Magnetoresistance anisotropy in ferromagnetic NiCu alloys

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The magnetoresistance anisotropy is calculated for ferromagnetic nickel-copper alloys. The model is based on *sd* impurity scattering at temperatures sufficiently low for the electron-magnon interaction to be negligible. The *d* bands as well as the conductivity integrals are treated in considerably more detail than previously reported. The results indicate that the majority-spin current favors the condition $\rho_{\parallel} < \rho_{\perp}$ and the minority-spin current favors $\rho_{\parallel} > \rho_{\perp}$. This is in opposition to previous work based on overly simplified band models. The feature of the band structure most responsible for producing a large, positive, magnetoresistance coefficient $(\rho_{\parallel} - \rho_{\perp})/\langle \rho \rangle_{av}$ appears to be a near-degeneracy at the Fermi energy between predominantly minority-spin bands.

I. INTRODUCTION

Ferromagnetic metals and alloys of the first-transition-series elements and copper exhibit remarkable magnetoresistance effects. In Ni_{85}-Fe_{15} (permalloy), for example, the anisotropic resistivity ratio $\Delta\rho/\langle\rho\rangle_{av} \equiv (\rho_{\parallel} - \rho_{\perp})/(\frac{1}{3}\rho_{\parallel} + \frac{2}{3}\rho_{\perp})$ is over 4% at 273 °K,[1] with $\rho_{\parallel} > \rho_{\perp}$ contrary to what one might intuitively guess. It is timely to reconsider the reasons for this, first because band-structure calculations have appeared for the ferromagnetic elements Ni (Refs. 2–4) and Fe, (Refs. 5, 6) and second because the effect has practical applications as a means of sensing magnetic fields in bubble devices[7] and magnetic recorders.[8]

Apparently, the explanation must go beyond ordinary transport theory, which is based on the force exerted on conduction electrons by the electric field $\vec{E}$ and magnetic induction $\vec{B} = \mu_0(\vec{H} + \vec{M}) \approx 1$ Wb/m^2. That this is so is evident from the $\omega\tau$ product, where $\omega = eB/m^*$ is the cyclotron frequency and τ the relaxation time. For the example cited above, an alloy near room temperature, $\omega\tau$ is certainly very small compared to unity. The $\omega\tau$ product is a measure of the distance traversed by electrons along with Fermi surface in $\vec{k}$ space. When $\omega\tau \ll 1$ this is only a small fraction of an orbit, be it open or closed, and the curvature of the Fermi surface simply is not important. Worse, ordinary magnetoresistance is a second-order effect in $\omega\tau$.

The applied magnetic field enters the problem only indirectly. It magnetizes the material, that is, aligns the spin system, and the spins affect the conductivity through the spin-orbit interaction as discussed below. This interaction causes an anisotropy in the leading term of the Jones-Zener expansion[9]

$$\sigma_{ij} = \sigma_{ij}^{(0)} + \sigma_{ijk}^{(1)} B_k + \sigma_{ijkl}^{(2)} B_k B_l + \cdots , \tag{1}$$

and makes it unnecessary to consider higher-order terms whenever $\omega\tau \ll 1$. In this regard, the Hall effect in ferromagnetic metals is more complicated than the magnetoresistance effect. The Hall effect requires that $\sigma_{ijk}^{(1)}$ be calculated with the spin-orbit interaction taken into account.

In the literature on the transport properties of ferromagnetic metals, reference is sometimes made to "ordinary" and "extraordinary" effects. The former are explicable in terms of ordinary transport theory; the latter are not. The distinction appears artificial in light of the Jones-Zener expansion with the coefficients $\sigma^{(0)}$, $\sigma^{(1)}$, and $\sigma^{(2)}$ properly calculated using the spin-orbit-perturbed wave functions. Higher-order terms in this expansion must be considered in pure metals at low temperature, where $\omega\tau \approx 1$, but in alloys at room temperature only the first term is important in the magnetoresistance problem.

It was pointed out by Mott[10] in 1936 that the relatively high resistivity of transition series metals is due to *sd* scattering with the mechanism being either the electron-phonon interaction or impurity scattering or both. The *d* bands are relatively flat, resulting in a low mobility for the *d* electrons, and consequently most of the current is carried by the more mobile *s* electrons. Mott's model explains the isotropic decrease in resistivity observed when the temperature is lowered through the Curie point on the basis of exchange-split *d* bands with one partially above and one totally below the Fermi level. In the magnetic state the density of available majority-spin *d* states would be zero were it not for the "tail" on the Fermi distribution function.

Smit,[11] in 1951, extended Mott's theory by introducing the spin-orbit interaction, which mixes states so that each *d* band is no longer characterized by a definite *z* component of spin. Whereas formerly at $T = 0$ only minority-spin *s* electrons could scatter into *d* states, there now exists a finite probability for electrons of either spin. Smit attributed the resistivity anisotropy to majority-spin electrons. He argued that the mixing of states is anisotropic, and that the *sd* scattering probability for majority-spin electrons is greatest for those

with $\vec{k}$ vector parallel to the magnetization $\vec{M}$. His model for the d bands is extremely simple: ten atomic $3d$ states exchange and crystal-field split into twofold and threefold degenerate levels.

In more recent years there have appeared calculations by additional authors, some[12,13] extending Smit's work to the case where $\vec{M}$ is not along a crystallographic axis, some[14,15] considering the term $L_z S_z$ in $\vec{L}\cdot\vec{S}$ which Smit dropped on the basis of a quenching argument, and some[16,17] attributing at least part of the anisotropy to electron-magnon scattering. In all cases the band structure is greatly simplified.

The purpose of the present work is to introduce a realistic band structure into the basic model of Smit and to calculate analytically the resistance anisotropy for face-centered-cubic single-crystal alloys of nickel and copper. It is assumed that an applied field exists of sufficient magnitude (about 250 Oe for nickel) to align the magnetization in the [001] direction. The results indicate that the mechanism works somewhat differently than Smit and others have concluded, at least when the Fermi level is near the top of the d bands. They also indicate those features of the bands that are important in producing a large anisotropy.

It is shown below that, for systems within the scope of the calculation, a resistance anisotropy with $\rho_{\parallel} > \rho_{\perp}$ results from *sd* scattering of *minority-spin* electrons and not majority-spin electrons as commonly believed. Moreover, energy separations between sheets of the Fermi surface of predominantly the *same* spin are more important in producing the condition $\rho_{\parallel} > \rho_{\perp}$ than are exchange splittings. In this calculation the Fermi level is assumed to lie near the top of uniformly exchange-split d bands. A small value of $\epsilon \equiv X_5 - X_2$, the splitting between uppermost d bands of like spin, tends to make $\Delta\rho/\langle\rho\rangle_{av} \equiv (\rho_{\parallel} - \rho_{\perp})/\langle\rho\rangle_{av}$ large and positive while a small exchange splitting constant 2γ tends to make $\Delta\rho/\langle\rho\rangle_{av}$ large and negative. There is a competition between these effects and $\Delta\rho/\langle\rho\rangle_{av}$ can be of either sign depending on the details of the bands and the location of the Fermi energy.

In Sec. II, a set of equations for the distribution functions for the various bands is obtained in terms of scattering probabilities. The distribution functions are written in terms of anisotropic, $\vec{k}$-dependent relaxation times. The spin-orbit interaction is considered in Sec. III, where it is used to compute first-order corrections to the Bloch functions that appear in the scattering-probability expressions. Impurity scattering is assumed to dominate phonon scattering, and this limits the applicability of the results to alloys. The unperturbed wave functions are obtained from Fletcher's tight-binding-method calculation[18] for d electrons but the relevant energy splittings are taken from more recent self-consistent calculations. The s electrons are represented by plane waves and *sd* hybridization is not considered. In Sec. IV the corrected wave functions are used to compute scattering probabilities and relaxation times. The conductivity integrals are evaluated in Sec. V and the results are discussed in Sec. VI. The NiCu system comes the closest in satisfying the assumptions made in the course of the calculation.

