PHYSICAL REVIEW B VOLUME 39, NUMBER 9 15 MARCH 1989-II

Structural, electronic, and magnetic properties of a Ni monolayer on Ag(001): Ni adsorption versus Ag surface segregation

Soon C. Hong and A. J. Freeman
Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208

C. L. Fu
Metals and Ceramics Division, P.O. Box 2008, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831

(Received 18 April 1988)

The structural, electronic, and magnetic properties of a $p(1\times1)$ Ni overlayer on Ag(001) are investigated with use of the highly precise all-electron total-energy full-potential linear–augmented-plane-wave (FLAPW) method. Although the Ni—Ag bond length remains essentially the same as that of $p(1\times1)$ Ni/Cu(001), we found that the Ni magnetic moment ($0.57\mu_B$) is enhanced by 50% from that ($0.39\mu_B$) of Ni/Cu(001) as a result of the effect of negative pressure. Nevertheless, the magnetic moment is reduced by about 20% compared with that ($0.70\mu_B$) of the surface layer in Ni(001) due to hybridization coupling of Ni and Ag. The magnetic hyperfine field is found to be reduced at the interface due to the direct contribution from conduction electrons. Self-consistent charge and spin densities, work function, single-particle energy bands, and layer-projected density of states for Ni/Ag(001) are also presented. The negligible exchange splitting observed in the photoemission experiment of Thompson *et al.* is explained in terms of possible Ni subsurface layer formation (Ag segregation to the surface) which is found, from separate self-consistent calculations, to have a lower total energy and a very small (nearly "dead") magnetic moment ($\leq 0.02\mu_B$).

I. INTRODUCTION

Early on, experimental reports of magnetically "dead" layers for the ferromagnetic transition-metal surface stimulated various experimental and theoretical studies on surface magnetism.[1,2] While recent experiments and theories have ruled out the possibility of magnetically "dead" layers for clean ferromagnetic transition-metal surfaces, considerable attention has been directed to investigations of interface magnetism in magnetic metallic layers grown epitaxially as strained overlayers or in their metastable states. To this end, high-quality ultrathin films—made available by recent progress in fabrication and property modification techniques—can now be obtained. Studies of ultrathin ferromagnetic layers on nonmagnetic materials have emphasized the effects of the substrate on the magnetism of overlayers and the possibility of induced two-dimensional (2D) magnetism.[3-14]

There have been extensive studies on the surface and interface magnetism of Ni. Eib and Alvarado[15] measured electron-spin-polarized photoemission spectra of a single-crystal Ni surface and obtained an exchange splitting of 0.33 eV. More recently, magnetic surface states on Ni(100) have been observed by angle-resolved photoelectron emission spectra (ARPES).[16] Finally, we note that magnetic hyperfine fields measured by Mössbauer spectroscopy were interpreted to indicate that the surface magnetic moment of ferromagnetic transition metals (Fe and Co) is about the same as their bulk value, but decreases more rapidly with increasing temperature as compared with that for the bulk magnetization.[17-20]

It is well known that Ni atoms are very sensitive to their environment. For example, the magnetism of Ni overlayers on a metal surface is affected greatly by the interaction with the surface. Kramer and Bergmann[21] investigated how different metallic substrates (Mg, In, Sn, Cu, Ag, and Au) affect the magnetism of Ni thin films. They found that while Mg, In, and Sn substrates completely suppress the magnetism of Ni when the thickness of Ni layers is less than 2.5 atomic layers, the noble-metal substrates do not cause Ni films to be magnetically dead even at the monolayer level. Thompson *et al.*, using ARPES, obtained an exchange splitting (ΔE_{ex}) of 0.32 eV for a $p(1\times1)$ monolayer Ni on Cu(100) (Ref. 13) while they obtained very small ΔE_{ex} for a $p(1\times1)$ Ni monolayer on Ag(100).[14]

