to three atomic layers. Our LMTO calculations have been carried out using theoretical lattice parameter of Cu (3.58 Å). In addition, we have done several calculations using the experimental Cu lattice parameter (3.61 Å). Unsignificant changes have been observed for the magnetic moment of the monolayer, but the magnetization of bulk Fe-rich alloys were found to be very sensitive to the lattice parameter, and we discuss this effect in Sec. III.

Secondly, we have employed the Korringa-Kohn-Rostoker (KKR) method in combination with coherent-potential approximation (CPA).[41] In the calculations we take into account s, p, d, f orbitals and use only spherical potentials within the MT sphere. The fixed-spin-moment is used in the calculations of total energy.[8,9,39] The infinite extent of the perturbation parallel to the surface is taken into account by exploiting the two-dimensional (2D) planar periodicity and performing a 2D Fourier transform with 1000 $k_\perp$ points. Integration over the two-dimensional part of irreducible Brillouin zone is performed with 50 $k_\parallel$ points. Energy integrals are calculated using 22 energy points in semicircular contour. The Broyden's method modified by Johnson[42] is used in self-consistency calculations.

In the surface calculations we used the KKR CPA method developed for planar defects together with the CPA formalism.[43–47] We treat the ideal surface as two-dimensional perturbation of the bulk and by removing the atomic potentials of seven monolayers we create two half-crystals. The Green's function of the ideal surface and the Green's function of the monolayers are calculated using the multiple scattering theory and the details can be found in Refs. 43–48. In the magnetic moment vs concentration of Fe calculations we used the experimental lattice constant of Cu (3.61 Å).

In Fig. 1 we compare the concentration dependence of the average magnetic moment of 1 ML $Fe_{1-x}Ni_x$ alloy film deposited on Cu(001) substrate calculated by the LMTO GF and the KKR methods. One can see excellent agreement between these two sets of calculations. We view this agreement as an additional support for the reliability of our results. Also, unless specified explicitly, we will not distinguish between the LMTO and the KKR calculations in the following discussion.

III. RESULTS AND DISCUSSION

In Fig. 2 we show the average magnetic moment in the fcc $Fe_{1-x}Ni_x$ alloy on the Cu substrate as a function of concentration for the 1 ML film (solid line, circles), as well as for the bulk calculated at the theoretical equilibrium lattice parameters of the alloys (solid line, squares, Ref. 15) and at the theoretical (dashed line) and the experimental (dot-dashed line) lattice parameters of the fcc Cu. The magnetic moment of the $Fe_{1-x}Ni_x$ alloy film increases monotonously from $\mu = 0.3\mu_B$ for Ni/Cu(001) to $\mu = 2.8\mu_B$ for Fe/Cu(001). Experimentally, very thin Fe-Ni films were found to give a ferromagnetic signal over the whole concentration

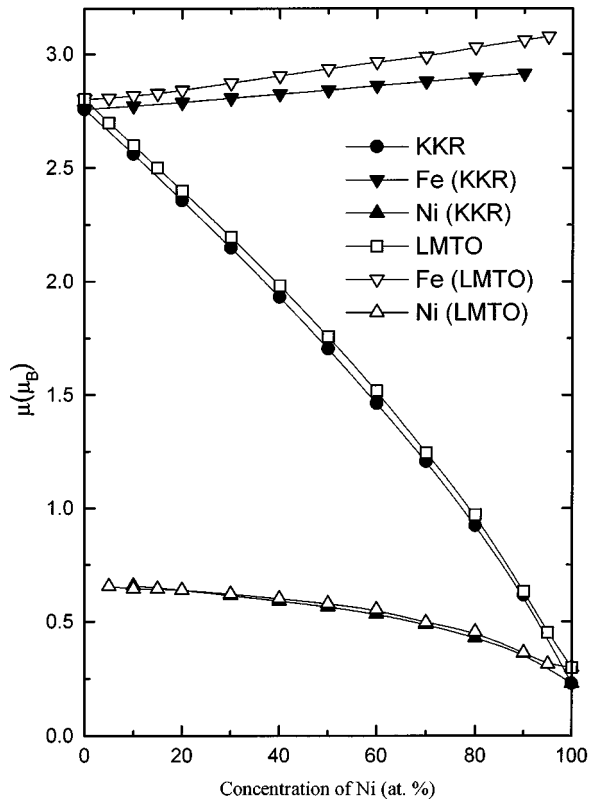

FIG. 1. Concentration dependence of magnetization and local moments of a single monolayer Fe-Ni film on Cu(001) calculated by the LMTO and the KKR methods.

interval,[26,28] in agreement with our finding. Also, as has been analyzed in Ref. 15, the results for bulk alloys are in good agreement with experimental data.

