

Calculated surface electronic structure of ferromagnetic iron and the ferromagnetic ordered iron-cobalt alloy

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The electronic and magnetic properties of the (100) and (110) surfaces of ferromagnetic iron and the ferromagnetic iron-cobalt ordered alloys are calculated self-consistently. It is found that (a) in pure bcc iron the spin polarization increases from a bulk value of 2.12 to 2.90 at the (100) surface and to 2.55 at the (110) surface; (b) the ordered FeCo alloy has a bulk spin polarization of 2.66 for the Fe constituent and 1.78 for the Co constituent, compared with 2.12 and 1.56 for the respective pure elements; (c) in the (100) surfaces of ordered FeCo, the spin polarizations are 2.95 for Fe and 2.03 for Co; (d) the (110) surface of ordered FeCo exhibits spin polarizations of 2.75 for Fe and 1.86 for Co; (e) an atomic (110) overlayer of Fe on ordered FeCo produces a surface spin polarization of 2.63 and 2.67 for the two inequivalent Fe atoms. Agreement with available experimental data is excellent. All results can be successfully interpreted based on the saturation magnetization of Co, the relatively weak electron-electron interaction of Fe, and the surface narrowing of the electronic d band.

I. INTRODUCTION

Recently, there has been considerable interest in the magnetism and related properties of $3d$ magnetic transition-metal alloys, surfaces, and overlayers. These transition metals (Fe, Co, and Ni) are itinerant-electron ferromagnets; that is, their magnetization derives from the spin polarization of the itinerant d electrons. In crossing the Periodic Table from Fe to Ni, there is an increase in the number of these d electrons and a consequent drop in the bulk magnetization¹ from 2.22 bohr magnetons (μ_B) per atom in Fe, to 1.72 in Co, and 0.61 in Ni. The magnetic properties also depend on the electronic structure because the d electrons are sensitive to local environment. Consequently, the presence of a dissimilar neighbor, as found in an alloy, or the absence of a neighbor, as found at a surface, may cause an atom to exhibit a wide variety of behaviors.

The effort to understand such varied behavior must start with the bulk material. Iron is an element of great technological importance and its properties have been extensively examined. For our purposes, it is sufficient to note that Fe possesses a g factor¹ of approximately 2.10 and thus a spin polarization of 2.12. This means that Fe is ferromagnetically weak, i.e., not all available d holes contribute to the magnetization. It was previously shown² that this is a direct consequence of a relatively weak electron-electron interaction.

The Fe-Co alloy is also technologically important.³ This alloy possesses several useful characteristics such as the largest known magnetization per atom and an extremely high Curie temperature. In particular, the ordered FeCo alloy, which consists of Fe and Co atoms arranged at the corner and body-centered positions of a

simple-cubic lattice, has a magnetization of $2.42\mu_B$ per atom.⁴ This is $0.45\mu_B$ higher than the average of its constituent elements. Neutron-diffraction studies⁵ indicate that the vast majority of the anomalous increase in the magnetization is caused by an increase in the Fe magnetic moment from $2.2\mu_B$ to approximately $3.0\mu_B$, while the Co magnetic moment increases only slightly. Meyer and Asch⁶ found the g factor of the equiatomic alloy to be approximately 2.15, thus suggesting that the spin polarization is 2.25 ± 0.01 . Schwarz and Salahub⁷ used the local-spin-density technique to calculate the properties of the ordered FeCo alloy and found a spin polarization of 2.18. Victora and Falicov² demonstrated that, at least for the disordered equiatomic alloy, the increased magnetization is caused by magnetic saturation made possible by the presence of the strong Co electron-electron interaction.

A wide variety of experimental techniques⁸⁻¹⁵ show that the surface layer of a magnetic $3d$ transition metal is magnetic, while recent theoretical studies demonstrate that the surface magnetization is, in fact, enhanced relative to the bulk value.¹⁶⁻¹⁸ In particular, theory predicts a spin polarization of 2.98 electrons for the Fe(100) surface¹⁸ and approximately 0.70 electrons for the Ni surfaces.^{16,17} The experimental evidence of Gradmann *et al.*¹⁵ suggests that the magnetization of the Fe(110) surface is enhanced by approximately 30%. It is found¹⁹ that Fe atoms segregate to the surface of the Fe-Co alloy.