On the theoretical side, Wang and Freeman[22] [using a self-consistent linear combination of atomic orbitals (LCAO) discrete-variational method] found that the surface layer of Ni(100) was not magnetically dead. Jepsen *et al.*[23] obtained an enhanced magnetic moment ($0.65\mu_B$) for a surface Ni atom compared to that ($0.61\mu_B$) of a central Ni layer from a five-Ni-layer single-slab calculation with use of the LAPW method. A more precise calculation,[24] using the full-potential linear–augmented-plane-wave (FLAPW) method,[25] obtained the result that the surface magnetic moment of Ni(100) is enhanced by 20% from its bulk value. This enhancement of the magnetic moment at the surface is partially due to the dehybridization of *p* electrons from the *d* band which is clearly related to the reduced number of nearest neighbors at the surface. As regards theoretical studies of magnetism at the Ni-Cu interface, using the LAPW approach Wang *et al.*[26] obtained values of $0.39\mu_B$ for the monolayer and $0.68\mu_B$ for the surface layer and $0.47\mu_B$ for the subsurface layer for the bilayer Ni coverage on Cu(001). The result for the monolayer coverage is quite consistent with the ARPES result. Other calculations yielded similar results for monolayer Ni on Cu(100): Huang *et al.*[27] obtained a magnetic moment of $0.24\mu_B$ using the self-consistent local-orbital method; Tersoff and Falicov[28] reported a small reduction of the Ni magnetic moment from that of the bulk as obtained by using a non-self-consistent parametrized Hartree-Fock method. In addition, Tersoff and Falicov[28] found for a monolayer of Ni on Cu(111), i.e., the closest-packed plane, that the Ni atom has a very small magnetic moment and concluded that the Ni atom may be magnetically "dead" as a result of the important interactions of the Ni *d* band with substrate states.

In this paper, we present theoretical results for the structural, electronic, and magnetic properties of a Ni monolayer on Ag(001), using the highly precise FLAPW method based on local-spin-density- (LSD) functional theory, in order to explain theoretically the experimental results that the exchange splitting of Ni/Ag(001) is much smaller than that of Ni/Cu(001). Both Ni as an adsorbate overlayer and as a subsurface layer (i.e., Ag segregation to the surface) are considered and compared. In Sec. II, the computational model and theoretical approach are described briefly. Our calculated results (magnetic moment, hyperfine field, and single-particle spectra) are presented in Sec. III, as is a discussion of the effect of the Ag substrate on the magnetism of the Ni and a comparison with corresponding theoretical results for the clean Ni(001) surface and Ni/Cu(001). Finally, results of total-energy calculations for Ni as a subsurface layer to Ag(001) are invoked to reconcile the discrepancy between the results of our calculation for Ni/Ag(001) and the ARPES experiment of Thompson *et al.*[14] A summary and conclusions are given in the final section.

II. METHODOLOGY AND COMPUTATIONAL MODEL

To investigate the structural, electronic, and magnetic properties of $p(1\times1)$ Ni/Ag(001), we model the system by a single slab consisting of five layers of Ag(001) with a Ni monolayer on each side of the slab. The two-dimensional lattice parameter and the Ag-Ag interlayer spacing are taken to be those of bulk Ag. The Ni-Ag interlayer spacing is determined from total-energy calculations.

The Kohn-Sham equations[29,30] are solved self-consistently employing the FLAPW method.[25] In this method, no shape approximations are made to the potential or the charge density in solving Poisson's equation. All the matrix elements corresponding to this general potential are rigorously taken into account in all parts of space. The lattice harmonics with angular momentum up to $l=8$ are used to expand the charge density and potential and to construct the wave functions inside the muffin-tin (MT) spheres. For the exchange-correlation potential we employ the explicit form of von Barth and Hedin[31] for the spin-polarized studies and the Hedin and Lunqvist form[32] for the paramagnetic state calculations.

The core electrons are treated fully relativistically, whereas the valence electrons are treated semirelativistically[33], i.e., including all other relativistic terms but spin-orbit coupling. About 2×240 basis functions are used for each of the 21 *k* points in the 1/8 irreducible wedge of the two-dimensional Brillouin zone. Self-consistency is assumed when the rms difference between the input and output spin and charge densities is less than $3\times10^{-4}\ e/(\text{a.u.})^3$.

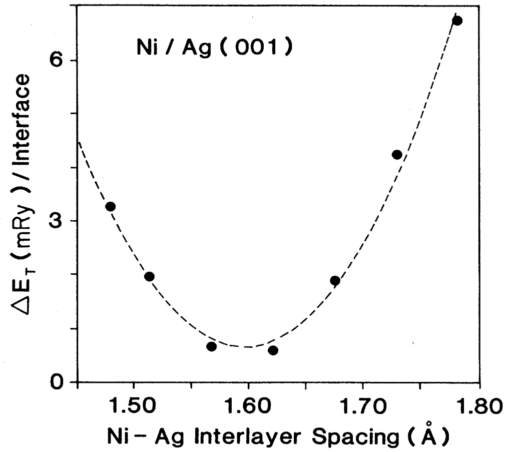

FIG. 1. Total energy of Ni/Ag(001) vs the Ni-Ag interlayer spacing. The circles denote calculated data points fitted by a parabolic curve (dashed line).