As we can see in Fig. 2, in a concentration interval $0.4 < x < 0.8$ our results for the monolayer and for the bulk are quite close to each other. However, we observe substantial deviations between the film and the bulk magnetization in Fe-rich, as well as in Ni-rich alloys. In particular, the magnetic moment of the bulk collapses in Fe-rich alloys, but it is enhanced in Fe-rich films. On the contrary, in the Ni-rich part of the diagram the bulk magnetic moment is substantially higher than one for the monolayer. Thus the behavior of the magnetic moment in the bulk and for a single monolayer of the fcc $Fe_{1-x}Ni_x$ alloy is quite different, and the most prominent feature of our results is the absence of a HS-LS magnetic transition in the film.

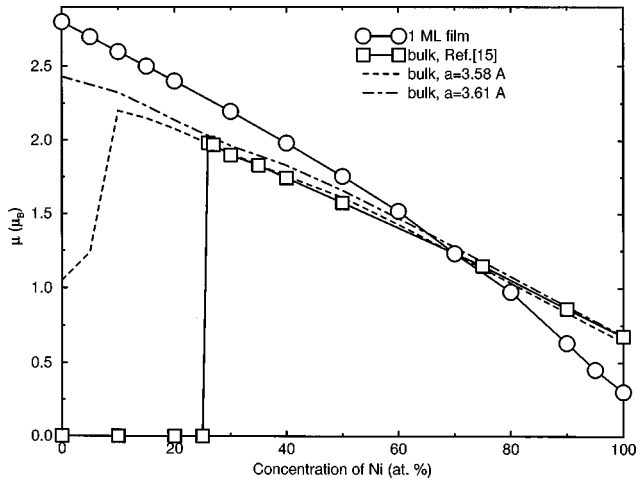

FIG. 2. Calculated average magnetic moment of single monolayer Fe-Ni film on Cu(001) substrate (solid line, circles) as a function of Ni concentration. Average magnetic moment of ferromagnetic bulk alloys, calculated at the theoretical equilibrium lattice parameters corresponding to this concentration (solid line, squares, Ref. 15), as well as at the fixed lattice parameters $a = 3.58$ Å (theoretical LMTO lattice parameter of bulk fcc Cu, dashed line) and $a = 3.61$ Å (experimental lattice parameter of bulk fcc Cu, dot-dashed line) are also shown.

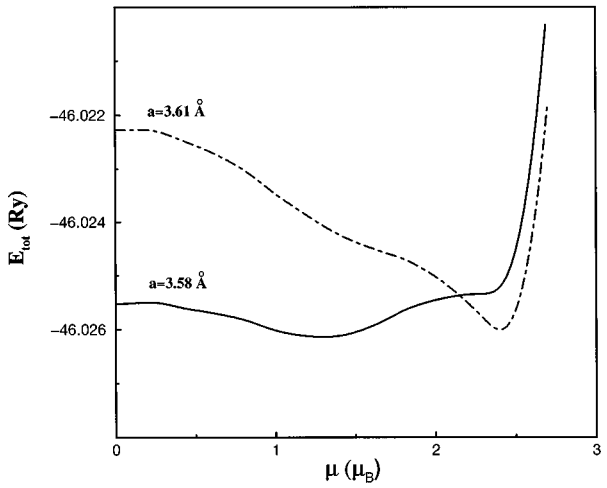

FIG. 3. Total energy as a function of constrained magnetic moment for the $Fe_{0.95}Ni_{0.05}$ alloy at different lattice parameters $a = 3.58$ Å (solid line) and $a = 3.61$ Å (dashed lane).

To explain the observed results one should note that there are at least three important factors which influence the surface calculations. (i) All our calculations have been performed for a fixed lattice parameter equal to the equilibrium lattice parameter of bulk fcc Cu, (ii) the dimensionality of the system is reduced, and (iii) there is an interaction between the monolayer and the substrate.