II. DISTRIBUTION FUNCTION AND RELAXATION TIME FORMALISMS

We distinguish 11 bands: the d bands, denoted by subscript n ($n = 1, 2, \ldots, 10$), and a single s band that is twofold degenerate due to spin. The d bands are nondegenerate due to the spin-orbit interaction. Associated with each band is a distribution function f (subscripts temporarily suppressed) satisfying

$$\left(\frac{\partial f}{\partial t}\right)_{\text{field}} + \left(\frac{\partial f}{\partial t}\right)_{\text{collisions}} = 0 \tag{2}$$

where, as usual,

$$\left(\frac{\partial f}{\partial t}\right)_{\text{field}} = -\frac{\partial f_0}{\partial \epsilon}\, e\vec{v}\cdot\vec{E} = -\frac{\partial f_0}{\partial \epsilon}\,\frac{e}{\hbar}\,\nabla_{\vec{k}}\epsilon(\vec{k})\cdot\vec{E}\,, \tag{3}$$

$$\left(\frac{\partial f_s}{\partial t}\right)_{\text{coll}} = [1 - f_s(\vec{k})]\int f_s(\vec{k}')P^{ss}_{\vec{k}',\vec{k}}\,dS' - f_s(\vec{k})\int [1 - f_s(\vec{k}')]P^{ss}_{\vec{k},\vec{k}'}\,dS'$$
$$+\sum_{n=1}^{10}\left([1 - f_s(\vec{k})]\int f_n(\vec{k}')P^{ns}_{\vec{k}',\vec{k}}\,dS' - f_s(\vec{k})\int [1 - f_n(\vec{k}')]P^{sn}_{\vec{k},\vec{k}'}\,dS'\right), \tag{4a}$$

and

$$\left(\frac{\partial f_n}{\partial t}\right)_{\text{coll}} = [1 - f_n(\vec{k})]\int f_s(\vec{k}')P^{sn}_{\vec{k}',\vec{k}}\,dS' - f_n(\vec{k})\int [1 - f_s(\vec{k}')]P^{ns}_{\vec{k},\vec{k}'}\,dS'$$
$$+\sum_{n'=1}^{10}\left([1 - f_n(\vec{k})]\int f_{n'}(\vec{k}')P^{n'n}_{\vec{k}',\vec{k}}\,dS' - f_n(\vec{k})\int [1 - f_{n'}(\vec{k}')]P^{mn'}_{\vec{k},\vec{k}'}\,dS'\right). \tag{4b}$$

In these equations $\vec{E}$ is the applied electric field, dS' denotes an integration over the appropriate sheet of the Fermi surface and, for example, $P^{sn}_{\vec{k}'\vec{k}}$ is the probability of scattering from a state $\vec{k}'$ in

the s band to a state $\vec{k}$ in the nth d band. Only elastic collisions are considered.

Also associated with each band is a relaxation time τ that, in general, is an anisotropic function of $\vec{k}$ and is *defined* by the equations

$$f_s(\vec{k}) = f_0 - \frac{\partial f_0}{\partial \epsilon}\tau_s(\vec{k})\vec{v}_s(\vec{k})\cdot e\vec{E} \tag{5a}$$

and

$$f_n(\vec{k}) = f_0 - \frac{\partial f_0}{\partial \epsilon}\tau_n(\vec{k})\vec{v}_n(\vec{k})\cdot e\vec{E}, \tag{5b}$$

where f_0 is the equilibrium distribution function. Note that the magnetic field does not enter the first-order term of these Jones-Zener expansions for f_s and f_n. In terms of $\tau_s(\vec{k})$ and $\tau_n(\vec{k})$ the linearized equation for $(\partial f_s/\partial t)_{\text{coll}}$ is

$$\begin{aligned}\left(\frac{\partial f_s}{\partial t}\right)_{\text{coll}} = -e\frac{\partial f_0}{\partial \epsilon}\Bigg[&\int \tau_s(\vec{k}')\vec{v}_s(\vec{k}')\cdot\vec{E}P^{ss}_{\vec{k}',\vec{k}}\,dS' \\ &- \tau_s(\vec{k})\vec{v}_s(\vec{k})\cdot\vec{E}\int P^{ss}_{\vec{k},\vec{k}'}\,dS' \\ &+\sum_{n=1}^{10}\left(\int \tau_n(\vec{k}')\vec{v}_n(\vec{k}')\cdot\vec{E}P^{ns}_{\vec{k}',\vec{k}}\,dS'\right. \\ &\left.- \tau_s(\vec{k})\vec{v}_s(\vec{k})\cdot\vec{E}\int P^{sn}_{\vec{k},\vec{k}'}\,dS'\right)\Bigg],\end{aligned} \tag{6}$$

with corresponding equations for $(\partial f_n/\partial t)_{\text{coll}}$.

According to the first Born approximation, the scattering probabilities are[19]

$$P^{sn}_{\vec{k},\vec{k}'} = \frac{(x/4\pi^2\hbar)\,|V^{sn}_{\vec{k},\vec{k}'}|^2}{|\nabla_{\vec{k}'}\epsilon_n|}, \tag{7a}$$

$$P^{ns}_{\vec{k},\vec{k}'} = \frac{(x/4\pi^2\hbar)\,|V^{ns}_{\vec{k},\vec{k}'}|^2}{|\nabla_{\vec{k}'}\epsilon_s|}, \tag{7b}$$

and

$$P^{ss}_{\vec{k},\vec{k}'} = \frac{(x/4\pi^2\hbar)\,|V^{ss}_{\vec{k},\vec{k}'}|}{|\nabla_{\vec{k}'}\epsilon_s|}, \tag{7c}$$

where

$$\begin{aligned}|V^{sn}_{\vec{k},\vec{k}'}|^2 &= |V^{ns}_{\vec{k}',\vec{k}}|^2 \\ &= \left|\int\sum_l e^{-i\vec{k}\cdot\vec{R}_l}\Psi^*_{n,\vec{k}'}(\vec{r}-\vec{R}_l)V_{\text{scat}}(r)\,e^{i\vec{k}\cdot\vec{r}}\chi^{\pm}\,d\tau\right|^2 \\ &\simeq \left|\int \Psi^*_{n,\vec{k}'}(r)V_{\text{scat}}(r)e^{i\vec{k}\cdot\vec{r}}\chi^{\pm}\,d\tau\right|^2,\end{aligned} \tag{8a}$$

and

$$|V^{ss}_{\vec{k},\vec{k}'}|^2 = \left|\int e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}V_{\text{scat}}(r)\,d^3r\right|^2\delta_{+,-}, \tag{8b}$$

where x is the impurity concentration (henceforth suppressed), $\vec{R}_l$ a lattice vector, $\vec{r}$ the position vector, $\chi^{\pm}$ the spin functions for minority- and majority-spin s electrons (positive and negative spin, respectively), and $d\tau$ designates an integration over both spatial and spin coordinates. These matrix elements are central to the magnetoresistance anisotropy and will be considered in detail below.

Eleven coupled integral equations for τ_n and τ_s are obtained upon demanding that the total rate of change of f be zero:

$$\begin{aligned}4\pi^2\hbar\vec{v}_s(\vec{k})\cdot\vec{E} = &-|\nabla_{\vec{k}}\epsilon_s|^{-1}\int\tau_s(\vec{k}')\vec{v}_s(\vec{k}')\cdot\vec{E}\,|V^{ss}_{\vec{k}',\vec{k}}|^2\,dS' + \tau_s(\vec{k})\vec{v}_s(\vec{k})\cdot\vec{E}\int|V^{ss}_{\vec{k},\vec{k}'}|^2|\nabla_{\vec{k}'}\epsilon_s|^{-1}\,dS' \\ &-|\nabla_{\vec{k}}\epsilon_s|^{-1}\sum_{n=1}^{10}\int\tau_n(\vec{k}')\vec{v}_n(\vec{k}')\cdot\vec{E}\,|V^{ns}_{\vec{k}',\vec{k}}|^2\,dS' + \tau_s(\vec{k})\vec{v}_s(\vec{k})\cdot\vec{E}\sum_{n=1}^{10}\int|V^{sn}_{\vec{k},\vec{k}'}|^2|\nabla_{\vec{k}'}\epsilon_n|^{-1}\,dS'\end{aligned} \tag{9a}$$

and

$$\begin{aligned}4\pi^2\hbar\vec{v}_n(\vec{k})\cdot\vec{E} = &-|\nabla_{\vec{k}}\epsilon_n|^{-1}\int\tau_s(\vec{k}')\vec{v}_s(\vec{k}')\cdot\vec{E}\,|V^{sn}_{\vec{k}',\vec{k}}|^2\,dS' + \tau_n(\vec{k})\vec{v}_n(\vec{k})\cdot\vec{E}\int|V^{ns}_{\vec{k},\vec{k}'}|^2|\nabla_{\vec{k}'}\epsilon_s|^{-1}\,dS' \\ &-|\nabla_{\vec{k}}\epsilon_n|^{-1}\sum_{n'=1}^{10}\int\tau_{n'}(\vec{k}')\vec{v}_{n'}(\vec{k}')\cdot\vec{E}\,|V^{n'n}_{\vec{k}',\vec{k}}|^2\,dS' + \tau_n(\vec{k})\vec{v}_n(\vec{k})\cdot\vec{E}\sum_{n'=1}^{10}\int|V^{nn'}_{\vec{k},\vec{k}'}|^2|\nabla_{\vec{k}'}\epsilon_n|^{-1}\,dS'.\end{aligned} \tag{9b}$$

The term $n' = n$ is included in the sum.