III. RESULTS

A. Total-energy studies: Structural properties

Before investigating the electronic structure and magnetism of a Ni monolayer on Ag(001), we first have to know the Ni-Ag interlayer spacing (bond length). Thus we calculate the total energy of Ni/Ag(001) in its paramagnetic state for seven different interlayer spacings and fit our calculated values to a parabolic curve, as shown in Fig. 1. The total-energy results yield a Ni-Ag interlayer spacing of 1.60 Å, i.e., Ni atoms are relaxed by 9.6% (here we define unrelaxed interlayer spacing as that determined by the average of the Ag—Ag and Ni—Ni bond lengths in bulk). The interlayer spacing of 1.60 Å corresponds to a bond length of 2.60 Å which is close to the bond length of Ni—Cu (2.56 Å) employed[26] in the investigation of the electronic and magnetic properties of Ni/Cu(001). Usually, self-consistent spin-polarized calculations result in a longer bond length compared to that obtained for a paramagnetic state because spin-up electrons fill antibonding states with spin-down bonding states due to the spin splitting of the bands. However, for weak ferromagnetic elements with a small exchange splitting such as Ni the bond length in a ferromagnetic state is almost the same as that in a paramagnetic state.[34] Thus, the spin-polarized calculations are performed for the Ni-Ag interlayer spacing at the minimum total energy.

B. Charge density and work function

We first discuss the charge density because it has direct physical significance in LSD theory and provides some insights for understanding the formation of the surface and interface. Contour mapping of the charge density for the (110) plane is plotted in Fig. 2. The delocalized electrons (*s*- and *p*-like) of Ni spill out into the vacuum to

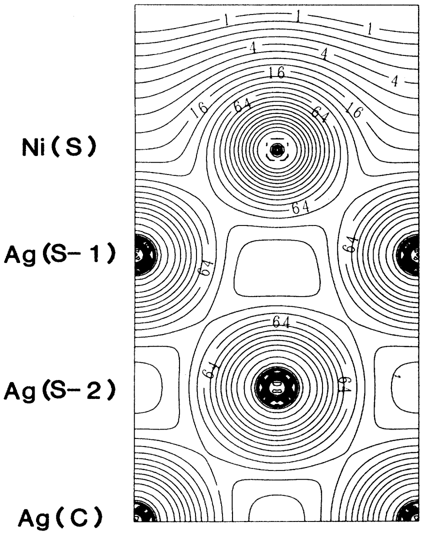

FIG. 2. Valence charge-density contour map for Ni/Ag(001) on the (110) plane in units of 1×10^{-3} $e/(\text{a.u.})^3$. Subsequent contour lines differ by a factor of $\sqrt{2}$.

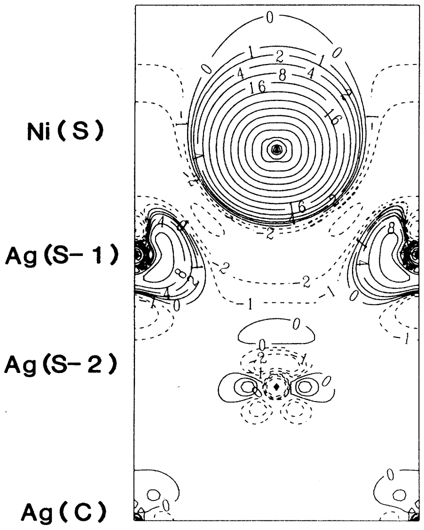

FIG. 3. Spin density contour map for Ni/Ag(001) on the (110) plane in units of 1×10^{-4} $e/(\text{a.u.})^3$. Subsequent contour lines differ by a factor of 2.

smooth the discontinuity at the surface. A more detailed picture of the charge configuration is obtained by partitioning the density into contributions from different layers, and by a further decomposition inside the atomic spheres into different l values as shown in Table I: (i) s- and p-like charges within the Ni MT spheres, coming partly from the tail of the d-like electrons of neighboring atoms, decrease from those of the clean Ni(001) surface due to the closed d-electron shell of the Ag atom; (ii) s- and p-like charges within the interface Ag MT spheres (which again originate partly from the tail of d electrons from neighboring Ni atoms) increase compared to the inner layer; and (iii) the short screening length manifests itself in the constant number of electrons within the Ag MT spheres just one layer below the interface.

The charge distribution near a surface, i.e., the spill out of electrons into the vacuum region and the charge transferred between Ni and interface Ag layers, gives rise to a surface dipole layer which consequently determines the work function. The calculated work function for Ni/Ag(001) is found to be 5.12 eV which is less than that (5.4 eV, Ref. 24) of the clean Ni(001) surface. The lowered work function is due to (i) the weak d-d coupling of Ni-Ni (due to the negative pressure effect) and Ni-Ag (due to the separation of their d bands) and (ii) charge transfer from the Ni layer to Ag atoms.

