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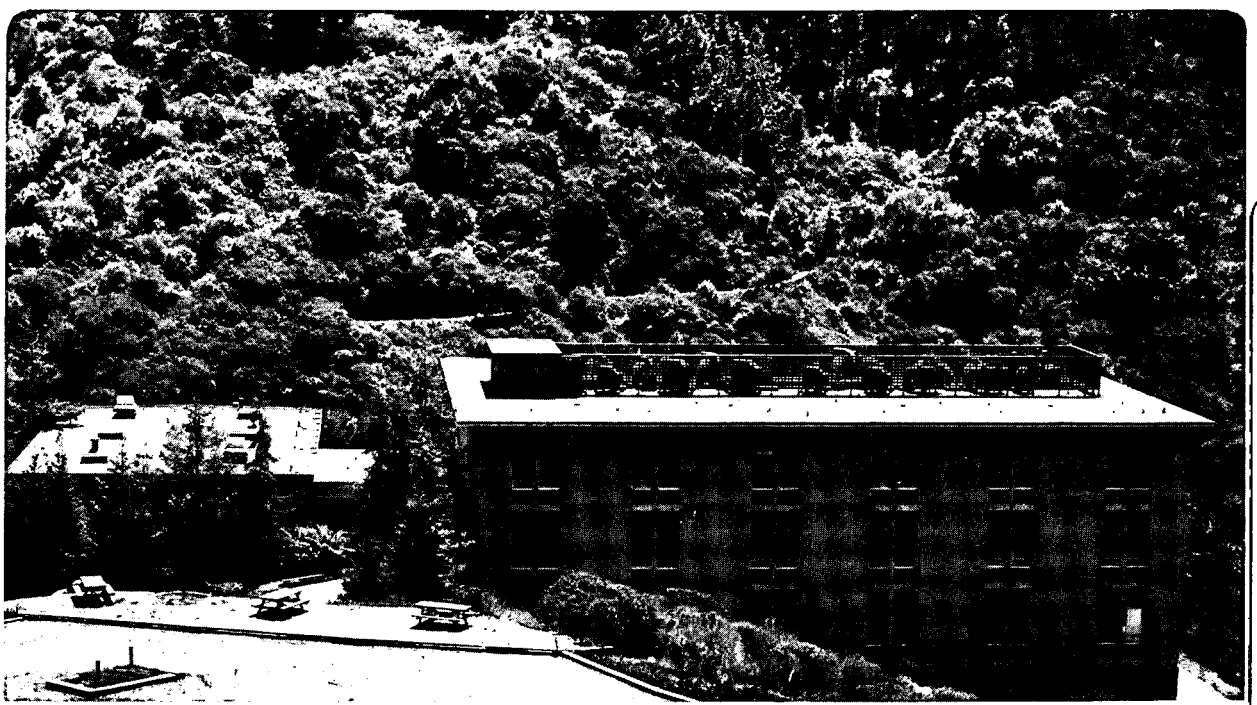

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ABSTRACT

The magnetic structure of {111} stacking faults in Nickel is investigated utilizing a fully self-consistent, layered Korringa-Kohn-Rostoker approach which does *not* require full three-dimensional symmetry or the use of finite-sized slabs. Localized electronic states appear at the faults. The spin polarization is calculated for a twin boundary, an intrinsic fault, an extrinsic fault, and several other stacking sequences. In all cases, the magnetic moment is found to be insensitive to the orientation of the nearest-neighbor atoms, but instead can be related to the distance

to the nearest atom in the direction perpendicular to the fault plane. Very simple empirical expressions for calculating the spin polarization and total energy of any stacking configuration are presented.

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Recently, there has been a great deal of interest in the magnetic properties of transition-metal films, interfaces and surfaces. Much of this interest stems from the development of new experimental techniques for performing spin-sensitive surface spectroscopy.[1–8] In addition, there have been numerous theoretical predictions of enhanced magnetism at the surface of many transition metals.[9–11] These predictions, based on electronic structure calculations, are often times at odds with experimental findings.[3]

Alloy and overlayer systems are complicated by many factors, but there have been some attempts to investigate their properties[12,13] in a systematic way. The aim of the current work is to investigate a much less complicated system, namely {111}

. stacking faults in nickel.[14,15]

The method used for studying the faults is the self-consistent layered-Korringa-Kohn-Rostoker[16] (LKKR) technique recently developed by MacLaren *et al.*[17] The electronic structure calcluation is based on the local approximation to spin-density functional theory[18] due to von Barth and Hedin[19], and includes the semi-relativistic corrections of Koelling and Harmon[20], which do *not* include the effects of spin-orbit coupling. (The neglect of spin-orbit effects is not expected to alter significantly the results reported below.) In LKKR, the properties of a solid are derived from the properties of its two-dimensional planar components. There is no need for three-dimensional periodicity, finite-sized slabs or "super-cells", and the problems associated with those approximations are completely avoided.