In order to understand the influence of a nonequilibrium lattice parameter on the magnetic properties of FeNi alloys, we have carried out calculations for bulk $Fe_{1-x}Ni_x$ alloys with two different lattice parameters $a = 3.58$ Å and 3.61 Å, corresponding to the theoretical (LMTO calculations) and the experimental lattice parameters of Cu, respectively. One can immediately see from Fig. 2 that in contrast to the calculations of the system with equilibrium lattice parameters, in which increasing concentration of Fe leads to a sharply decreasing magnetic moment reaching zero at $x = 0.25$, the changes in the magnetization with concentration are not so dramatic when the lattice parameter is fixed. For $a = 3.58$ Å we observe transition from the HS state to the intermediate spin (IS) state, while at $a = 3.61$ Å this transition is suppressed.

As a matter of fact, it is known that at the lattice parameter close to that of Cu the magnetic state of pure fcc Fe is most probably antiferromagnetic or a spin-spiral, and is very complicated.[22,49–51] If one neglects these configurations, as is the case in the present work, then the most stable state is the IS state,[10,15,18,41] but there are also two competing states, the

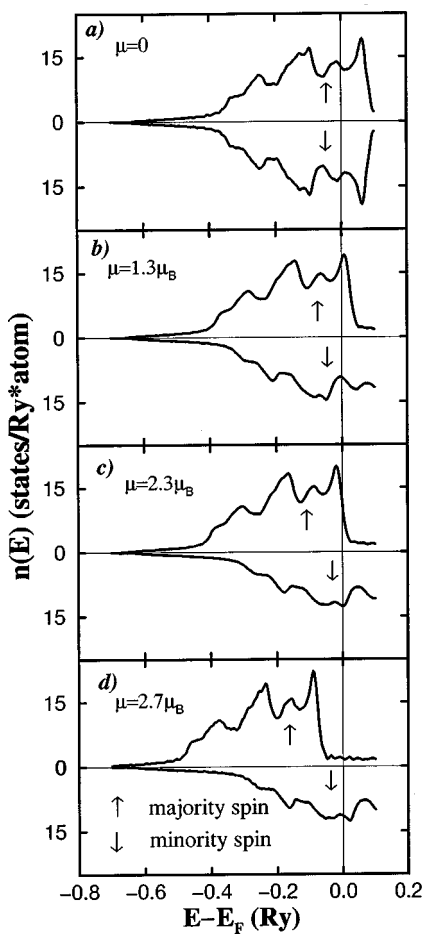

FIG. 4. Calculated density of states (DOS) $n(E)$ as a function of energy (relative to the Fermi energy E_F) for the bulk $Fe_{0.95}Ni_{0.05}$ alloy calculated for different constrained magnetic moments, paramagnetic (a), $\mu=1.3\mu_B$ (b), $\mu=2.3\mu_B$ (c), and $\mu=2.7\mu_B$ (d). The DOS for majority- and minority-spin channels are denoted by ↑ and ↓, respectively.

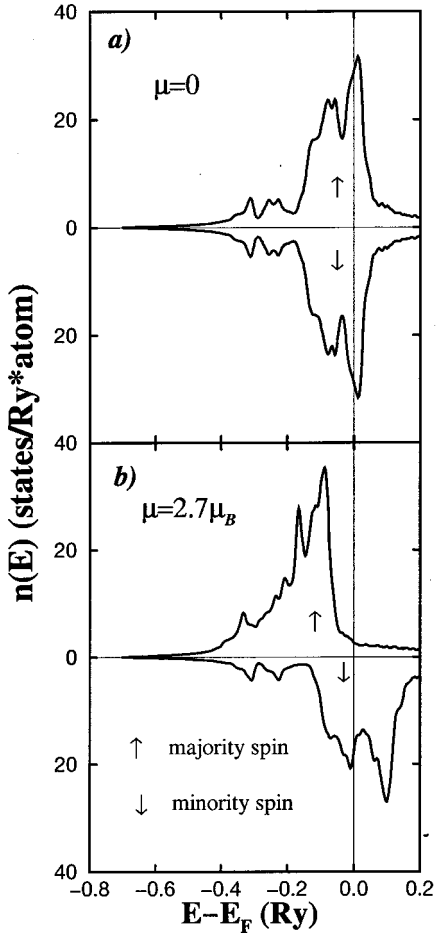

FIG. 5. Calculated paramagnetic (a) and ferromagnetic [$\mu=2.7\mu_B$, (b)] density of states (DOS) $n(E)$ as a function of energy (relative to the Fermi energy E_F) for a single monolayer $Fe_{0.95}Ni_{0.05}$ alloy on Cu(001) substrate. The DOS for majority- and minority-spin channels are denoted by ↑ and ↓, respectively.