TABLE I. Orbital decomposition of the total number of valence electrons within the muffin-tin spheres where S, I, $I-1$, and C denote the surface, interface, subinterface, and center layers, respectively.

	s	p	d	Total
Ni(S)	0.396	0.207	8.400	9.023
Ag(I)	0.364	0.265	8.874	9.531
Ag($I-1$)	0.340	0.221	8.907	9.485
Ag(C)	0.341	0.220	8.906	9.485

C. Spin density and magnetic moment

A contour plot of the self-consistent spin density obtained for Ni/Ag(001) for the (110) plane is shown in Fig. 3. The Ni-atom spin density swells into the vacuum and the interface Ag layer is positively polarized. The interstitial region of the surface Ni and interface Ag atoms is negatively polarized by the delocalized s,p electrons. The spin-density configuration tells us also that the interface effects on magnetism is confined again to just the interface (as confirmed by an angular momentum decomposition of magnetic moment within the MT spheres).

The magnetic moment of the Ni atom, found to be $0.57\mu_B$, is reduced compared to that of the clean Ni(001) ($0.70\mu_B$, Ref. 24) even though the Ni d electrons in Ni/Ag(001) are more localized, as discussed in the next section. The magnetic moment of the Ni atoms in Ni/Ag(001) is larger, however, than that ($0.39\mu_B$, Ref. 26) of the Ni atoms in Ni/Cu(001). These facts indicate that unlike the case of Fe and Cr,[35] the interaction of the Ni 3d with the substrate plays a more important role in determining the magnetic moment of Ni than does the localization of the Ni d electrons. The importance of this coupling was pointed out theoretically by Tersoff and Falicov[36] and experimentally by Kramer and Bergmann.[21] The polarization of the d electrons of the interface Ag atoms results in a small magnetic moment ($0.012\mu_B$); however, the negative polarization of the delocalized s and p electrons reduces the total magnetic moment of the interface Ag to a negligible value.

D. Contact magnetic hyperfine fields

The electronic spin density at the nucleus is the key quantity for the interpretation of the hyperfine interaction which probes the coupling of the electronic spin density to the nuclear magnetic moment. The spin density at

TABLE II. Magnetic moment and Fermi-contact magnetic hyperfine fields (in kG) broken down into contributions from the core and conduction electrons for (a) the Ni overlayer on the Ag(001) and (b) Ni diffused below the Ag(001) surface.

Magn.	Moment	Core	CE	Total	H_c(core)/M
(a) Ni(S)/Ag(001)	0.57	-87.5	46.5	-41.0	-153.0
(b) Ag/Ni($S-1$)/Ag(001)	0.02	-3.8	0.3	-4.1	

the nucleus gives rise to the Fermi-contact field (H_c) which is substantially larger than the positive contributions from unquenched orbital angular momentum and dipolar fields.[37] For convenience H_c is decomposed into two parts: (i) the negative contribution from core-electron polarization; and (ii) the contribution from the conduction electrons (CE) (cf. Table II).

As is now well established even for bulk metals and their surfaces, the core contribution scales with the local magnetic moment regardless of the metallic environment because the core electrons lie inside the 3*d* electrons which are principally responsible for the local magnetic moment.[37–40] As shown in Table II the value of H_c(core)/M for a Ni atom on Ag(001) is -153 kG/μ_B. This value is close to those obtained (with different computational approaches) for such diverse systems as the free Ni atom (-150 kG/μ_B),[37] the clean Ni(001) surface (-146 kG/μ_B),[24] Ni overlayers on Cu(001) (-146 kG/μ_B),[26] and Ni overlayers on Fe(001) (-154 kG/μ_B).[40] Unlike the case of ferromagnetic bulk materials, where the CE contribution is governed by the indirect negative polarization, for the Ni overlayer on Ag(001) the CE contribution becomes positive due to the direct polarization. The CE contribution (46.5 kG) is much higher than that (2.9 kG, Ref. 24) of the clean Ni(001) because of negligible indirect polarization induced by neighboring Ni (due to the larger Ni—Ni bond length) and Ag (due to its negligible magnetic moment). The higher positive CE contribution reduces the total H_c to -41.0 kG which is about 1/3 of the bulklike value (-118.6 kG).[24]

E. Single-particle spectra

To explore the physical background for understanding surface and interface formation, we discuss the layer-projected density of states (LDOS) and band structure of Ni/Ag(001). The LDOS is plotted in Fig. 4 where the left-hand (right-hand) side represents majority (minority) spin states. The *d*-band width of Ni on Ag(001) is much narrower compared to the clean Ni(001) surface,[24] bulk Ni,[34] and Ni/Cu(001).[26] This *d*-band narrowing indicates that the *d* band of the Ni layer hardly interacts with the low-lying *d* states of the substrate Ag atoms. Despite this narrowing of the *d* band which contributes to the enhanced surface magnetic moment in the cases of Fe and Cr overlayers on nonmagnetic metals,[35] the magnetic moment of Ni atoms on Ag(001) is reduced with respect to that of the clean Ni(001) surface. Thus we may conclude, as pointed out by Tersoff and Falicov,[36] that the hybridization of the Ni *d* band with the *s,p* states of Ag, even though weak, reduces the exchange splitting to about 0.45 eV and results in the reduction of the magnetic moment. But this exchange splitting is larger than that (0.37 eV, Ref. 26) of Ni atoms on Cu(001) where the *d-d* hybridization between Ni and Cu is stronger compared to that between Ni and Ag due to overlap of their *d* bands.