Two important approximations are now made. The first is that the density of d states is large compared to the density of s states, so that a simultaneous solution of these integral equations for τ_s and τ_n can be avoided:

$$\frac{1}{\tau_s(\vec{k})} \simeq \frac{1}{\tau_{sd}(\vec{k})} \equiv \frac{1}{4\pi^2\hbar}\sum_n\int\frac{|V^{sn}_{\vec{k},\vec{k}'}|^2}{|\nabla_{\vec{k}'}\epsilon_n|}\,dS'_n. \tag{10}$$

The second is that the d bands are mostly below the Fermi level so that the character of the d wave functions $\Psi_{n,\vec{k}}$ is not appreciably different from that at the top of the bands, which occurs at X. Recall that $V^{sn}_{\vec{k},\vec{k}'}$ depends on $\vec{k}'$ through the coefficients $a_{n,m}(\vec{k}')$ in $\Psi_{n,\vec{k}'}$. This approximation allows us to write

$$\begin{aligned}\frac{1}{\tau_{sd}(\vec{k})} &\simeq \frac{1}{4\pi^2\hbar}\sum_n|\nabla^{sn}_{\vec{k},\vec{k}'}|^2\int\frac{dS'_n}{|\nabla_{\vec{k}'}\epsilon_n|} \\ &= \frac{2\pi}{\hbar}\sum_n N_n(\epsilon_f)\,|V^{sn}_{\vec{k},\vec{k}'}|^2,\end{aligned} \tag{11}$$

where $\vec{k}'$ is $(2\pi/a, 0, 0)$, $(0, 2\pi/a, 0)$, or $(0, 0, 2\pi/a)$

as appropriate and $N_n(\epsilon_f)$ is the density of states at the Fermi energy for the nth surface. These approximations enormously simplify the calculation, but are not essential to the basic theory.

Thus, prior to considering the spin-orbit interaction, we assume that the Fermi surface consists of three relatively small hole surfaces centered on X, characterized by a large effective mass and spin $+\frac{1}{2}$, and a single electron surface for both spins, which we take to be spherical. We recognize that these two approximations are not strictly compatible for NiCu alloys since even for Ni one of the electron surfaces deriving from the 4s level touches the Brillouin zone boundary and resembles the Fermi surface of Cu. We believe, however, that the errors incurred by assuming a spherical surface largely cancel when calculating an *anisotropic* effect such as $(\rho_{\parallel}-\rho_{\perp})/\langle\rho\rangle_{\rm av}$.

When ss scattering is considered alone, as is appropriate when the d bands lie entirely below the Fermi level, the integral equations reduce to

$$\frac{1}{\tau_s}=\frac{1}{\tau_{ss}}\equiv\int\left(1-\frac{\vec{v}(\vec{k}')\cdot\vec{E}}{\vec{v}(\vec{k})\cdot\vec{E}}\right)P^{ss}_{\vec{k},\vec{k}'}\,dS' \,. \tag{12}$$

This equation has a well-known and $\vec{k}$-independent solution[20] when the Fermi surface is spherical and scattering is due to a spherically symmetrical potential.

When both scattering mechanisms are present, we avoid solving the coupled integral equations by invoking Matthiessen's rule,[21] which assumes the probabilities of ss and sd scattering are independent (which they are not):

$$\frac{1}{\tau_s(\vec{k})}=\frac{1}{\tau_{ss}}+\frac{1}{\tau_{sd}(\vec{k})} \,. \tag{13}$$

It must be emphasized, however, that this is not an exact solution to the integral equations.

III. SPIN-ORBIT INTERACTION AND BAND STRUCTURE

In the tight-binding approximation

$$\Psi^0_{n,\vec{k}}=\sum_{l,m}e^{i\vec{k}\cdot\vec{R}_l}a_{n,m}(\vec{k})\,\varphi_m(\vec{r}-\vec{R}_l) \tag{14}$$

where φ_m are the atomic wave functions

$$\begin{aligned}
&\varphi_1=yzf(r)\chi^-, && \varphi_6=yzf(r)\chi^+,\\
&\varphi_2=zxf(r)\chi^-, && \varphi_7=zxf(r)\chi^+,\\
&\varphi_3=xyf(r)\chi^-, && \varphi_8=xyf(r)\chi^+,\\
&\varphi_4=\tfrac{1}{2}(x^2-y^2)f(r)\chi^-, && \varphi_9=\tfrac{1}{2}(x^2-y^2)f(r)\chi^+,\\
&\varphi_5=\frac{1}{2\sqrt{3}}(3z^2-r^2)f(r)\chi^-, && \varphi_{10}=\frac{1}{2\sqrt{3}}(3z^2-r^2)f(r)\chi^+,
\end{aligned} \tag{15}$$

where $f(r)$ is a radial function, χ a spin function, and the superscript on $\Psi^0_{n,\vec{k}}$ emphasizes that these are the zero-order wave functions for the perturbation calculation that follows. Although more accurate self-consistently determined radial functions exist, it is sufficient for our purpose to take $f(r)$ proportional to a Laguerre polynomial divided by r^2:

$$f(r)=\left(\frac{15}{4\pi}\right)^{1/2}\frac{R_{3,2}(r)}{r^2}=\frac{1}{81}\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{Z}{a_0}\right)^{7/2}e^{-Zr/3a_0} \,, \tag{16}$$

where Z is an effective charge, reduced because of shielding. In our notation $a_{n,m}(\vec{k})$ is a block-diagonal 10×10 array with two equal 5×5 blocks. The elements of each block satisfy

$$\sum_m(H_{n,m}-E_n\delta_{n,m})a_{n,m}(\vec{k})=0, \quad n,\ m=1,2,3,4,5, \tag{17}$$

where $H_{n,m}$ is essentially a matrix element of the difference between the crystalline and isolated-atom potential. Fletcher[18] has calculated these coefficients for Ni, and finds that the top of the 3d band occurs at the symmetry points X on the Brillouin zone boundary [that is, at $(2\pi/a,\ 0,\ 0)$, $(0,\ 2\pi/a,\ 0)$, and $(0,\ 0,\ 2\pi/a)$]. His coefficients and energies at X are summarized in our notation in Table I.

The matrix elements of the spin-orbit interaction are

$$\langle\Psi^0_{n,\vec{k}}|K\vec{L}\cdot\vec{S}|\Psi^0_{n',\vec{k}'}\rangle=K\sum_{m,m'}a^*_{n,m}(\vec{k})a_{n',m'}(\vec{k})\times\langle\varphi_m|\vec{L}\cdot\vec{S}|\varphi_{m'}\rangle\delta_{\vec{k},\vec{k}'} \,, \tag{18}$$

provided the potential is predominantly radial in regions where the probability amplitude is large, and provided the "spin-other-orbit" interaction[22] is negligible. The matrix elements of $\vec{L}\cdot\vec{S}$ with the atomic states $\varphi_1=yzf(r)\chi^-$, etc., are evaluated by writing

$$\vec{L}\cdot\vec{S}=L_zS_z+\tfrac{1}{2}(L^+S^-+L^-S^+) \,, \tag{19}$$

where $L^{\pm}$ and $S^{\pm}$ are raising and lowering opera-

TABLE I. Tight-binding coefficients and energies at symmetry points X (from Fletcher, Ref. 18).

ϵ_n[a] or $a_{n,m}$[b]	$(2\pi/a,0,0)$	$(0,2\pi/a,0)$	$(0,0,2\pi/a)$
$\epsilon_1,\ \epsilon_6-2\gamma$	-2.6979	0	0
$\epsilon_2,\ \epsilon_7-2\gamma$	0	-2.6979	0
$\epsilon_3,\ \epsilon_8-2\gamma$	0	0.0	-2.6979
$\epsilon_4,\ \epsilon_9-2\gamma$	-0.0464[c]	-0.0464[c]	-0.0464[c]
$\epsilon_5,\ \epsilon_{10}-2\gamma$	-2.4303	-2.4303	-2.4303
$a_{1,1};\ a_{6,6}$	1	1	1
$a_{2,2};\ a_{7,7}$	1	1	1
$a_{3,3};\ a_{8,8}$	1	1	1
$a_{4,4};\ a_{9,9}$	1/2	$-1/2$	1
$a_{4,5},\ a_{9,10}$	$\sqrt{3}/2$	$\sqrt{3}/2$	0
$a_{5,4};\ a_{10,9}$	$-1/2$	1/2	0
$a_{5,5},\ a_{10,10}$	$\sqrt{3}/2$	$\sqrt{3}/2$	1

[a] In eV from top of d band.

[b] All unlisted coefficients are zero.

[c] More recent values are 0.27 (Ref. 2) and 0.14 (Ref. 4).

tors, and by rewriting the φ_m in terms of spherical harmonics. For example,

$$\varphi_2 = R_{3,2}(1/\sqrt{2})(Y_{2,1} - Y_{2,-1})\chi^- ,$$

$$\vec{L}\cdot\vec{S}\,|\varphi_2\rangle = R_{3,2}[-(1/2\sqrt{2})(Y_{2,1} + Y_{2,-1})\chi^- + (1/2\sqrt{2})(Y_{2,0} - Y_{2,-2})\chi^+]$$

$$= -\tfrac{1}{2}i\varphi_1 + \tfrac{1}{4}i\varphi_8 - \tfrac{1}{4}\varphi_4 + (1/2\sqrt{2})\varphi_{10} , \qquad (20)$$

giving

$$\langle\varphi_1\,|\vec{L}\cdot\vec{S}\,|\varphi_2\rangle = -\tfrac{1}{2}i . \qquad (21)$$

The remaining matrix elements are listed in Table II.