LS and the HS, that are very close in energy. The existence of metamagnetism in pure fcc Fe has been understood from the shape of the canonical density of states for the fcc lattice.[6,7] In alloys the shape of DOS is influenced by the disorder, and already at 25% of Ni metamagnetism disappears.[15] However, in dilute alloys one can expect the metamagnetism to survive, and we illustrate this in Fig. 3 where the total energy of the $Fe_{0.95}Ni_{0.05}$ bulk alloy, obtained from fixed spin moment calculations, is plotted as a function of magnetic moment for two lattice parameters 3.58 and 3.61 Å.

One can see in Fig. 3, that at the smaller lattice parameter the total energy curve has only one minimum at $\mu=1.3\mu_B$, but there are indications of two other minima, corresponding to the metamagnetic states of pure fcc Fe. Similar to the analysis given by Andersen *et al.*[6] and by Roy and Pettifor,[7] this situation can be understood in terms of the underlying electronic structure of the alloy. In Fig. 4 we show an evolution of the $Fe_{0.95}Ni_{0.05}$ alloy density of states (DOS) (lattice parameter is equal 3.58 Å) with increasing magnetic moment. In the paramagnetic state the Fermi energy is situated on the decreasing side of the peak of the DOS, and in fact is quite close to the DOS valley, which explains the slow variation of the total energy when the magnetic moment is close to zero. The equilibrium magnetic moment $\mu=1.3\mu_B$ at this lattice parameter corresponds to the situation where the Fermi level is pinned in a valley of the minority band, in agreement with the ''band-gap'' arguments of Malozemoff *et al.*[52] It costs some energy to increase the band splitting due to the fact that it is necessary to overcome the peak of the DOS in the majority band. So the state with $\mu=2.3\mu_B$ is less energetically stable. However, this energy balance is quite fragile, and already at a slightly larger lattice parameter 3.61 Å the high spin state with $\mu=2.3\mu_B$ becomes more stable than the IS state. Thus, the suppression of the HS to the LS phase transition in the 1 ML Fe-Ni film can be partly explained by the effect of the fixed lattice parameter. However, one can see in Fig. 2 that the equilibrium magnetization of the film is even higher than that of the HS bulk alloy ($a=3.61$ Å), thus there is an additional enhancement of magnetization due to interactions with substrate.

In order to explain this fact let us compare the paramagnetic DOS of the bulk [Fig. 4(a)] and of the monolayer [Fig. 5(a)] in the $Fe_{0.95}Ni_{0.05}$ alloy. As a matter of fact the discussion of the bulk DOS presented above indicates an extreme sensitivity of the equilibrium magnetic moment in Fe-Ni to the details of the electronic structure, and one can expect that