Figure 5 displays the band structure along the high-symmetry lines of the irreducible 2D BZ for Ni/Ag(001). The left-hand (right-hand) side panels represent majority (minority) spin states. The bands are sorted for clarity according to their mirror reflection symmetries. Top (bottom) panels present the odd (even) parities with respect to the given symmetry line and the dashed (dotted) lines stand for the odd (even) symmetry states with respect to *z* reflection symmetry. Surface states, drawn by heavy solid lines, are defined as having more than 50% of their wave function localized in the Ni surface.

The minority spin band structure is very similar to that for majority spin except for the exchange splitting of the surface states just as for Ni atoms in other environments.[24,26,34] The Ni bands are seen to be almost completely separated in energy from the Ag bands. The $\overline{M}_3$ surface state (d_{xy}-like), localized at the Ni surface by more than 98%, is occupied and lies 0.32 eV below E_F

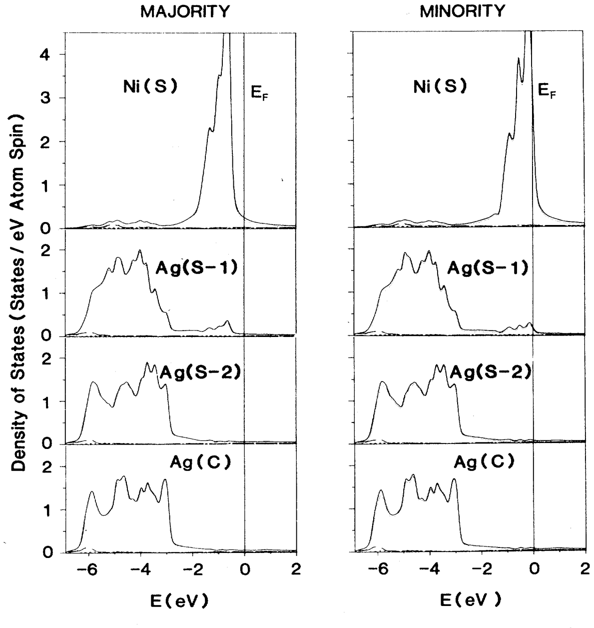

FIG. 4. Layer-projected partial density of states in units of states/eV spin for Ni/Ag(001). Dotted lines indicate *d* states and dashed lines represent *s,p* contributions.