The first-order wave functions at $(2\pi/a,\ 0,\ 0)$ and $(0,\ 2\pi/a,\ 0)$ are

$$\Psi^1_{n,\vec{k}} = \Psi^0_{n,\vec{k}} + K\sum_{n'\neq n}\frac{\langle\Psi^0_{n',\vec{k}}|\vec{L}\cdot\vec{S}|\Psi^0_{n,\vec{k}}\rangle}{\epsilon_n(\vec{k}) - \epsilon_{n'}(\vec{k})}\Psi^0_{n',\vec{k}} \qquad (22)$$

or

$$\Psi^1_{n,\vec{k}} = \Psi^0_{n,\vec{k}} + K\sum_{n'\neq n,\,m,\,m'}\frac{a^*_{n',m'}(\vec{k})a_{n,m}(\vec{k})\langle\varphi_{m'}|\vec{L}\cdot\vec{S}|\varphi_m\rangle}{\epsilon_n(\vec{k}) - \epsilon_{n'}(\vec{k})} \times\Psi^0_{n',\vec{k}} . \qquad (23)$$

Tables I and II indicate that degenerate perturbation theory is needed at $(0,\ 0,\ 2\pi/a)$. This can be avoided by introducing new zeroth-order wave functions [for $(0,\ 0,\ 2\pi/a)$ only], given by Eq. (14) with

$$\begin{aligned} &a_{1,1} = a_{2,1} = a_{6,6} = a_{7,6} = 1/\sqrt{2} ,\\ &-a_{1,2} = a_{2,2} = a_{6,7} = -a_{7,7} = i/\sqrt{2} ,\\ &a_{3,3} = a_{4,4} = a_{5,5} = a_{8,8} = a_{9,9} = a_{10,10} = 1 ,\\ &(\text{all remaining } a\text{'s}) = 0 , \end{aligned} \qquad (24)$$

and by computing Ψ^1 from Eq. (22) using the matrix elements given in Table III.

The top of the d bands at the three nonequivalent points X is shown in Fig. 1. Let $\epsilon \equiv X_5 - X_2$ be the splitting between the twofold degenerate and nondegenerate bands and 2γ the uniform exchange splitting. The remaining bands are at least 2 eV lower and are neglected since only wave functions for the highest band are of interest. The first-order wave functions for $\vec{k}$ near X now can be written with the aid of Tables I, II, and III: at $\vec{k} = (2\pi/a,\ 0,\ 0)$,

$$\begin{aligned} \Psi^1_7 &= \Psi^0_7 + \sum_{n'}\frac{K}{\epsilon_7 - \epsilon_{n'}}\left[\tfrac{1}{4}a^*_{n',3} + \tfrac{1}{4}a^*_{n',4} - (1/2\sqrt{2})a^*_{n',5} + \tfrac{1}{2}ia^*_{n',6}\right]\Psi^0_{n'} \\ &\simeq \Psi^0_7 + \frac{i}{4}\frac{K}{2\gamma}\Psi^0_3 + \frac{1-\sqrt{6}}{8}\frac{K}{2\gamma+\epsilon}\Psi^0_4 \\ &= \sum_l e^{i2\pi R_{x,l}/a}\varphi^{(x)}_7(\vec{r} - \vec{R}_l) , \end{aligned} \qquad (25)$$

where

$$\varphi^{(x)}_7 = \varphi_7 + \frac{i}{4}\frac{K}{2\gamma}\varphi_3 + \frac{1-\sqrt{6}}{16}\frac{K}{2\gamma+\epsilon}(\varphi_4 + \sqrt{3}\varphi_5) \qquad (26a)$$

and where terms with energy denominators greater than $2\gamma + \epsilon$ have been dropped. Similarly,

$$\varphi^{(x)}_8 = \varphi_8 - \frac{i}{4}\frac{K}{2\gamma}\varphi_2 - \frac{i}{4}\frac{K}{\epsilon}(\varphi_9 + \sqrt{3}\varphi_{10}) . \qquad (26b)$$

At $\vec{k} = (0,\ 2\pi/a,\ 0)$,

$$\varphi^{(y)}_6 = \varphi_6 + \frac{1}{4}\frac{K}{2\gamma}\varphi_3 + i\frac{1-\sqrt{6}}{16}\frac{K}{2\gamma+\epsilon}(-\varphi_4 + \sqrt{3}\varphi_5) \qquad (26c)$$

and

$$\varphi^{(y)}_8 = \varphi_8 - \frac{1}{4}\frac{K}{2\gamma}\varphi_1 + \frac{i}{4}\frac{K}{\epsilon}(-\varphi_9 + \sqrt{3}\varphi_{10}) . \qquad (26d)$$

At $\vec{k} = (0,\ 0,\ 2\pi/a)$,

$$\varphi^{(z)}_6 = \frac{1}{\sqrt{2}}\varphi_6 + \frac{i}{\sqrt{2}}\varphi_7 \qquad (26e)$$

TABLE II. Matrix elements $\langle\varphi_{m'}|\vec{L}\cdot\vec{S}|\varphi_m\rangle$.

m' \ m	1	2	3	4	5	6	7	8	9	10
1		$-\frac{i}{2}$						$-\frac{1}{4}$	$\frac{i}{4}$	$\frac{i}{2\sqrt{2}}$
2	$\frac{i}{2}$							$-\frac{i}{4}$	$-\frac{1}{4}$	$\frac{1}{2\sqrt{2}}$
3				$-i$		$\frac{1}{4}$	$\frac{i}{4}$			
4			i			$-\frac{i}{4}$	$\frac{1}{4}$			
5						$\frac{i}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$			
6			$\frac{1}{4}$	$\frac{i}{4}$	$\frac{i}{2\sqrt{2}}$		$\frac{i}{2}$			
7			$-\frac{i}{4}$	$\frac{1}{4}$	$\frac{1}{2\sqrt{2}}$	$-\frac{i}{2}$				
8	$-\frac{1}{4}$	$\frac{i}{4}$							i	
9	$-\frac{i}{4}$	$-\frac{1}{4}$						$-i$		
10	$\frac{i}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$								

TABLE III. Matrix elements $\langle\Psi^0_{n',\vec{k}}|\vec{L}\cdot\vec{S}|\Psi^0_{n,\vec{k}}\rangle$ at $\vec{k} = (0,\ 0,\ 2\pi/a)$.

n' \ n	1	2	3	4	5	6	7	8	9	10
1	$-\frac{1}{2}$									
2		$\frac{1}{2}$						$\frac{1}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$\frac{i}{2}$
3				$-i$			$\frac{1}{2\sqrt{2}}$			
4			i				$-\frac{i}{2\sqrt{2}}$			
5							$-\frac{i}{2}$			
6						$-\frac{1}{2}$				
7			$\frac{1}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$\frac{i}{2}$		$\frac{1}{2}$			
8		$-\frac{1}{2\sqrt{2}}$							i	
9		$-\frac{i}{2\sqrt{2}}$						$-i$		
10		$-\frac{i}{2}$								

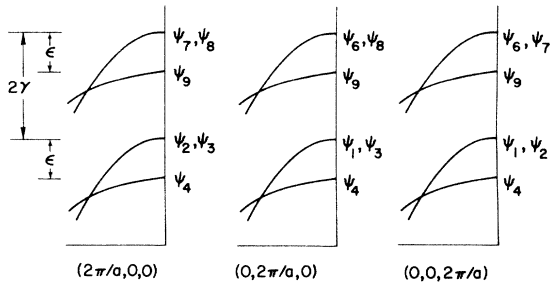

FIG. 1. Labeling of wave functions at X.

and

$$\varphi_7^{(z)} = \frac{1}{\sqrt{2}}\varphi_6 - \frac{i}{\sqrt{2}}\varphi_7 - \frac{i}{2\sqrt{2}}\frac{K}{2\gamma+\epsilon}\varphi_4 . \tag{26f}$$

IV. SCATTERING POTENTIAL MATRIX ELEMENTS AND τ_{sd}

Let the nuclear charge of the impurity differ from that of the host lattice by $e\Delta Z$, with ΔZ about 1 or 2 so that the Born approximation remains valid, and consider scattering due to the spherically symmetrical scattering potential

$$V(r) = (\Delta Z e^2/r)e^{-qr} . \tag{27}$$

The matrix elements of $V(r)$ involve integrals of the form

$$\begin{aligned}\int e^{i\vec{k}\cdot\vec{r}} V(r) f(r) x_i x_j d^3r &= -\frac{\partial^2}{\partial k_i \partial k_j}\int e^{i\vec{k}\cdot\vec{r}} V(r) f(r)\, d^3r \\ &= \frac{4(2\pi)^{1/2}\Delta Z e^2}{81}\frac{\partial^2}{\partial k_i \partial k_j}\frac{1}{k^2+(q+Z/3a_0)^2} \\ &= C_{sd}\left[\tfrac{1}{4}(k_f^2+q^2)\delta_{ij} - k_i k_j\right]\end{aligned} \tag{28}$$

where $f(r)$ is given by Eq. (16), $x_i = x$, y, or z, and the constant is

$$C_{sd} = \frac{32(2\pi)^{1/2}\Delta Z e^2}{81(k_f^2+q^2)[k_f^2+(q+Z/3a_0)^2]^2}\left(\frac{Z}{a_0}\right)^{7/2} . \tag{29}$$