In this paper we present results of calculations for the magnetic and electronic properties of the (100) and (110) surfaces for Fe and the ordered FeCo alloy. We also perform calculations for the Fe segregated (110) surface. We use the Slater-Koster parametrized tight-binding scheme in which the one- and two-center integrals are fitted to the bulk band structure. The exchange interaction is treated

self-consistently in a single-site approximation. This scheme has been previously used and produced excellent agreement with both experiment and state-of-the-art calculations.

II. CALCULATION

In this section we describe our calculations. In Sec. IIA we describe the Hamiltonian and in Sec. IIB we examine the numerical accuracy of our work and the possible errors introduced by our major approximations.

A. Hamiltonian

We take our Hamiltonian to be the sum of a one-electron term H_0 and an electron-electron-interaction term H_{e-e} . For H_0 we choose the parametrized tight-binding scheme of Slater and Koster.²⁰ The Hamiltonian H_0 is written in terms of one- and two-center integrals, which are treated as parameters chosen to fit the bulk band structure. In Co (as in Ni) there is a marked discrepancy between the calculated and the experimentally measured bandwidth (photoemission experiments). For both Co and Fe we have chosen the calculated paramagnetic band structure of Moruzzi *et al.*^{21,22} (see Ref. 2) with the belief that discrepancies with photoemission data are caused by additional many-body effects, as has been argued^{23,24} for Ni. We include s , p , and d orbitals, with interactions up to second-nearest neighbors. For the matrix elements between Co and Fe we take the geometric mean of the respective Co-Co and Fe-Fe matrix elements. The two sets of intersite matrix elements are similar, so the results are insensitive to the precise scheme for choosing the Co-Fe matrix elements.

The choice of on-site energies has been the focus of debate.²⁵ We have experimented with several choices^{26,27} of energy difference between the Fe and Co band centers and found that, depending on choice, there exists small charge transfers of less than 0.05 electrons between the Fe and the Co. The direction of the transfer depends on the choice of energy difference. To avoid this ambivalence, we have chosen the energy levels so that there is no charge transfer.

For the Fe or Co electron-electron interaction we use a single-site approximation which has been extensively discussed,²⁸

$$H_{e-e} = \sum_{i,\sigma,\sigma'} \sum_{\alpha,\beta,\gamma,\delta} U_{\alpha\beta\gamma\delta} c_{i\alpha\sigma}^\dagger c_{i\beta\sigma'}^\dagger c_{i\gamma\sigma} c_{i\delta\sigma} \quad (1)$$

where $c_{i\alpha\sigma}^\dagger$ creates an orbital of symmetry α and spin σ at site i .

We treat H_{e-e} in the Hartree-Fock approach; we can, with some approximations, reduce H_{e-e} to a simple form for the on-site potential shifts,

$$\begin{aligned} \Delta E_{d\nu\sigma} &= -\frac{1}{2}(U-J)\langle m_{d\nu\sigma} \rangle - \frac{1}{2}J\langle m_{d\sigma} \rangle \\ &\quad + \frac{1}{2}(U-2U'+J)\langle n_{d\nu} - n_{d\nu}^0 \rangle \\ &\quad + V_{sd}\langle n_s - n_s^0 \rangle + V_{dd}\langle n_d - n_d^0 \rangle, \\ \Delta E_{s\sigma} &= V_{ss}\langle n_s - n_s^0 \rangle + V_{sd}\langle n_d - n_d^0 \rangle. \end{aligned} \quad (2)$$

Here, $\Delta E_{d\nu\sigma}$ is the on-site potential shift for a d orbital of symmetry ν and spin σ , measured relative to the value for the pure paramagnetic metal. By $m_{d\nu\sigma}$ we denote the spin polarization ($n_{d\nu\sigma} - n_{d\nu\bar{\sigma}}$) in the d orbital of symmetry ν at a given site, and $m_{d\sigma} \equiv \sum_{\nu} m_{d\nu\sigma}$. The total d occupancy at the site is denoted by $n_d \equiv \sum_{\nu,\sigma} n_{d\nu\sigma}$, and the value for the respective pure metal is n_d^0 . Quantities for s and p orbitals are similarly defined. In (2), s refers to the entire sp complex.