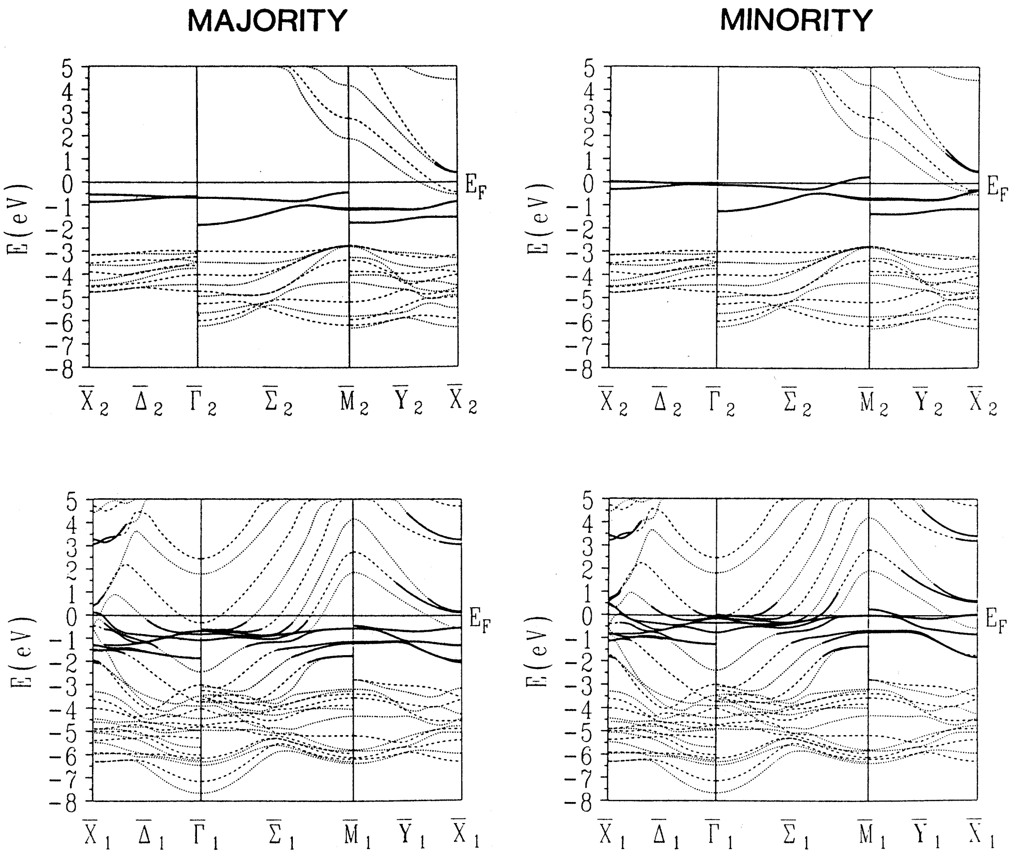

FIG. 5. Energy bands for Ni/Ag(001) of majority spin and minority spin along high-symmetry directions in the 2D Brillouin zone. Top and lower panels show odd and even symmetries with respect to the given symmetry line. Dashed and dotted lines represent odd and even parities with respect to the central plane. Solid lines indicate surface states whose wave functions have more than 50% weight within the surface Ni layer.

for majority spin. The corresponding minority spin state exists at 0.28 eV above E_F and results in an exchange splitting of 0.60 eV. As expected from the values of the magnetic moment, this exchange splitting is smaller than that at the Ni(001) surface ($\Delta E_{\text{ex}}=0.78$ eV),[24] but larger than that of Ni/Cu(001) ($\Delta E_{\text{ex}}=0.37$ eV).[26] Our calculate exchange splitting for Ni on Ag(001) is very different from ARPES results[14] which concluded that the exchange splitting is much smaller that that for Ni on Cu(001). To explain the discrepancy between the theoretical and the experimental results we investigate the possibility that Ni atoms diffuse below the Ag(001) surface (i.e., segregation of Ag atoms to the surface).

F. Diffusion of Ni into the Ag substrate

Metallic Ni has a higher surface energy than does Ag.[41] Hence, it may be that Ag atoms may segregate to the surface in order to lower the surface energy. To examine this possibility we have calculated the total energy of the slab with Ni as a subsurface layer [Ag/Ni($S-1$)/Ag(001)] while keeping the Ni—Ag bond length at its equilibrium value (i.e., we interchange the layer stacking sequence of the Ag interface layer and Ni surface for the overlayer case). For Ag/Ni($S-1$)/Ag(001), the total energy is found to be lower than that of Ni/Ag(001) by a relatively large amount (0.6 eV). Hence it is very possible for deposited Ni atoms to diffuse into the Ag substrate.

To investigate the magnetism of Ag/Ni($S-1$)/Ag(001) we carried out spin-polarized calculations. A contour map of the spin density for this system drawn on the (110) plane is shown in Fig. 6. The result is very different from that of the Ni overlayer on Ag(001). The magnetic moment at the Ni sites is drastically reduced and the spin density at the Ag sites do not show any polarization due to the small magnetic moment of the neighbor Ni atoms. We found that the magnetic moment and hyperfine field of Ni in this system is reduced drastically to $0.02\mu_B$ and -3.8 kG, respectively (cf. Table II), with the ferromagnetic state stable compared to the paramagnetic state by only a small amount (ΔE_T-8 meV).

Finally, we consider the single-particle spectra as a way to provide a physical understanding for the drastic reduction of the magnetic moment. Figure 7 represents the LDOS of the Ni layer in the Ni subsurface system. The LDOS, especially the bandwidth, is almost the same as

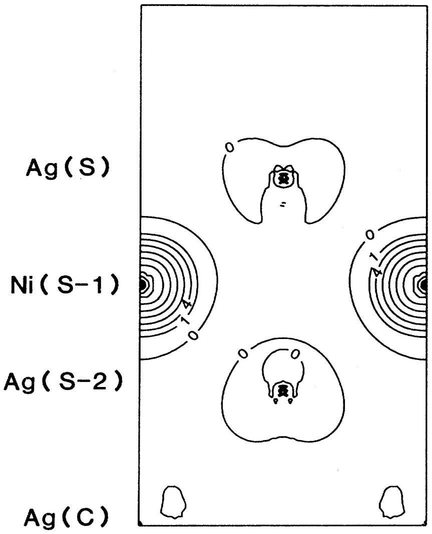

FIG. 6. Spin-density contour map for Ag/Ni($S-1$)/Ag(001) on the (110) plane in units of 1×10^{-4} e/(a.u.)^3. Subsequent contour lines differ by a factor of 2.