The matrix elements for $\vec{k} = (2\pi/a,\ 0,\ 0)$, $(0,\ 2\pi/a,\ 0)$, and $(0,\ 0,\ 2\pi/a)$ are denoted by superscripts x, y, and z, respectively. A subscript + or − indicates the s-electron spin, which now must be explicitly considered. Those matrix elements relevant to the top of the d bands are

$$\begin{aligned}|V_{-,7}^{(x)}|^2 &= \left|\int \varphi_7^{(x)} V(r) e^{i\vec{K}\cdot\vec{r}}\chi^- d\tau\right|^2 \\ &= \left|\frac{i}{4}\frac{K}{2\gamma}\int xyf(r)V(r)e^{i\vec{K}\cdot\vec{r}}d^3r \right. \\ &\quad \left. + \frac{1-\sqrt{6}}{16}\frac{K}{2\gamma+\epsilon}\int (z^2-y^2)f(r)V(r)e^{i\vec{K}\cdot\vec{r}}d^3r\right|^2 \\ &= C_{sd}^2\left[\frac{1}{16}\left(\frac{K}{2\gamma}\right)^2 k_x^2k_y^2 + \left(\frac{1-\sqrt{6}}{16}\right)^2\left(\frac{K}{2\gamma+\epsilon}\right)^2 \right. \\ &\quad \left. \times (k_z^2-k_y^2)^2\right],\end{aligned} \tag{30a}$$

$$|V_{+,7}^{(x)}|^2 = C_{sd}^2 k_z^2k_x^2 , \tag{30b}$$

$$|V_{-,8}^{(x)}|^2 = C_{sd}^2 \tfrac{1}{16}(K/2\gamma)^2 k_z^2k_x^2 , \tag{30c}$$

$$|V_{+,8}^{(x)}|^2 = C_{sd}^2\left[k_x^2k_y^2 + \tfrac{1}{16}(K/\epsilon)^2(k_z^2-k_y^2)^2\right], \tag{30d}$$

$$\begin{aligned}|V_{-,6}^{(y)}|^2 &= C_{sd}^2\left[\frac{1}{16}\left(\frac{K}{2\gamma}\right)^2 k_x^2k_y^2 \right. \\ &\quad \left. + \left(\frac{1-\sqrt{6}}{16}\right)^2\left(\frac{K}{2\gamma+\epsilon}\right)^2 (k_z^2-k_x^2)^2\right],\end{aligned} \tag{30e}$$

$$|V_{+,6}^{(y)}|^2 = C_{sd}^2 k_y^2k_z^2 , \tag{30f}$$

$$|V_{-,8}^{(y)}|^2 = C_{sd}^2 \tfrac{1}{16}(K/2\gamma)^2 k_y^2k_z^2 , \tag{30g}$$

$$|V_{+,8}^{(y)}|^2 = C_{sd}^2\left[k_x^2k_y^2 + \tfrac{1}{16}(K/\epsilon)^2(k_z^2-k_x^2)^2\right], \tag{30h}$$

$$|V_{-,6}^{(z)}|^2 = 0 , \tag{30i}$$

$$|V_{+,6}^{(z)}|^2 = C_{sd}^2(\tfrac{1}{2}k_y^2k_z^2 + \tfrac{1}{2}k_z^2k_x^2) , \tag{30j}$$

$$|V_{-,7}^{(z)}|^2 = C_{sd}^2\frac{1}{32}\left(\frac{K}{2\gamma+\epsilon}\right)^2 (k_x^2-k_y^2)^2 , \tag{30k}$$

and

$$|V_{+,7}^{(z)}|^2 = C_{sd}^2(\tfrac{1}{2}k_y^2k_z^2 + \tfrac{1}{2}k_z^2k_x^2) . \tag{30l}$$

According to Eq. (11) the reciprocal sd relaxation time for minority-spin or majority-spin s electrons is proportional to the sum of $|V_+|^2$ or $|V_-|^2$, respectively. Upon taking the sum and after a modest amount of algebra, we obtain

$$\frac{1}{\tau_{s+d}} = \frac{4\pi}{\hbar}C_{sd}^2 N_d\left[k_y^2k_z^2 + k_z^2k_x^2 + k_x^2k_y^2 + \frac{1}{96}\left(\frac{K}{\epsilon}\right)^2\left[(k_y^2-k_z^2)^2 + (k_z^2-k_x^2)^2 + (k_x^2-k_y^2)^2\right] + \frac{1}{96}\left(\frac{K}{\epsilon}\right)^2(2k_z^2-k_x^2-k_y^2)^2\right] \tag{31a}$$

and

$$\begin{aligned}\frac{1}{\tau_{s-d}} = \frac{4\pi}{\hbar}C_{sd}^2 N_d\left\{\frac{1}{16}\left(\frac{K}{2\gamma}\right)^2(k_y^2k_z^2 + k_z^2k_x^2 + k_x^2k_y^2) + \frac{1}{6}\left[\frac{1}{8} + \left(\frac{1-\sqrt{6}}{16}\right)^2\right]\left(\frac{K}{2\gamma+\epsilon}\right)^2\left[(k_y^2-k_z^2)^2 + (k_z^2-k_x^2)^2 + (k_x^2-k_y^2)^2\right]\right. \\ \left. - \frac{1}{6}\left[\frac{1}{16} - \left(\frac{1-\sqrt{6}}{16}\right)^2\right]\left(\frac{K}{2\gamma+\epsilon}\right)^2(2k_z^2-k_x^2-k_y^2)^2 - \frac{1}{32}\left(\frac{K}{2\gamma}\right)^2(k_x^2+k_y^2)k_z^2\right\} .\end{aligned} \tag{31b}$$

It is assumed in Eqs. (31a) and (31b) that each of the three hole pockets contributes equally to the total density of d states, N_d. This is not strictly true, because the spin-orbit interaction splits the

twofold degenerate band near (0, 0, $2\pi/a$) by an amount K (Table III) and enlarges the pocket centered about this point. When the Fermi energy is so high that the remaining two pockets disappear, the *sd* relaxation times simplify to

$$\frac{1}{\tau_{s+d}} = \frac{2\pi}{\hbar} C_{sd}^2 N_d (k_x^2 + k_y^2) k_z^2 \tag{31c}$$

and

$$\frac{1}{\tau_{s-d}} = \frac{\pi}{8\hbar} C_{sd}^2 N_d \left(\frac{K}{2\gamma + \epsilon}\right)^2 (k_x^2 - k_y^2)^2 . \tag{31d}$$

At this point several observations can be made. The first is that both $1/\tau_{s+d}$ and $1/\tau_{s-d}$ consist of cubic-symmetry terms and anisotropic terms that are a function of the polar angle θ alone, as required by the symmetry of the system. For example, when only one hole surface exists $1/\tau_{s+d}$ [Eq. (31c)] varies as $\sin^2\theta\cos^2\theta$ or $\cos 4\theta$. Second, as observed by Smit, the spin-orbit interaction allows *sd* scattering for majority-spin electrons. But, contrary to what Smit found, this more detailed calculation indicates that

$$\frac{1}{\tau_{s-d}(\theta = 0)} < \frac{1}{\tau_{s-d}(\theta = \pi/2)} \tag{32a}$$

[for both Eqs. (31b) and (31d)], which implies $\rho_\parallel < \rho_\perp$ if the anisotropy is due to majority-spin electrons. However,

$$\frac{1}{\tau_{s+d}(\theta = 0)} \geq \frac{1}{\tau_{s+d}(\theta = \pi/2)} \tag{32b}$$

which leads us to believe that in the preponderance of alloy systems, where experimentally $\rho_\parallel > \rho_\perp$, the resistance anisotropy is dominated by the scattering of minority-spin electrons. It is reasonable that *a priori* the two effects should be of comparable magnitude, because just as the spin-orbit interaction increases the density of available majority-spin d states at the Fermi energy, it also decreases the density of minority-spin states.

V. CALCULATION OF THE CURRENT

The assumption that spin is conserved during scattering allows the conductivities for minority- and majority-spin electrons to be computed independently and then added. The conduction of d electrons is neglected. Symmetry considerations[23] indicate that the final result must have the form $\sigma = \sigma_0 + \sigma_2 \cos 2\theta + \sigma_4 \cos 4\theta$, where θ is the angle between the electric field and the z-directed magnetization. The coefficient of $\cos 2\theta$ is obtained by calculating $\sigma_{zz} \equiv \sigma_\parallel$ and $\sigma_{xx} \equiv \sigma_\perp$. The coefficient of $\cos 4\theta$ is smaller and this term vanishes upon taking a polycrystalline average. It is not considered here.

The required conductivity integrals are

$$\sigma_\parallel^\pm = \frac{3 n_{s\pm} e^2}{4\pi m_s} \int_0^\pi d\theta \int_0^{2\pi} d\phi\, \tau_{s\pm}(\theta, \phi) \cos^2\theta \sin\theta \tag{33a}$$

and

$$\sigma_\perp^\pm = \frac{3 n_{s\pm} e^2}{4\pi m_s} \int_0^\pi d\theta \int_0^{2\pi} d\phi\, \tau_{s\pm}(\theta, \phi) \sin^3\theta \cos^2\phi , \tag{33b}$$

where

$$\tau_{s\pm}(\theta, \phi) = [1/\tau_{ss} + 1/\tau_{s\pm d}(\theta, \phi)]^{-1} . \tag{34}$$

Departures from a Fermi surface with cubic symmetry are ignored for now and $1/\tau_{s\pm d}$ are given by Eqs. (31a) and (31b). The effect of lower symmetry is discussed below. The quantity

$$\frac{1}{\tau_{ss}} = \frac{2\pi N_s(\epsilon_f)(\Delta Z)^2 e^4}{\hbar k_f} \left(\ln\frac{4k_f^2 + q^2}{q^2} - \frac{4k_f^2}{4k_f^2 + q^2}\right) \tag{35}$$

is the standard expression[22] for ss scattering (with impurity concentration x in numerator suppressed) where $e\Delta Z$ is the difference in nuclear charge, q the screening parameter in the screened Coulomb potential, and $N_s(\epsilon_f)$ the density of s states counting both spins.