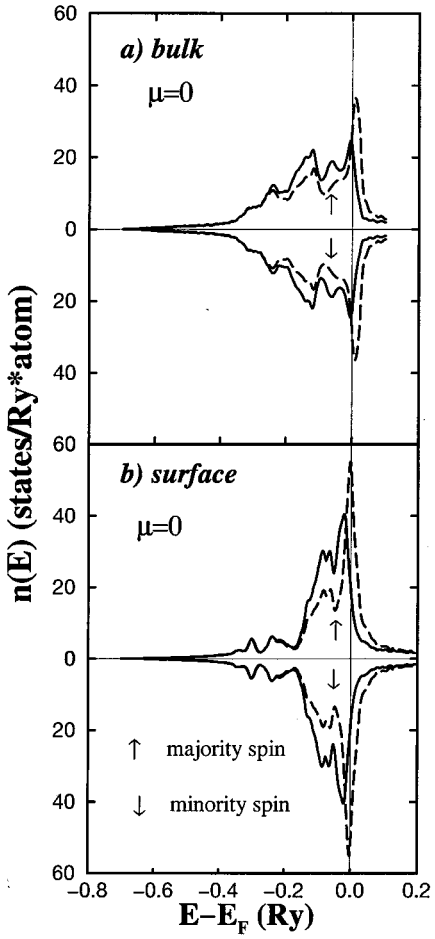

FIG. 6. Calculated paramagnetic density of states (DOS) $n(E)$ as a function of energy (relative to the Fermi energy E_F) for bulk alloy $Fe_{0.05}Ni_{0.95}$ (a) and for single monolayer $Fe_{0.05}Ni_{0.95}$ on Cu(001) surface (b). The partial DOS of Fe is shown by dashed line. The DOS for a majority- and minority-spin channels are denoted by ↑ and ↓, respectively.

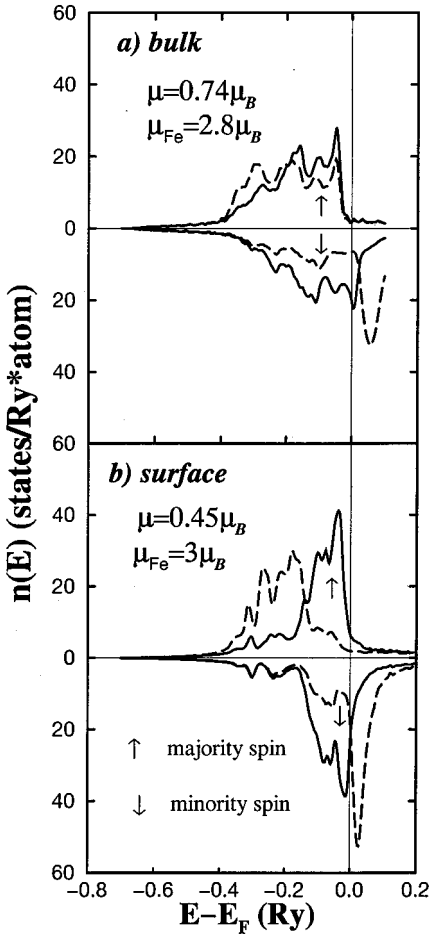

FIG. 7. Calculated density of states (DOS) $n(E)$ as a function of energy (relative to the Fermi energy E_F) for bulk alloy $Fe_{0.05}Ni_{0.95}$ ($\mu=0.74\mu_B$) (a) and for single monolayer $Fe_{0.05}Ni_{0.95}$ on the Cu(001) surface ($\mu=0.45\mu_B$) (b). The partial DOS of Fe shown by dashed line. The DOS for a majority- and minority-spin channels are denoted by ↑ and ↓, respectively.

significant changes of the DOS are followed by a substantial change of the magnetic moment. The electronic structure of the bulk differs from that of the film because of two reasons. First, there is a band narrowing effect at the surface, which is clearly seen in the paramagnetic DOS of the monolayer (Fig. 5). This effect is due to the lower coordination number of surface atoms. The band narrowing at the surface leads to a shift of the center of gravity of the *d* band towards the Fermi level for metals with a more than half filled *d* band, such as Fe, Ni, and Cu, and contributes to an increasing DOS at the Fermi level. Second, one has to account for the interaction of the Fe and Ni *d* electrons with the substrate. Because the Cu *d* band is filled, and therefore is situated well below the Fermi level, the *d* electrons of the film can only hybridize weakly with the Cu *sp* electrons.[53] As has been shown recently by Pourovskii *et al.*,[54] this effect is most pronounced for the states with ''out-plane'' symmetry, which could become so localized, as to form a virtual bound state, similar to the case of a single transition metal impurity in Cu.[22,55] Note that the *d* band of the paramagnetic Fe is not filled, and therefore it is pinned by the Fermi energy. Because the total DOS of the Fe-rich alloy is dominated by the local DOS of Fe, its value at E_F increases substantially compared to that of the bulk alloy.