that of the Ni in the Ni overlayer system. However, the exchange splitting energy is reduced greatly up to 0.02 eV, compared to that of Ni/Ag(001). This fact also supports the statement made in Sec. III E that the band narrowing in Ni atoms does not play a role in the determination of the magnetic moment of the Ni atoms; instead, the hybridization of Ni d and Ag s states, even though very weak, is responsible for the large reduction of the exchange splitting and results in very small magnetic moment of the Ni atom in this subsurface system. This small exchange splitting may explain the experimental results[14] which reported that the Ni on Ag(001) has a significantly smaller exchange splitting than that of Ni on Cu(001).

IV. SUMMARY

We have presented results of high-precision, self-consistent, all-electron local-density-functional total-energy calculations using the FLAPW method for a Ni monolayer on Ag(001). The Ni—Ag bond length was determined as 2.60 Å from total-energy calculations obtained at seven different bond lengths.

The almost complete separation of the Ni d bands from the Ag d states and the increased Ni-Ni spacing enhances the magnetic moment ($0.57\mu_B$) on the Ni site by 50% compared to that ($0.39\mu_B$) of Ni/Cu(001); however, the coupling between the Ni and Ag atoms, even though it is very weak, reduces the magnetic moment with respect to that ($0.70\mu_B$) of the clean Ni(001) surface. Unlike Fe and Cr atoms, the Ni band narrowing does not play an important role in determining the magnetic moment of the Ni atoms.

The magnetic hyperfine field on the Ni site in Ni/Ag(001) is greatly reduced compared to that of bulk Ni due to a large direct positive contribution from the conduction electrons.

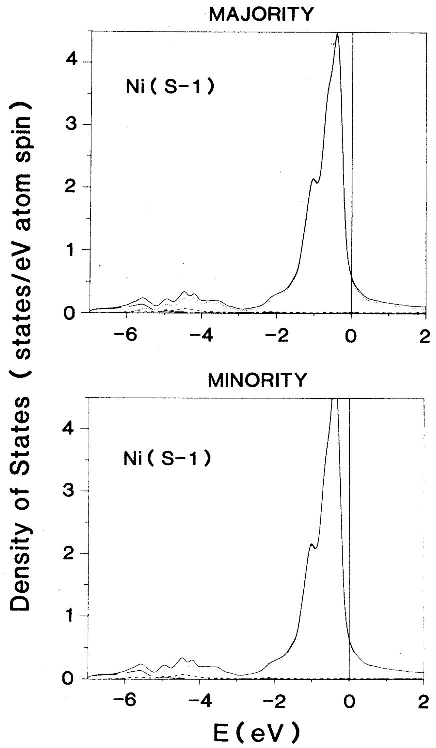

FIG. 7. Layer-projected partial density of states in units of states/eV spin for Ni layer in Ag/Ni($S-1$)/Ag(001). Dotted lines indicate d states and dashed lines represent s,p contributions.

The exchange splitting between spin-up and -down states is about 0.45 eV and the $\overline{M}_3$ state with majority spin, localized at the Ni atoms with a weight of more than 98%, is occupied with a binding energy of 0.32 eV. The work function is reduced with respect to the clean Ni(001) surface and is caused by the weakness of the d-d coupling between the Ni atoms themselves and between the Ni-Ag atoms.

Finally, we find that the total energy of the system having Ni atoms as a subsurface layer is reduced. Hence, the diffusion of Ni atoms below the Ag surface layer is very possible when Ni atoms are deposited on Ag(001). The magnetic moment ($0.02\mu_B$) of this system is much lower than that of Ni/Ag(001), and appears to explain recent ARPES experiments.[14]

ACKNOWLEDGMENTS

Work at Northwestern University supported by the U.S. Office of Naval Research (Grant No. 00041-81-K-0438) and by a computing grant from the Pittsburgh Superconducting Center, which is supported by the Division of Advanced Scientific Computing, National Science Foundation. Work at Oak Ridge National Laboratory sponsored by the Division of Materials Science, U.S. Department of Energy, under Contract No. DE-AC-05-84OR21400 with Martin Marietta Systems, Inc.

[1] L. N. Liebermann, D. R. Fredkin, and H. B. Shore, Phys. Rev. Lett. **22**, 539 (1969).

[2] L. N. Liebermann, J. Clinton, D. M. Edwards, and J. Mathon, Phys. Rev. Lett. **25**, 232 (1970).

[3] M. Pryzbylski and U. Gradmann, Phys. Rev. Lett. **59**, 1152 (1987).

[4] N. C. Koon, B. T. Jonker, F. A. Volkening, J. J. Krebs, and G. A. Prinz, Phys. Rev. Lett. **59**, 2463 (1987).