The majority-spin electronic conductivity is limited mostly by ss scattering and is the easier of the two to calculate. An expansion of τ_{s-} is possible (for σ^- only) because all terms in $1/\tau_{s-d}$ are of order $(K/2\gamma)^2$ or $[K/(2\gamma + \epsilon)]^2$. The term in $1/\tau_{s-d}$ proportional to $(k_y^2 - k_z^2)^2 + (k_z^2 - k_x^2)^2 + (k_x^2 - k_y^2)^2$ can be eliminated in favor of a more tractable one involving $k_x^4 + k_y^4 + k_z^4$ through use of simple identities, giving, in spherical coordinates,

$$\tau_{s-} \simeq \tau_{ss} - \frac{4\pi\tau_{ss}^2 C_{sd}^2 k_f^5}{\hbar k_f} \frac{N_d}{N_s} \left\{ \left[\frac{1}{16}\left(\frac{K}{2\gamma}\right)^2 - \frac{39 - 2\sqrt{6}}{24\times 32}\left(\frac{K}{2\gamma + \epsilon}\right)^2\right](\sin^2\theta\cos^2\theta + \sin^2\phi\cos^2\phi\sin^4\theta) \right.$$
$$\left. + \frac{39 - 2\sqrt{6}}{24\times 32}\left(\frac{K}{2\gamma + \epsilon}\right)^2 (\cos^4\phi\sin^4\theta + \sin^4\phi\sin^4\theta + \cos^4\theta) - \frac{9 - 2\sqrt{6}}{48\times 32}\left(\frac{K}{2\gamma + \epsilon}\right)^2 (3\cos^2\theta - 1)^2 - \frac{1}{32}\left(\frac{K}{2\gamma}\right)^2 \sin^2\theta\cos^2\theta \right\} . \tag{36}$$

The integrations for $\sigma_\parallel^-$ and $\sigma_\perp^-$ are elementary, and the results are

$$\sigma_\parallel^- = \sigma_0 \left\{1 - \frac{1}{140\beta}\frac{N_d}{N_s}\left[\left(\frac{K}{2\gamma}\right)^2 + \frac{5 + 2\sqrt{6}}{24}\left(\frac{K}{2\gamma + \epsilon}\right)^2\right]\right\} \tag{37a}$$

and

$$\sigma_{\perp}^{-}=\sigma_0\left\{1-\frac{1}{140\beta}\frac{N_d}{N_s}\left[\frac{5}{4}\left(\frac{K}{2\gamma}\right)^2+\frac{19-2\sqrt{6}}{8}\left(\frac{K}{2\gamma+\epsilon}\right)^2\right]\right\}, \tag{37b}$$

where $\sigma_0=n_{s+}e^2\tau_{ss}/m_s=n_{s-}e^2\tau_{ss}/m_s$ and the dimensionless constant β (which also appears in σ^+) is defined as

$$\beta=\frac{\hbar k_f}{4\pi k_f^5 C_{sd}^2 N_s \tau_{ss}}=\frac{3}{32\pi}\left(\frac{3k_f a_0}{2Z}\right)^7\left(1+\frac{q^2}{k_f^2}\right)^2\left[1+\left(\frac{Z+3qa_0}{3k_f a_0}\right)^2\right]^4\left(\ln\frac{4k_f^2+q^2}{q^2}-\frac{4k_f^2}{4k_f^2+q^2}\right). \tag{38}$$

where a_0 is the Bohr radius. Note that $\sigma_{\perp}^{-}<\sigma_{\parallel}^{-}$.

The probability of *sd* scattering for minority-spin electrons is large, especially for those with $\vec{k}$ vectors near the $\langle 111\rangle$ axes, since the existence of available *d* states does not depend solely on the spin-orbit interaction. This precludes an expansion of τ_{s+d} similar to the one used for τ_{s-d} and requires the evaluation of integrals of the form

$$\sigma^{+}\propto\frac{1}{N_d}\int\frac{k_x^2k_f^2\sin\theta\,d\theta\,d\phi}{k_y^2k_z^2+k_z^2k_x^2+k_x^2k_y^2+k_f^4[(K/\epsilon)^2f(\theta,\phi)+\beta N_s/N_d]}, \tag{39}$$

where the sought-after anisotropy resides in $f(\theta,\phi)$ and $\beta N_s/N_d$ is a term due to *ss* scattering. The second term in $1/\tau_{s+d}$ [Eq. (31a)] is small and of cubic symmetry and can be replaced by $k_f^4(K/\epsilon)^2/48$ with the result that $f(\theta,\phi)$ becomes a function of θ alone. The ϕ integrations now can be performed by contour integration with results as follows:

$$\sigma_{\parallel}^{+}=\sigma_0\frac{3\beta}{4\pi}\frac{N_s}{N_d}\int_0^{\pi}d\theta\frac{\cos^2\theta}{\sin^3\theta}\int_0^{2\pi}d\phi\frac{1}{\sin^2\phi\cos^2\phi+g(\theta)}=\sigma_0 12\beta\frac{N_s}{N_d}\int_0^{\pi}d\theta\frac{\cos^2\theta}{\sin^3\theta\{[1+8g(\theta)]^2-1\}^{1/2}}$$

$$=\sigma_0 3\beta\frac{N_s}{N_d}\int_0^{\pi}d\theta\frac{\cos^2\theta\sin\theta}{\{[\sin^2\theta\cos^2\theta+\lambda(\theta)][\sin^4\theta+4\sin^2\theta\cos^2\theta+4\lambda(\theta)]\}^{1/2}}, \tag{40a}$$

and

$$\sigma_{\perp}^{+}=\sigma_0\frac{3\beta}{4\pi}\frac{N_s}{N_d}\int_0^{\pi}d\theta\frac{1}{\sin\theta}\int_0^{2\pi}d\phi\frac{\cos^2\phi}{\sin^2\phi\cos^2\phi+g(\theta)}=\sigma_0 6\beta\frac{N_s}{N_d}\int_0^{\pi}d\theta\frac{1}{\sin\theta\{[1+8g(\theta)]^2-1\}^{1/2}}$$

$$=\sigma_0\frac{3\beta}{2}\frac{N_s}{N_d}\int_0^{\pi}d\theta\frac{\sin^3\theta}{\{[\sin^2\theta\cos^2\theta+\lambda(\theta)][\sin^4\theta+4\sin^2\theta\cos^2\theta+4\lambda(\theta)]\}^{1/2}}, \tag{40b}$$

where the functions $g(\theta)$ and $\lambda(\theta)$, introduced for brevity, are defined by

$$g(\theta)=\frac{\cos^2\theta}{\sin^2\theta}+\frac{\lambda(\theta)}{\sin^4\theta} \tag{40c}$$

and

$$\lambda(\theta)=\frac{1}{48}\left(\frac{K}{\epsilon}\right)^2+\frac{1}{96}\left(\frac{K}{\epsilon}\right)^2(3\cos^2\theta-1)^2+\beta\frac{N_s}{N_d}. \tag{40d}$$

The remaining integrations over θ are worse than elliptic even for the special case where $\lambda(\theta)$ is replaced by a constant. The maximum value of $\lambda(\theta)$ is small compared to unity but the integrals diverge as λ_{max} approaches zero. The major contribution $\sigma_{\parallel}^{+}$ and $\sigma_{\perp}^{+}$ occurs near $\theta=0$ or $\pi/2$, respectively. The approach taken is to determine the asymptotic form of σ^{+} for constant λ and then replace λ by $\lambda(0)$ or $\lambda(\pi/2)$ as appropriate. It is shown in the Appendix that

$$\sigma_{\parallel}^{+}\text{ and }\sigma_{\perp}^{+}\underset{\lambda\to 0}{\longrightarrow}-\sigma_0\frac{3\sqrt{3}\beta}{2}\frac{N_s}{N_d}\ln\lambda. \tag{41}$$

This gives

$$\sigma_{\parallel}^{+}=-\sigma_0\frac{3\sqrt{3}\beta}{2}\frac{N_s}{N_d}\ln\left[\frac{1}{16}\left(\frac{K}{\epsilon}\right)^2+\beta\frac{N_s}{N_d}\right] \tag{42a}$$

and

$$\sigma_{\perp}^{+}=-\sigma_0\frac{3\sqrt{3}\beta}{2}\frac{N_s}{N_d}\ln\left[\frac{1}{32}\left(\frac{K}{\epsilon}\right)^2+\beta\frac{N_s}{N_d}\right], \tag{42b}$$

with $\sigma_{\perp}^{+}>\sigma_{\parallel}^{+}$.