We define U as the on-site direct Coulomb integral between d orbitals of the same symmetry (rescaled by correlation effects; see below), U' is the integral between d orbitals of different symmetry, and J is the exchange integral. We define $V_{dd} \equiv U' - \frac{1}{2}J$, which gives the effective (repulsive) interaction between d electrons, aside from magnetic effects. We similarly define an effective interaction V_{ss} among sp electrons, and V_{sd} between sp and d electrons. We neglect the on-site exchange integrals other than those between d orbitals. Atomic symmetry demands that $U = U' + 2J$. The ratio $U:J$ is taken to be 5:1 as suggested by Herring.²⁹ The absolute magnitude of U is scaled to give the correct bulk magnetization, $\mu = 1.72\mu_B$ for Co and $\mu = 2.22\mu_B$ for Fe. We use Auger-electron spectroscopy data³⁰ to set V_{dd} for Fe and Co. The ratios of V_{sd} and V_{ss} to V_{dd} are taken to be the ratios of the atomic values.

It is difficult within the tight-binding approximation to treat charge transfer accurately at the surface. To avoid this problem and still treat charge transfer and potential shifts at the surface in a simple way, we impose upon our potential the constraint

$$\Delta n_{sp} = \Delta n_d = 0. \quad (3)$$

That is, the average on-site potentials of the d orbitals and of the s and p orbitals are fixed by the requirement that the total occupancies of the sp and d complexes at any site should not differ from the bulk values. More fully-self-consistent calculations^{17,18,31} suggest that the d band gains or loses no more than 0.1 electrons at the surface. By neglecting this, we may expect to alter the calculated surface magnetization by less than $0.1\mu_B$ per atom, an acceptable level of error.

B. Accuracy

We discuss first the numerical accuracy of our calculation, and second the crucial approximations in our Hamiltonian and their effect on the reliability of the model.

Our calculation uses a finite slab seven layers thick to represent the metal and its surfaces. Comparison with a five-layer calculation shows only a slight (less than 0.01 electrons) difference in the surface spin polarization, thus suggesting adequate convergence with respect to slab thickness. Additional evidence is produced by comparing the central layer of the slab with a bulk calculation. There is very close agreement (approximately 0.01 electrons) for the FeCo calculation and close agreement (less than 0.04 electrons) for the Fe(110) calculation. Only for the Fe(100) calculation is the disagreement noticeable: We find the central layer in the surface calculation to have a spin polarization 0.07 electrons larger than the bulk result. Interestingly, this is similar to the result obtained by

Ohnishi *et al.*¹⁸ for the central atom of a seven-layer slab; however, we do not find any Friedel oscillation of the spin moment. In any case, the conclusion to be drawn is that finite-slab effects are very unlikely to cause substantial errors, i.e., greater than 0.1 electrons, in the surface spin polarization.

Convergence with respect to wave-vector sample is provided by 36 wave vectors evenly distributed throughout the irreducible (100) surface Brillouin zone and 25 wave vectors evenly distributed throughout the irreducible (110) Brillouin zone. The adequacy of this sample is shown by the close agreement of the slab calculations with the bulk calculations, which used an unimpeachable 350 wave vectors per irreducible Brillouin zone.

We now recapitulate the most crucial approximations in our Hamiltonian and consider their effects. Our zero-charge-transfer requirement for the FeCo bulk is obviously incorrect. However, we find that the total moment per unit cell is independent of small charge transfers. Of course, the distribution of the magnetization between atoms does depend on the location of the available d holes as influenced by charge transfer. Thus, our approximation limits the accuracy of our calculated distribution of magnetization to about 0.05 electrons.