[5] M. F. Onellion, C. L. Fu, M. A. Thompson, J. L. Erskine, and A. J. Freeman, Phys. Rev. B **33**, 7322 (1986).

[6] D. Pescia, M. Stampanoni, G. L. Bona, A. Vaterlaus, R. F. Willis, and F. Meier, Phys. Rev. Lett. **58**, 2126 (1987).

[7] D. Pescia, G. Zampieri, M. Stampanoni, G. L. Bona, R. F. Willis, and F. Meier, Phys. Rev. Lett. **58**, 933 (1987).

[8] R. Kurzawa, K. P. Kämper, W. Schmitt, and G. Güntherodt, Solid State Commun. **60**, 777 (1986).

[9] B. T. Jonker, K. H. Walker, E. Kisker, G. A. Prinz, and C. Carbone, Phys. Rev. Lett. **57**, 142 (1986).

[10] S. D. Bader, E. R. Moog, and P. Grünberg, J. Magn. Magn. Mater. **53**, L295 (1986).

[11] J. Korecki and U. Gradmann, Phys. Rev. Lett. **55**, 2491 (1985).

[12] J. Tyson, A. H. Owens, and J. C. Walker, J. Appl. Phys. **52**, 2487 (1981).

[13] M. A. Thompson and J. L. Erskine, Phys. Rev. B **31**, 6832 (1985).

[14] M. A. Thompson, M. Onellion, and J. L. Erskine, Bull. Am. Phys. Soc. **31**, 675 (1986).

[15] W. Eib and S. F. Alvarado, Phys. Rev. Lett. **37**, 444 (1976).

[16] E. W. Plummer and W. Eberhardt, Phys. Rev. B **20**, 1444 (1979).

[17] T. Shinjo, T. Matsuzawa, T. Takada, S. Nasu, and Y. Murukami, Jpn. J. Phys. Soc. Jpn. **35**, 1032 (1973).

[18] T. Shinjo, T. Matsuzawa, T. Mizutani, and T. Takada, Jpn. J. Phys. Suppl. 2, Pt. 2, 729 (1974).

[19] U. Gradmann, K. Ullrich, J. Pebler, and K. Schmidt, J. Magn. Magn. Mater. **5**, 339 (1977).

[20] J. Lauer, V. Keune, and T. Shinjo, Physica B+C **86-88B**, 1409 (1977).

[21] I. Kramer and G. Bergmann, Phys. Rev. B **27**, 7271 (1983).

[22] C. S. Wang and A. J. Freeman, Phys. Rev. B **21**, 4585 (1980).

[23] O. Jepsen, J. Madsen, and O. K. Andersen, Phys. Rev. B **26**, 2790 (1982).

[24] E. Wimmer, A. J. Freeman, and H. Krakauer, Phys. Rev. B **30**, 3113 (1984).

[25] E. Wimmer, H. Krakauer, M. Weinert, and A. J. Freeman, Phys. Rev. B **24**, 864 (1981), and references therein.

[26] D.-S. Wang, A. J. Freeman, and H. Krakauer, Phys. Rev. B **26**, 1340 (1982).

[27] H. Huang, X.-y, Zhu, and J. Hermanson, Phys. Rev. B **29**, 2270 (1984).

[28] J. Tersoff and L. M. Falicov, Phys. Rev. B **26**, 6186 (1982).

[29] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).

[30] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).

[31] U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).

[32] L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971).

[33] D. D. Koelling and B. N. Harmon, J. Phys. C **10**, 3107 (1977).

[34] V. L. Moruzzi, J. F. Janak, and A. R. Williams, *Calculated Electronic Properties of Metals* (Pergamon, New York, 1978).

[35] C. L. Fu and A. J. Freeman, J. Magn. Magn. Mater. **54-57**, 777 (1986).

[36] J. Tersoff and L. M. Falicov, Phys. Rev. B **26**, 459 (1982).

[37] A. J. Freeman and R. E. Watson, in *Magnetism,* edited by G. T. Rado and H. Shul (Academic, New York, 1964), Vol. IIA, p. 167.

[38] J. I. Lee, C. L. Fu, and A. J. Freeman, J. Magn. Magn. Mater. **62**, 93 (1986).

[39] A. J. Freeman, C. L. Fu, M. Weinert, and S. Ohnishi, Hyperfine Interact. **33**, 531 (1987), and references therein.

[40] J. I. Lee, C. L. Fu, and A. J. Freeman (unpublished).

[41] R. Richter, J. R. Smith, and J. G. Gay, in *The Structure of Surfaces,* edited by M. A. Van Hove and S. Y. Tong (Springer-Verlag, Berlin, 1985), p. 35.