The final portion of the calculation consists of adding the spin-up and spin-down currents and computing $\Delta\rho/\langle\rho\rangle_{av}$. The result is

$$\frac{\Delta\rho}{\langle\rho\rangle_{av}}=\frac{\rho_{\parallel}-\rho_{\perp}}{\frac{1}{3}\rho_{\parallel}+\frac{2}{3}\rho_{\perp}}=\frac{3(\sigma_{\perp}-\sigma_{\parallel})}{\sigma_{\perp}+2\sigma_{\parallel}}, \tag{43}$$

where

$$\sigma_{\parallel}=\sigma_0\left\{1-\frac{1}{140\beta}\frac{N_d}{N_s}\left[\left(\frac{K}{2\gamma}\right)^2+\frac{5+2\sqrt{6}}{24}\left(\frac{K}{2\gamma+\epsilon}\right)^2\right]-\frac{3\sqrt{3}\beta}{2}\frac{N_s}{N_d}\ln\left[\frac{1}{16}\left(\frac{K}{\epsilon}\right)^2+\beta\frac{N_s}{N_d}\right]\right\} \tag{44a}$$

and

$$\sigma_{\perp}=\sigma_0\left\{1-\frac{1}{140\beta}\frac{N_d}{N_s}\left[\frac{5}{4}\left(\frac{K}{2\gamma}\right)^2+\frac{19-2\sqrt{6}}{8}\left(\frac{K}{2\gamma+\epsilon}\right)^2\right]-\frac{3\sqrt{3}\beta}{2}\frac{N_s}{N_d}\ln\left[\frac{1}{32}\left(\frac{K}{\epsilon}\right)^2+\beta\frac{N_s}{N_d}\right]\right\}. \tag{44b}$$

These expressions are applicable only when the second terms and the arguments of the logarithms

are small compared to unity.

VI. DISCUSSION

The resistivity anisotropy $\Delta\rho/\langle\rho\rangle_{av}$ is basically a second-order effect. The magnetization affects the wave functions to first order in $K/\Delta\epsilon$ through the spin-orbit interaction, where $\Delta\epsilon$ is an energy separation between bands. The electron scattering probabilities involve $(K/\Delta\epsilon)^2$ and are computed using the perturbed wave functions and Born approximation. These probabilities appear in a set of 11 coupled integral equations for the Fermi distribution functions or, in this formalism, relaxation times. Only the relaxation times τ_{s+} and τ_{s-} for s-like electrons of both spins are considered because the effective mass of d electrons is large. The elements σ_{ij} of the conductivity tensor are found by integrating $k_i k_j \tau_{s-}(\vec{k})$ and $k_i k_j \tau_{s+}(\vec{k})$ over spherical Fermi surfaces and adding the results.

The purpose of the calculation is to indicate those features of the band structure likely to be important in causing a large resistivity anisotropy in NiCu alloys and to outline the course that a more general calculation for other alloys might take. In the interest of carrying the calculation through to a conclusion, a number of simplifying assumptions and approximations are made. Matthiessen's rule is invoked in place of a solution to the coupled integral equations. The Fermi level is assumed to be near the top of the d bands so that an additional integration involving the $\vec{k}$ dependence of the tight-binding wave-function coefficients $a_{n,m}(\vec{k})$ is not required. The least important approximations are those relating to the cubic-symmetry aspects of the problem, for example, the assumption of spherical Fermi surfaces for the s electrons. More important are those approximations that affect the anisotropy directly, such as taking the three hole pockets to be of equal size, as is done throughout most of the calculation. In view of the foregoing, predicted values of $\Delta\rho/\langle\rho\rangle_{av}$ can only be regarded as qualitative.

Values for the band parameters $2\gamma = \Delta\Gamma_{25'}$ and $\epsilon = X_5 - X_2$ are obtainable from recent self-consistent calculations for ferromagnetic nickel. Connolly's APW calculation[2] using an averaged exchange potential of $\frac{2}{3}$ the free-electron value gives $2\gamma = 0.81$ and $\epsilon = 0.27$ eV. Callaway and Wang[4] obtain $2\gamma = 0.70$ and $\epsilon = 0.14$ eV using the tight-binding method. Both values of ϵ are so close to the spin-orbit energy[24] $K = 0.1$ eV that the use of first-order perturbation theory would not be justified in a rigorous calculation. With this difficulty in mind we adopt the ratios $K/\epsilon = \frac{1}{3}$ and $K/(2\gamma+\epsilon) = \frac{1}{11}$.

The constant β gives the importance of ss scattering relative to sd scattering for fixed N_d/N_s. It is a sensitive function of Fermi wave vector k_F, effective charge Z, and screening length $1/q$. Based on $Z = 3$, the nearly-free-electron value $k_F = 0.60 \times 10^8$ cm^{-1} (lattice constant 3.52 Å, 0.54 electrons/atom) and the Thomas-Fermi estimate[25] of the electron screening length $1/q = 0.60 \times 10^{-8}$ cm, Eq. (38) gives $\beta = 0.36$. The value of β is not critical to understanding the predictions of the theory because β enters only as $N_d/\beta N_s$.

An estimate of N_d/N_s as a function of percentage Cu in Ni can be made assuming rigid bands and using Callaway and Wang's[4] density of states curves for Ni. The Fermi level for Ni is such that the addition of Cu first increases and then decreases N_d, while N_s is nearly constant. Precise values are difficult to obtain from the figures, but the behavior is roughly given by (in units of electron states/atom Ry)

$$N_s = 4 \quad \text{(counting both spins)}, \tag{45}$$

$$N_d(\epsilon) = \begin{cases} 20 + 1000\epsilon & (0 \le \epsilon \le 0.01) \\ 45 - 1500\epsilon & (0.01 \le \epsilon \le 0.03) \end{cases}$$

where ϵ (in rydbergs) is measured upwards from the Fermi energy of pure Ni. The percentage of Cu which raises the Fermi energy by an amount $\Delta\epsilon_f$ is

$$100 \int_0^{\Delta\epsilon_f} [N_s + N_d(\epsilon)]\, d\epsilon\,. \tag{46}$$

This gives $N_d/N_s = 5$ for pure Ni, $N_d/N_s = 7.5$ (the maximum value) at 29-at.% Cu, $N_d/N_s = 3.75$ at 54-at.% Cu, and $N_d/N_s = 0$ at 65-at.% Cu.

The averaged conductivities of minority- and majority-spin electrons, $\langle\sigma^{\pm}\rangle_{av} \equiv \frac{1}{3}\sigma_{\parallel}^{\pm} + \frac{2}{3}\sigma_{\perp}^{\pm}$, are shown in Fig. 2 as a function of $N_d/\beta N_s$, and the resistivity anisotropy $\Delta\rho/\langle\rho\rangle_{av}$ appears in Fig. 3. According to the estimates given above, nearly pure Ni would correspond to $N_d/\beta N_s = 14$, and Ni_{71}-Cu_{29} to $N_d/\beta N_s = 21$. There is considerable uncer-

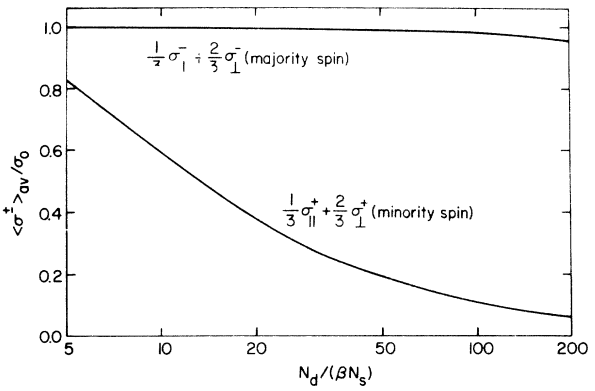

FIG. 2. Averaged and normalized conductivity for majority- and minority-spin electrons according to Eqs. (37) and (42) with $K/\epsilon = 1/3$ and $K/(2\gamma+\epsilon) = 1/11$. Constant β is about 0.36 and depends on screening length and radial portion of d wave functions.

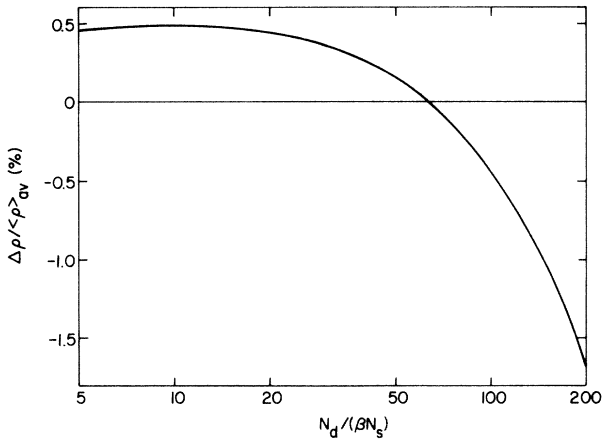

FIG. 3. Normalized resistivity anisotropy according to Eqs. (43) and (44). $N_d/(\beta N_s)=20$ corresponds to about Ni_{70}-Cu_{30} (see text).

tainty in this correspondence, mostly because of β, and for this reason the results are not reexpressed in terms of alloy composition. Note that $N_d/\beta N_s$ is not a monotonic function of percent Cu.