A more stringent approximation, as represented by Eq. (3), is made in the surface calculations. Here no charge transfer relative to the bulk is permitted either between atoms or between the sp - and d -projected subbands. Comparison with fully-self-consistent calculations^{17,18,31} suggests that this is an excellent approximation. Still, the uncertainty of up to 0.1 electron in the local d occupancy corresponds to a possible error of up to $0.1\mu_B$, which may be measurable for Fe or FeCo systems. However, there is no evidence that any available methods are accurate to better than $0.1\mu_B$ for inhomogeneous systems in any case. Approximation (3) also neglects the crystal-field splitting of the on-site potential.

Our Hartree-Fock treatment necessarily exaggerates the exchange splitting, which is reduced by correlation effects. Our restriction that the elemental Fe and Co have the correct magnetic moment will reduce the possible effects of this error. Nonetheless, it is possible that the exaggerated splitting may produce undesired consequences such as a slight distortion of the calculated density of states (DOS) which might make comparison with photoemission more difficult.

The use of a tight-binding Hamiltonian should be analyzed with care. This method provides a rather good treatment of the d band, but the handling of the sp band is less accurate. Since $sp-d$ hybridization plays an important role here, the tight-binding approximation introduces some risk of reduced quantitative accuracy.

Finally, it is important to note that, if many-body effects are important, the one-electron DOS which we calculate may not be the same as the excitation spectrum which is measured by photoemission. In particular, bulk Co and Ni exhibit a compressed photoionization spectrum^{32,33} compared to the calculated DOS. Since the Fermi energy is fixed, it is the lowest-energy peaks which experience the largest displacement. In the FeCo system, this effect is probably reduced due to the considerable hy-

bridization between the two elements. Nonetheless, substantial deviations between calculated and measured band structures are possible, particularly at the lower energies.

Ultimately, we must base our assessment of overall accuracy upon comparison with reported results of fully-self-consistent calculations for simple systems, and with experiment. Such comparisons are few, but they suggest that our methods reliably predict the quantitative magnetization of heterogeneous systems.^{2,16} Other important conclusions which we draw either involve comparisons of different systems, in which case our errors should approximately cancel, or appear to be model independent.

III. RESULTS

In this section we discuss the results of our calculations and compare them with other relevant calculations and experiments. In Sec. IIIA we discuss our calculation of the Fe surfaces. In other sections we consider the bulk FeCo (Sec. IIIB) and its surfaces (Sec. IIIC). The segregated system is discussed in Sec. IIID and a summary of the spin-polarization results for all systems is given in Table I.

A. Fe surfaces

The (100) and (110) surfaces of Fe are shown in Fig. 1. Our calculation gives a surface spin polarization for the (100) surface of 2.90 electrons. The enhanced magnetization penetrates some distance into the bulk: The second, third, and center layers have spin polarizations of 2.30, 2.24, and 2.18 electrons, respectively. These results are very similar to those of Ohnishi *et al.*¹⁸ In particular, their surface spin polarization is 2.98 electrons and their calculated DOS's also resemble ours, although 5–10% narrower. This excellent agreement between two different calculational techniques confirms the accuracy of our methods.

The calculated surface DOS of the Fe(110) surface is shown in comparison with bulk iron in Fig. 2. Two features in the surface DOS are immediately apparent: the appearance of a minority surface state near the Fermi energy and the absence at the surface of a small majority peak in the DOS found near the Fermi energy of the bulk. It may also be apparent from the DOS that the magnetization increases at the surface; in fact, the surface spin polarization is 2.55 versus 2.12 in the bulk. This is in

TABLE I. Spin-polarization results for all systems.