The calculations of the electronic structures of the close-packed bulk systems *(fcc, hcp,* and *dhcp* defined below) were iterated until the Fermi energies were stable to 10 microHartrees, and the spin polarizations were stable to better than $\pm$ 0.002 μ_B (where μ_B is the Bohr magneton). The stacking fault calculations were iterated to a similar accuracy. The reported effects are small, but are believed to be indicative of the real physical mechanisms.

The [111]-direction of the face-centered-cubic *(fcc)* lattice is defined to be the z-direction, as (111)-planes will be stacked to form the three-dimensional solid. The "ABC" stacking notation[21] is used to describe stacking sequences. In this notation, the *fcc* structure is indicated by (...<ABC>...) where the "..." indicates that the structure within the brackets is repeated to infinity in the direction of the bracket adjacent to the "...". In addition to the *fcc* and the hexagonal-close-packed *(hcp)* (...<AB>...) structures, the stacking sequences studied are the double-hexagonal-close-packed *(dhcp)* lattice: (...<ABAC>...); the twin boundary: (...<ABC>ABA<CBA>...); the intrinsic fault: (...<ABC>ABAB<CAB>...); the extrinsic fault: (...<ABC>ABACA<BCA>...); the "super-extrinsic" fault: (...<ABC>ACBA<BCA>...) and the "hyper-extrinsic" fault:

(...<ABC>ACBAC<ABC>...).

The calculated spin polarization within the muffin-tin of an atom in bulk *fcc* nickel is 0.614 μ_B. The interstitial charge is polarized antiferromagnetically relative to that within the muffin-tin, and reduces the net spin polarization (the spin polarization of the charge within the Wigner-Seitz sphere is 0.597 μ_B). The layer-dependent changes in the net spin polarization are accurately reflected in the muffin-tin spin polarizations, which are quoted throughout the remainder of this paper.

The results for the spin polarization of the stacking faults are presented in table I. Since the spin polarizations of the layers are symmetric about the midpoints of the faults (the midpoints of the faults are indicated by a arrow, $\rightarrow$), only the spin polarization of the upper half of each fault is shown. The labeling of the layers in table I corresponds to that given above. The first entry in the table for each of the stacking faults is a layer fixed so as to have the properties of the bulk, the electronic structures of the remaining layers were allowed to adjust to the presence of the fault; the atomic positions were fixed. States localized at the faults are present for both spin polarizations. The calculated spin polarization for hypothetical *hcp* nickel is 0.583 μ_B and for hypothetical *dhcp* nickel, the polarization of the A layers is 0.592 μ_B and the polarization on layers B and C is 0.612 μ_B.

The most striking feature of table I is that the spin polarization of a site appears to be independent of the orientation of the nearest- and next nearest-neighbors. The apex layer of the twin boundary, the central B layer in the stacking (...<ABC>ABA<CBA>...), has its nearest- and next-nearest neighbors in the positions they would occupy in the *hcp* lattice, but the spin polarization is that of the *fcc* bulk. In contrast, the layers adjacent to the apex layer of the twin, labeled A in the stacking (...<ABC>ABA<CBA>...) have the local structure of the *fcc* lattice, but the spin polarization is depressed. This behavior is exactly the opposite of what is to be naively expected.

One physical interpretation of this result is that in the close-packed structures, the potential caused by nearby atoms is so nearly spherical that the exact positions of the atoms do not matter; each atomic site "sees" only a spherical potential. This reasoning implies that the loss of near-spherical symmetry may alter the spin polarization of a site.

The spin-polarization results show a correlation between the depression of the spin polarization of a layer and the presence of a nearby atom in the z-direction. For example, in the *fcc* case, the nearest neighbors in the z-direction are on the third layer from that under consideration whereas in the *hcp* structure these neighbors are only two-planes distant (thirty-three percent closer). The calculated spin polarization of nickel in the *hcp* structure is five percent less than that of *fcc* nickel. Similar reductions are present in all the stacking sequences investigated.

It is not surprising that stacking faults affect the spin polarization of the layers near the fault. It is, however, surprising that the spin polarization depends on the distance to the nearest neighbor in the z-direction. A simplified explanation of this effect is that it is only possible to have two neighbors at the distance of two planes away, and the resulting potential cannot possibly appear spherical. Consequently, the spin polarization is affected. More specifically, for nickel, the calculated decrease in spin polarization appears to be related to a local broadening in the density of states brought about by the close proximity of atoms in the z-direction.