The prediction $\Delta\rho/\langle\rho\rangle_{av}=0.44\%$ for Ni_{71}-Cu_{29} is in good (perhaps fortuitous) agreement with the experimental result[26] 0.37% for Ni_{70}-Cu_{30}.

These curves are obtained by ignoring the distortion of the Fermi surface caused by the spin-orbit interaction, and they overestimate $\Delta\rho/\langle\rho\rangle_{av}$ for small $N_d/\beta N_s$. As $N_d/\beta N_s$ approaches zero Eqs. (31c) and (31d) become appropriate, since these equations apply for a single hole surface. Also, σ^+ must be reevaluated, as it was assumed $N_d/\beta N_s \gg 1$. It is clear from Eqs. (31c) and (31d) that this extension of the calculation would lower $\Delta\rho/\langle\rho\rangle_{av}$ for small $N_d/\beta N_s$, because $1/\tau_{s+d}$ [Eq. (31c)] varies as $\cos 4\theta$ and makes no contribution to $\Delta\rho$, whereas $1/\tau_{s-d}(0) < 1/\tau_{s-d}(\pi/2)$ [Eq. (31d)]. In fact, the model predicts that $\Delta\rho/\langle\rho\rangle_{av}$ should be negative and very small when $N_d/\beta N_s \simeq 0$.

The reason for the sudden decrease in $\Delta\rho/\langle\rho\rangle_{av}$ for large $N_d/\beta N_s$ is related to the assumption that the hole pockets are so small that d states at the Fermi energy can be approximated by states at X. A near degeneracy (small ϵ) involving these states is very effective in producing a large and positive $\Delta\rho/\langle\rho\rangle_{av}$. A similar observation regarding degeneracies has been made by Berger.[15] The two highest d bands for pure nickel, which are separated by less than 0.3 eV at X, cross very near the Fermi level. It is clear, therefore, that as the percentage of copper in nickel decreases, ϵ will decrease and $\Delta\rho/\langle\rho\rangle_{av}$ will continue to increase in accordance with the experimental result. On the other hand, for small values of β and under certain additional conditions, the theory does indeed predict a negative $\Delta\rho/\langle\rho\rangle_{av}$. It is notable that a negative value is observed in at least one alloy of nickel[26]: $\Delta\rho/\langle\rho\rangle_{av}=-0.24\%$ for $Ni_{93.75}$-$Cr_{6.25}$ at 14 °K.

In conclusion, we find that the role of the majority-spin current is to drive $\Delta\rho/\langle\rho\rangle_{av}$ negative and that a *positive* $\Delta\rho/\langle\rho\rangle_{av}$ can arise only from the *minority-spin* current. The spin-orbit interaction allows majority-spin electrons to scatter into d states as previously observed by Smit. It also causes, with roughly equal effectiveness, an anisotropy in the scattering of minority-spin electrons (those that could scatter without this interaction), and this is the mechanism that we believe is important in NiCu alloys at low temperature.

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APPENDIX

The integrals under consideration are

$$I_{\parallel}=\int_0^{\pi}\frac{\cos^2\theta\sin\theta\,d\theta}{\{[\sin^2\theta\cos^2\theta+\lambda(\theta)][\sin^4\theta+4\sin^2\theta\cos^2\theta+4\lambda(\theta)]\}^{1/2}} \tag{A1a}$$

and

$$I_{\perp}=\int_0^{\pi}\frac{\sin^3\theta\,d\theta}{\{[\sin^2\theta\cos^2\theta+\lambda(\theta)][\sin^4\theta+4\sin^2\theta\cos^2\theta+4\lambda(\theta)]\}^{1/2}}\,, \tag{A1b}$$

which can be rewritten, for constant λ, as

$$I_{\parallel}=\int_0^1\frac{u\,du}{[u(u-u_1)(u-u_2)(u-u_3)(u-u_4)]^{1/2}}\,,\quad I_{\perp}=\int_0^1\frac{(1-u)\,du}{[u(u-u_1)(u-u_2)(u-u_3)(u-u_4)]^{1/2}} \tag{A2}$$

where

$$u_1=\tfrac{1}{2}-\tfrac{1}{2}(1+4\lambda)^{1/2}\simeq-\lambda,\quad u_2=\tfrac{1}{2}+\tfrac{1}{2}(1+4\lambda)^{1/2}\simeq1+\lambda,\quad u_3=\tfrac{1}{3}-\tfrac{2}{3}(1+3\lambda)^{1/2}\simeq-\tfrac{1}{3}-\lambda,\quad u_4=\tfrac{1}{3}+\tfrac{2}{3}(1+3\lambda)^{1/2}\simeq1+\lambda\,. \tag{A3}$$

These integrals can be expressed in terms of elliptic functions only if $\lambda \ll 1$. When this is the case the roots u_i ($i=1, 2, 3, 4$) can be expanded to lowest order in λ, giving

$$I_{\parallel}=\int_0^1 \frac{u\,du}{(1+\lambda-u)[u(u+\lambda)(u+\lambda+\frac{1}{3})]^{1/2}}=\int_0^1 \frac{(1+\lambda)\,du}{(1+\lambda-u)[u(u+\lambda)(u+\lambda+\frac{1}{3})]^{1/2}}-\int_0^1 \frac{du}{[u(u+\lambda)(u+\lambda+\frac{1}{3})]^{1/2}}$$

$$=\frac{2(3\lambda)^{1/2}}{(1+3\lambda)^{1/2}(1+2\lambda)}\left[\Pi\left(\frac{1+2\lambda}{1+\lambda};\ \frac{1}{1+3\lambda},\ \sin^{-1}\frac{1}{(1+\lambda)^{1/2}}\right)-F\left(\frac{1}{1+3\lambda},\ \sin^{-1}\frac{1}{(1+\lambda)^{1/2}}\right)\right], \tag{A4a}$$

$$I_{\perp}=\int_0^1 \frac{(1-u)\,du}{(1+\lambda-u)[u(u+\lambda)(u+\lambda+\frac{1}{3})]^{1/2}}=\int_0^1 \frac{du}{u(u+\lambda)(u+\lambda+\frac{1}{3})}-\int_0^1 \frac{\lambda\,du}{(1+\lambda-u)[u(u+\lambda)(u+\lambda+\frac{1}{3})]^{1/2}}$$

$$=\frac{2\sqrt{3}}{(1+3\lambda)^{1/2}(1+2\lambda)}\left[(1+\lambda)F\left(\frac{1}{1+3\lambda},\ \sin^{-1}\frac{1}{(1+\lambda)^{1/2}}\right)-\frac{\lambda^2}{1+\lambda}\Pi\left(\frac{1+2\lambda}{1+\lambda};\ \frac{1}{1+3\lambda},\ \sin^{-1}\frac{1}{(1+\lambda)^{1/2}}\right)\right], \tag{A4b}$$

where

$$\Pi(n;k^2,\phi)=\int_0^{\phi}\frac{d\alpha}{(1-n\sin^2\alpha)(1-k^2\sin^2\alpha)^{1/2}} \tag{A5}$$

and

$$F(k^2,\phi)=\int_0^{\phi}\frac{d\alpha}{(1-k^2\sin^2\alpha)^{1/2}} \tag{A6}$$

are incomplete elliptic integrals of the third and first kind, and where use was made of the transformation

$$u=\frac{\lambda\sin^2\alpha}{1-\sin^2\alpha}\,. \tag{A7}$$

Asymptotic forms for Π and F are needed. For this purpose it is necessary to transform Π as it appears in $I_{\parallel}$ and $I_{\perp}$ so that its characteristic, n, is less than unity. This can be done using the relationship[27]

$$\Pi(n;k^2,\phi)=F(k^2,\phi)-\Pi(k^2/n;k,\phi)+\left(\frac{n}{(1-n)(n-k^2)}\right)^{1/2}\times\tan^{-1}\left(\frac{(1-n)(n-k^2)}{n(1-k^2\sin^2\phi)}\right)^{1/2}\tan\phi\,. \tag{A8}$$

The dominant term in this relationship as $\lambda\to 0$ is the last one, which is easily expanded, giving

$$\Pi\left(\frac{1+2\lambda}{1+\lambda},\ \frac{1}{1+3\lambda},\ \sin^{-1}\frac{1}{(1+\lambda)^{1/2}}\right)\underset{\lambda\to 0}{\longrightarrow}\frac{1}{4\lambda}\ln\left(\frac{1}{\lambda}\right). \tag{A9}$$

The asymptotic form of F is obtainable from series expansions given in Gradshteyn and Ryzhik[28]:

$$F\left(\frac{1}{1+3\lambda},\ \sin^{-1}\frac{1}{(1+\lambda)^{1/2}}\right)\underset{\lambda\to 0}{\longrightarrow}\frac{1}{2}\ln\left(\frac{1}{\lambda}\right). \tag{A10}$$

It follows that

$$I_{\parallel}\underset{\lambda\to 0}{\longrightarrow}\tfrac{1}{2}\sqrt{3}\ln(1/\lambda) \tag{A11a}$$

and

$$I_{\perp}\underset{\lambda\to 0}{\longrightarrow}\tfrac{1}{2}\sqrt{3}\ln(1/\lambda)\,. \tag{A11b}$$

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