System	Spin polarization	
	Fe	Co
Pure elements	2.12	1.56
Fe-Co alloy	2.66	1.78
(100) Fe surface	2.90	
(110) Fe surface	2.55	
(100) FeCo surfaces	2.95	2.03
(110) FeCo surface	2.75	1.86
(110) Fe overlayer		
Co position	2.63	
Fe position	2.67	

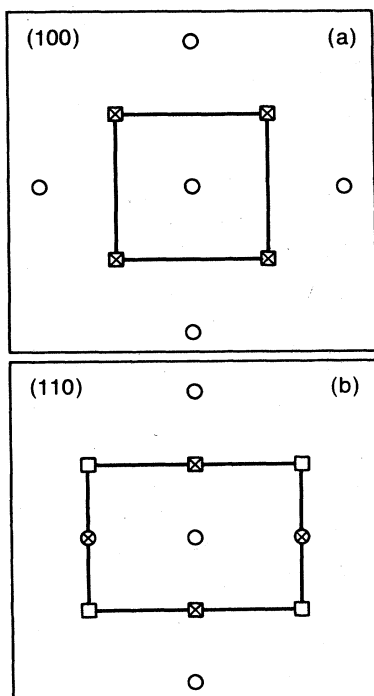


FIG. 1. Unit surface cells. Circles represent iron atoms; squares represent cobalt atoms in FeCo surfaces or Fe atoms in pure iron surfaces. Uncrossed atoms are located on the surface; crossed atoms are located on the first layer below the surface.

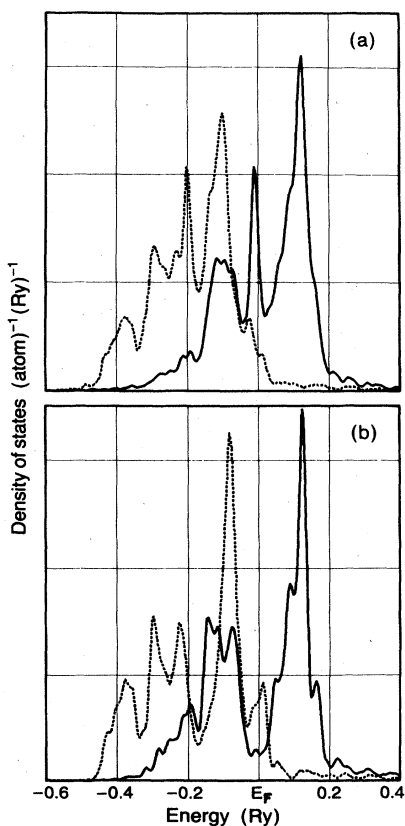


FIG. 2. Projected density of states. (a) Fe(110) surface layer; (b) bulk Fe. Solid lines are minority states; dashed lines are majority states.

agreement with the experimental results of Gradmann *et al.*¹⁵ The relative magnetizations of bulk Fe and the two surfaces are easily explained by noting that nearest-neighbor interactions dominate the d -band width [matrix elements are proportional³⁴ to (distance)⁻⁵ and the first-nearest-neighbor distance is $\frac{1}{2}\sqrt{3}$ smaller than the second-nearest neighbor (distance)]. The bulk atom in the bcc structure has eight nearest neighbors, an atom on the (110) surface has six, and an atom on the (100) surface has four. Thus the (100) surface has the fewest neighbors, smallest bandwidth, the same electron-electron interaction as the other geometries, and consequently the highest magnetization. The atom on the (110) surface has an intermediate number of neighbors and consequently will have an intermediate magnetization.

B. Bulk FeCo

Calculated DOS's for the ordered FeCo alloy are shown in Fig. 3. The majority DOS's have almost identical projections on the Fe and on the Co atoms. The minority DOS has more electrons projected on the Co atom and more holes projected on the Fe atom, which merely corresponds to Fe having fewer electrons than Co. Even in the minority DOS, there are very strong similarities between the two atoms in the location of projected peaks. Clearly, there is considerable hybridization of states between the two atoms; the amount of mixing is quite similar to that