The total energies (relative to *fcc* nickel) of the stacking sequences are tabulated in table II. The energies of the *hcp* and *dhcp* structures are quoted in (mJ/m^2) per (111)-plane over the energy of the *fcc* structure. The energies of the stacking faults are quoted in (mJ/m^2) per fault.

A very simple fitting procedure has been developed to allow estimates of the spin polarizations and energies of any stacking configuration.

The spin polarizations are fitted to a linear equation of the form

$$\mu = M_o + \alpha_2 \eta_2 + \alpha_3 \eta_3 \tag{1}$$

where M_o, α_2 and α_3 are fitting parameters and η_2 and η_3 are defined to be the number of layers of the same type (A, B, or C) as the layer under consideration, at a distance of two and three planes away, respectively. For example, for the *fcc* lattice, $\eta_2 = 0$ and $\eta_3 = 2$, whereas for the *hcp* lattice, $\eta_2 = 2$ and $\eta_3 = 0$.

The values of the fitting parameters were calculated using the results of the twin boundary and all the stacking-fault calculations discussed above (*not* including the *hcp* and *dhcp* results). The resulting fitting parameters are $M_o = 0.604\ \mu_B$, $\alpha_2 = -0.010\ \mu_B$, and $\alpha_3 = 0.003\ \mu_B$. Figure 1 compares the spin polarizations resulting from the fits with LKKR results for the hyper-extrinsic and the *dhcp* stacking sequences. The trends in spin polarization are accurately reproduced, even for *dhcp* nickel, which demonstrates the predictive power of the simple formula. The apparent systematic error in the fit for the *dhcp* configuration stems from the fact that the fitting parameters are those based on an *fcc* bulk structure, not the *dhcp* bulk.

The internal energy is fitted to a similar formula:

$$E = \sum_{layers} \left\{ E_{hcp} + \sum_{i=2}^{3} \xi_i \gamma_i \right\}. \tag{2}$$

In this expression, E_{hcp} is zero if the layer has local *fcc* structure (i.e. layer B in the stacking ABC), and is a constant (to be determined by a least-squares fit of all the stacking sequences) if the layer has the local *hcp* structure (i.e. layer B in the sequence ABA). The γ_i are also fitting parameters. The ξ_i are defined to the number of planes at a distance of i atomic layers away which are different from what they would be in the *fcc* lattice. For example, $\xi_2 = 2$ and $\xi_3 = 2$ for the *hcp* configuration. Table II contains the results of the fit. The values of the fitting parameters are $E_{hcp} = 89\ (mJ/m^2)$, $\xi_2 = -8\ (mJ/m^2)$, and $\xi_3 = 6\ (mJ/m^2)$. The trends in energy are

reproduced reasonably well by the simple formula.

In conclusion, the magnetic properties of {111} stacking faults in ferromagnetic nickel have been calculated using a self-consistent layered-Korringa-Kohn-Rostoker formalism which does not require the use of finite-sized slabs or "super-cells". Localized states appear at all of the faults studied. The spin polarization of a site does not depend on the orientation of the nearest- and next-nearest neighbors. Instead, the spin polarization depends directly on the distance to the nearest neighbor in the z-direction, and is most reduced by the presence of neighbors directly above and below at the (minimum possible) distance of two layers away.

Simple formulas for calculating the spin polarization and internal energy of any stacking configuration are presented. These formulas should be useful for rough estimates of the properties of {111} stacking faults in nickel.

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Table Captions

Table I The muffin-tin spin polarizations for the stacking fault structures. The first entry in each column is a layer fixed to be "bulk-like". The electronic structure of the remaining layers was allowed to rearrange in the presence of the fault. The midpoints of the faults are indicated by arrows. Since the polarizations of the layers are symmetric about the midpoints of the faults, only the polarization for half of each stacking fault is displayed. The polarization is reduced on the layers which have a layer of the same type at a distance of two atomic layers.

Table II The LKKR total energies and the energies resulting from the simple fitting procedure [equation (2) of the text] of the investigated stacking sequences. The energy of the *hcp* and *dhcp* structures are quoted in (mJ/m^2) per (111)-plane over the total energy of *fcc* nickel. The energies of the stacking faults are quoted in (mJ/m^2) per fault. The simple fitting procedure provides a reasonable estimate of the energy of any stacking sequence.

Figure Captions

Figure 1 Comparison of the results of the simple fit with LKKR results for the spin polarization of the layers of the (a) hyper-extrinsic fault and (b) *dhcp* bulk structure. (The lines are guides for the eye.) The fits accurately reproduce the trends in both the sign of the change in and the absolute magnitude of the spin polarization for the stacking-fault configurations, but are only capable of predicting the sign of the change in spin polarization for other bulk configurations.