Now, if we compare the paramagnetic DOS in the bulk and in the film, we see that its value at the Fermi level $[n(E_f)]$ for the later case is almost twice as high as DOS in the bulk alloy. Therefore, according to the Stoner theory,[56] we can expect that the magnetic moment of the surface layer will increase substantially in comparison with the bulk value. This expectation is fully supported by our first-principles calculations. If we next consider the ferromagnetic DOS of the film [Fig. 5(b)] and compare it with that of the bulk, calculated for the same value of the magnetic moment $\mu=2.7\mu_B$ [Fig. 4(d)], we observe, that the band narrowing effect produces a considerably deeper gap of the minority band DOS near E_F. The Fermi level is pinned in this gap and this additionally contributes to the stability of the high-spin state in the film and to the enhancement of the magnetic moment.

Let us now consider the case of a Ni-rich alloy. As a representative example we choose $Fe_{0.05}Ni_{0.95}$ alloy, and present its paramagnetic and ferromagnetic DOS in Figs. 6 and 7, respectively. First, we notice that the total DOS is

almost completely dominated by the local DOS of Ni atoms. The *d* electrons of Ni experience the same two effects, as has been discussed above for the case of Fe-rich alloys, that is, band narrowing due to decreasing coordination at the surface and hybridization with *sp* electrons of the Cu substrate. However, in contrast to Fe, the *d* band of the paramagnetic Ni is nearly filled. For a single Ni impurity in Cu this leads to a shift of the virtual bound state away from the Fermi energy. Similar situation occurs for the monolayer film, and the value of the Ni DOS at E_F decreases. This effect is well known for films of pure Ni on the Cu(001) surface,[53,54] and we show in Fig. 6 that the situation is in principal the same for the 1 monolayer $Fe_{0.05}Ni_{0.95}$ alloy film on Cu(001). The PM DOS of the film is lower than that of the bulk alloy, and the total average magnetic moment decreases, as observed in our self-consistent calculations.

However, in an alloy the situation is more complicated due to the presence of Fe. In the paramagnetic phase the Fe *d* states are pinned by the Fermi energy, as has been discussed above. Because of low Fe concentration these electrons become virtually bound to the Fe sites and produce very high value of the local Fe DOS at the Fermi level. So, though the average magnetic moment of the film decreases, the local magnetic moment on Fe atoms increases, and in the Ni-rich films it takes its saturated value $\mu = 3\mu_B$. This leads to an interesting modification of the electronic structure of the ferromagnetic film as compared to the bulk ferromagnetic $Fe_{0.05}Ni_{0.95}$ alloy (Fig. 7). Indeed, in the bulk we observe a situation which is typical for an alloy between two transition metals. Band centers of the majority spin bands for the two alloy components are close to each other in energy, while those of the minority spin bands are separated due to different spin splitting for Fe and for Ni. As a result, the minority spin band is as a rule more influenced by the disorder. In the film the magnetization of Fe is $3\mu_B$, and its majority spin band is completely filled. Thus, similar to the filled *d* band of Cu it moves away from the Fermi energy, and the separation between the majority band centers of Fe and Ni increases as compared to the bulk alloy. This, however, does not lead to a formation of a Fe spin-up virtual bound state, similar to one that is seen in the minority spin band of Fe just above E_F. The reason is that the majority band Fe electrons can now hybridize with *d* electrons of the Cu substrate, situated in the same energy interval.

IV. CONCLUSIONS

A detailed theoretical study of magnetic properties of a single monolayer of an epitaxial $Fe_{1-x}Ni_x$ alloy on a Cu(001) substrate has been carried out over the whole concentration interval by means of the surface Greens-function technique. A comparison with the bulk magnetization of fcc FeNi is presented. We have shown that the monolayer films of iron-nickel remain in the high-spin state for all concentrations, in contrast to the bulk alloys that exhibit a high-spin–low-spin magnetic phase transition. The explanation of the difference between the behavior of the magnetic moments in bulk and in the film is given in terms of three major effects. First, we have shown that the HS-LS transition is partly suppressed due to the nonequilibrium lattice parameter of the Fe-Ni film. Second, we conclude that the electronic structure, and therefore properties of Fe-Ni films, depend crucially on the two-dimensional symmetry of the system. Third, the interaction of the deposited monolayer with the substrate leads to the enhancement of magnetization of Fe-rich alloys and to a suppression of the magnetic moment of the Ni-rich alloy. Therefore, we have shown that a direct extrapolation of surface investigations towards the bulk property in the Fe-Ni system is not appropriate.

ACKNOWLEDGMENTS

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