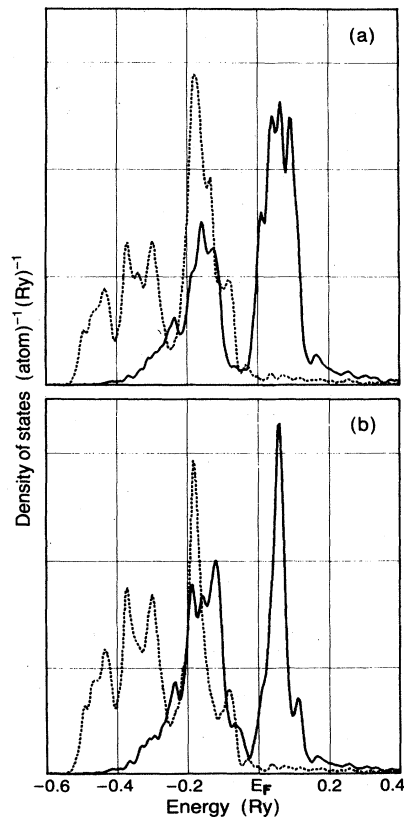


FIG. 3. Projected density of states for bulk FeCo. (a) Fe atom; (b) Co atom. Solid lines are minority states; dashed lines are majority states.

found between identical atoms in the pure elemental bulks.

In agreement with experiment, we find a substantially enhanced FeCo magnetization relative to the average of the constituent elements in their pure bulk form. In particular, we find the spin polarization of Fe to equal 2.66 electrons and the spin polarization of Co to equal 1.78 electrons, giving a total of 4.44 electrons per unit cell. Experiment finds a total spin polarization⁴ of 4.50 ± 0.02 electrons and individual spin polarization⁵ of 2.79 ± 0.1 for Fe and 1.68 ± 0.1 for Co. (In listing the experimental individual spin polarizations, we have assumed that the alloy g factor, 2.15, applies to each atom individually.) These values may be compared to the bulk spin polarizations: 2.12 for Fe and 1.56 for Co. Our calculation finds 93% of the experimental enhancement of the spin polarization (0.77 versus 0.83 experimentally), and we find, in agreement with experiment, that most of the enhancement occurs on the Fe atom.

Explanation for the enhancement is found in ideas proposed² for a similar enhancement in the disordered Fe-Co alloy. It was noted that Co is magnetically saturated, i.e., its magnetization is limited by the number of available d holes, while Fe is magnetically weak because of an insufficient electron-electron-interaction to bandwidth ratio. It was found that, for disordered Fe-Co alloys with greater than 30 at. % Co, the electron-electron interaction is sufficient to saturate the magnetic moment. This suggests that the rather large Co electron-electron interaction assists the weaker Fe electron-electron interaction in saturating the moment on the Fe as well as on the Co. It is clear from the considerable hybridization of Fe and Co states as shown in Fig. 3 that such assistance is possible. Additional evidence for the assistance mechanism is provided by the large increase in the Fe exchange splitting relative to pure Fe. One concludes that the strong electron-electron interaction of Co is sufficient to help increase the exchange splitting of the Fe atom, consequently saturating the magnetization without substantially diminishing the Co moment.

The slightly enhanced Co moment is caused by two structural effects. Body-centered-cubic cobalt has been constructed by sandwiching Co layers between Cr layers,³⁵ and, while the experimental resolution is insufficient to determine which structure of Co has the higher magnetization, a local-density calculation³⁶ conducted at the experimental lattice constant indicates an enhanced moment for the bcc structure (1.65 versus 1.56). Another contribution to the enhancement comes from the larger lattice constant of FeCo relative to the sandwiched bcc Co. A larger lattice constant means smaller bandwidth and higher magnetization. We find the spin polarization of bcc Co evaluated at the FeCo lattice constant to be 1.80 electrons. This gives a total enhancement relative to fcc Co of 0.24 electrons caused by structural effects. The presence of iron in the FeCo alloy affects this only marginally, making the final spin polarization 1.78.