Table I

Muffin-Tin Spin-Polarization (μ_B)

twin		int.		ext.		sup. ext.		hyp. ext.	
lay.	pol.	lay.	pol.	lay.	pol.	lay.	pol.	lay.	pol.
A	0.614	A	0.614	A	0.614	A	0.614	A	0.614
B	0.611	B	0.609	B	0.610	B	0.609	B	0.607
C	0.611	C	0.609	C	0.607	C	0.596	C	0.599
A	0.603	A	0.597	A	0.595	A	0.606	A	0.608
→B	0.614	B	0.594	B	0.598	C	0.595	C	0.600
		→		→A	0.582	→		→B	0.604

Table II

system	LKKR energy (mJ/m^2)	fitted energy (mJ/m^2)
hcp	101	85
dhcp	54	54
twin	105	90
intrinsic	176	185
extrinsic	161	181
super-extrinsic	160	167
hyper-extrinsic	200	181

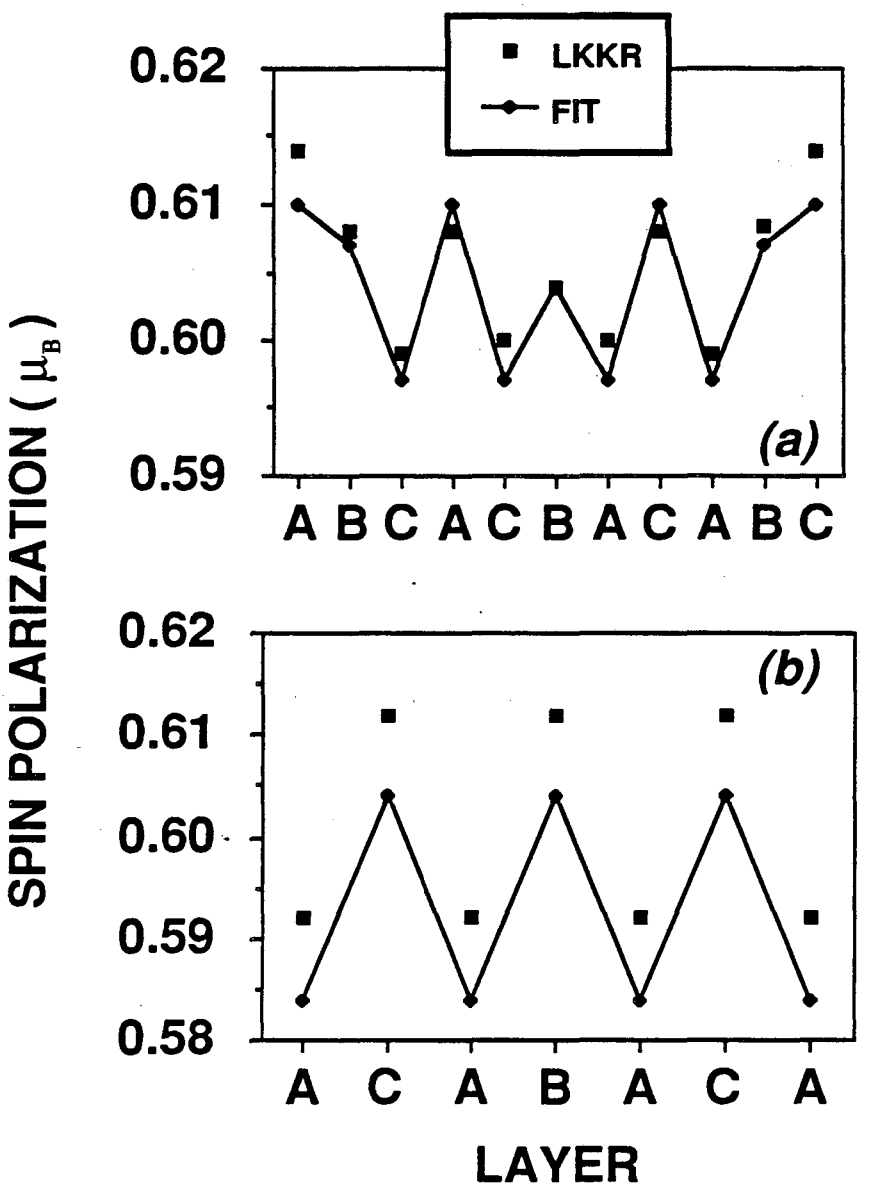
LKKR
FIT
0.62
0.61
0.60
0.59
(a)
A B C A C B A C A B C
0.62
0.61
0.60
0.59
0.58
(b)
A C A B A C A
LAYER
SPIN POLARIZATION (μ_B)

Figure 1

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