C. FeCo surfaces

The simple-cubic FeCo structure may be cut by the (100) plane, leaving either all Fe atoms at the surface or

all Co atoms. The DOS of the Fe surface is shown in Fig. 4(a). This density of states bears a strong resemblance to the DOS at the elemental Fe(100) surface. The spin polarization is 2.95 electrons, which is also very similar to the Fe(100) result of 2.90 electrons. These results suggest that the presence of the (100) surface is the dominant effect and that the precise nature of the second layer is not too important for the surface Fe layer. This is reasonable since, as previously observed, the effect of Co is to increase the effective electron-electron-interaction to bandwidth ratio at the Fe atom and it is clear from Fe(100) results that a (100) surface can do this much more effectively. Consequently, the presence of Co instead of Fe is somewhat unimportant. The one major difference is that the surface effects are not able to penetrate even one layer deep into the bulk. This is presumably because Co, unlike Fe, has a saturated magnetization. Consequently, spin polarization and related properties are less susceptible to perturbation.

The density of states for the all-Co surface is shown in Fig. 4(b). It has slightly larger exchange splitting and spin polarization than the bulk (2.03 versus 1.78 electrons). Interestingly, there is a very slight (0.1 electron) decrease in the spin polarization of the underlying Fe layer. However, even this effect vanishes at the next Co layer and

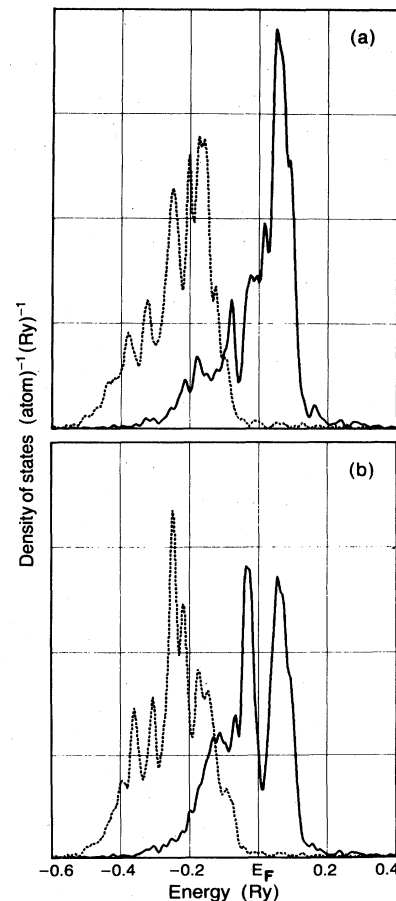


FIG. 4. Projected density of states for the two FeCo(100) surfaces. (a) Surface Fe atom; (b) surface Co atom. Solid lines are minority states; dashed lines are majority states.

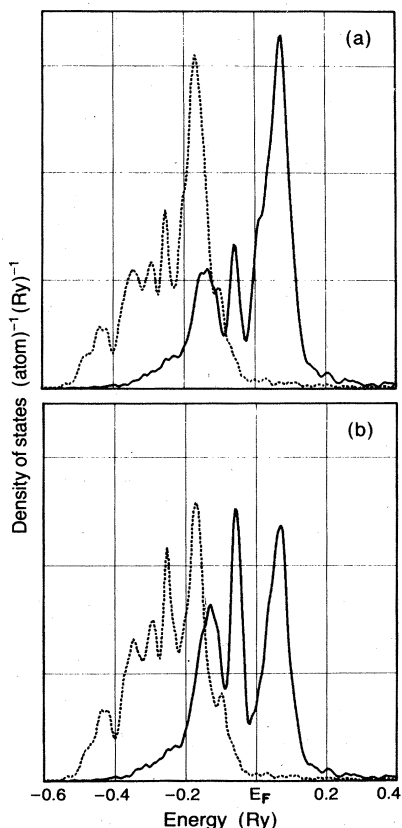


FIG. 5. Projected density of states for FeCo(110) surface. (a) Surface Fe atom; (b) surface Co atom. Solid lines are minority states; dashed lines are majority states.

deeper. Overall, the surface behaves like Ni surfaces^{16,17} in that the surface DOS is narrowed and new features appear, but the magnetic saturation allows only small increases in the magnetization.

The (110) surface of FeCo contains both Fe and Co atoms arranged in a two-atom unit surface cell. The surface DOS is shown in Fig. 5. As expected from the nearest-neighbor arguments given in Sec. III A, the (110) surface displays behavior intermediate between bulk FeCo and the (100) FeCo surfaces. The calculated spin polarizations at the surface are 2.75 electrons for Fe and 1.86 electrons for Co. There is very little penetration of surface effects into the bulk.

D. Fe segregated surface

Experimental and theoretical¹³ studies indicate that Fe tends to segregate to the surface of the FeCo alloy. To represent this, we have calculated the electronic properties of a Fe (110) overlayer, one atom thick, atop the FeCo alloy. The density of states for the two distinct surface Fe atoms is shown in Fig. 6. The spin polarizations are 2.63 electrons for the Fe atom occupying the Co position and 2.67 electrons for the Fe atom occupying the normal position. Clearly, the two Fe atoms have very similar electronic properties. It is to be noted that their properties are intermediate between the Fe(110) surface and the FeCo(110) surface.

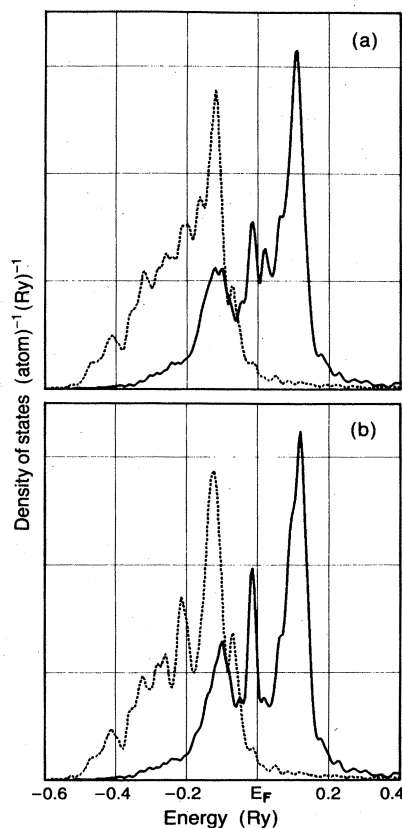


FIG. 6. Projected density of states for an Fe overlayer on the FeCo(110) surface. (a) Surface Fe atom at normal position; (b) surface Fe atom at the "Co" position. Solid lines are minority states; dashed lines are majority states.

IV. CONCLUSION

The complicated magnetic and electronic properties of FeCo surfaces have been calculated and the results explained through examination of two simpler systems: bulk FeCo and pure-Fe surfaces. The spin polarization of bulk FeCo is calculated to be 4.44 electrons per unit cell, thus capturing more than 90% of the experimental enhancement observed in the alloy relative to the average of the pure elemental magnetization. Most of the increase is found to occur on the Fe atom, where the presence of eight neighboring Co atoms helps increase the effective electron-electron interaction and saturates the moment. The much smaller magnetic enhancement found on the Co atom is caused by the shift from fcc to bcc structures and possibly a slight swelling in the lattice constant as iron is added.

For both Fe and FeCo, the (100) surface has substantially higher magnetization than the (110) surface, which is in turn more magnetic than the bulk. The effect is particularly vivid in Fe where the spin polarization increases from its bulk value of 2.12 electrons to 2.90 at the (100) surface. These effects may be understood in terms of simple bandwidth arguments, where it is noted that an atom at the (100) surface has only four nearest neighbors, at the (110) surface six nearest neighbors, and in bulk eight. Consequently, the (100) surface has the smallest band-

width and the largest magnetization. This argument applies to FeCo, as well as Fe, because the nearest-neighbor Co atoms hybridize exceedingly well with their neighboring Fe atoms and consequently produce a larger contribution to the Fe bandwidth than the second-nearest-neighbor Fe atoms. The Fe-overlayered surface on FeCo presents behavior intermediate between the pure Fe(110) surface and the ordinary FeCo(110) surface.

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