Effects of spin-orbit interaction upon impurity scattering in dilute alloys

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An earlier treatment of impurity scattering in dilute noble-metal alloys based on exact solutions of the Schrödinger equation for a lattice of muffin-tin potentials, is extended to take into account relativistic effects. For a nonrelativistic impurity in a relativistic host, the effects of spin-orbit interaction upon the host Fermi surface and impurity-induced Dingle-temperature anisotropies are calculated. Experimental Dingle-temperature anisotropies of Au(Cu), Au(Zn), and Au(Ag) are analyzed to yield phase shifts that describe scattering of conduction electrons at the Fermi level by the impurity atoms. For a relativistic impurity in a nonrelativistic host, Dingle-temperature anisotropies and spin-flip relaxation rates for conduction-electron spin resonance are discussed. A model calculation shows that host-lattice backscattering effects contribute significantly to the spin-flip scattering time T_1. Dingle-temperature anisotropies and spin-flip relaxation rates for Cu(Ge) and Cu(Au) are analyzed to yield the spin-orbit parameters of the impurity atoms in these alloys.

I. INTRODUCTION

In a recent series of papers,[1-5] an accurate procedure has been developed for the nonrelativistic analysis of impurity scattering in dilute alloys. This analysis is based upon an exact treatment of impurity scattering for the muffin-tin model of a single impurity in an otherwise perfect host lattice, by an extension of the Green's-function or Korringa-Kohn-Rostoker[6] (KKR) method of band-structure calculation. In this treatment, impurity scattering is completely determined by the "atomic" phase shifts of the host atom and of the impurity atom, together with the appropriate structure factors. It is well suited for semiempirical analysis of experiments involving impurity scattering of electrons at the Fermi level, and has been successfully applied to the analysis of Dingle-temperature anisotropy data for dilute substitutional[1-4] and interstitial[5] alloys in noble-metal hosts. The impurity-atom phase shifts inferred from these data contain information about effective impurity potentials for various metallic environments.

The purpose of the present paper is to discuss the qualitative and quantitative modifications of this nonrelativistic description of impurity scattering that are introduced by spin-orbit interaction. The spin-orbit interaction is the interaction between the spin of a conduction electron and the effective magnetic field generated by its motion through a spatially varying atomic potential. In the muffin-tin model the potential variation, and therefore the spin-orbit interaction, is confined within the muffin-tin spheres. The corresponding relativistic phase shifts for the host $[\eta^h_{lj}(E)]$ and impurity $[\eta^i_{lj}(E)]$ atoms are then characterized by both orbital (l) and total (orbital plus spin; $j = l \pm \frac{1}{2}$) angular momenta. It is convenient to define a spin-orbit parameter for each nonzero orbital angular momentum, proportional to the difference between the $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$ phase shifts:

$$\Delta^{(a)}_l(E) \equiv \eta^{(a)}_{l,\,l+1/2}(E) - \eta^{(a)}_{l,\,l-1/2}(E) , \qquad (1)$$

where (a) denotes h or i for host or impurity atoms, respectively. The extent to which $\Delta^{(a)}_l$ deviates from zero is a measure of the strength of the spin-orbit interaction on the atom (a). The potential gradient is greatest in the spatial region near the atomic core; its magnitude depends upon the nuclear charge of the atom and on how effectively this charge is screened by the electrons. The spin-orbit parameter is thus expected to be appreciable for elements of large atomic number such as Au ($Z = 79$) and to increase for elements across the periodic table, such as for Ga, Ge, and As, corresponding to the addition of s and p electrons which incompletely screen the additional nuclear charge.[7]

The qualitative effects of spin-orbit interaction can be summarized as follows. As a consequence of the coupling of spin with orbital motion of the electron within the muffin-tin spheres, the relativistic eigenstates of the lattice containing a single impurity differ from the nonrelativistic eigenstates in two respects. Firstly, they are characterized by the double-point-group representations ($\tilde{\Gamma}\tilde{\gamma}$) rather than the single-point-group representations ($\Gamma\gamma$) of the crystal symmetry. Secondly, for a lattice with inversion symmetry as considered here, the electronic eigenstates of the host lattice remain doubly degenerate, corresponding to the two generalized spin orientations ($\theta = \uparrow, \downarrow$) of the electron in a magnetic field. However,

since the strength of the spin-orbit interaction on the impurity atom is generally different from that on the host atom, the impurity can induce transitions between Bloch states of the host lattice of opposite generalized spin (e.g., $\uparrow \rightarrow \downarrow$) as well as of the same generalized spin (e.g., $\uparrow \rightarrow \uparrow$). This spin-flip process contributes to the linewidth of conduction-electron spin-resonance measurements; both processes contribute to the inverse lifetime of a Bloch state as measured in Dingle-temperature experiments.

In the present paper, the impurity is assumed to be substitutional and the lattice is assumed to have cubic symmetry. Our relativistic treatment of impurity scattering is based upon an exact solution of the Dirac equation for the muffin-tin model, as developed in more detail in Ref. 3. All relativistic interactions are thus included in the present treatment although attention is focused upon the spin-orbit interaction. Brown and Morgan[8] have shown that the mass-velocity and Darwin interactions introduce appreciable effects upon impurity scattering in heavy-noble-metal alloys. However, unlike the spin-orbit interaction, the effects of these interactions can be expressed as corrections to the nonrelativistic phase shifts. We shall illustrate the relativistic analysis for some dilute nonmagnetic noble-metal alloys, considering separately those effects associated with a relativistic host and those effects associated with a relativistic impurity. By comparing the results of relativistic and nonrelativistic analyses, the importance of the spin-orbit interaction in characterizing experimental data is assessed for various alloy systems. Two different types of experiment are considered: the anisotropy of the Dingle temperature and the relaxation of conduction-electron spin polarization.

The outline of the paper is as follows. In Sec. II, the relativistic theory of impurity scattering is briefly reviewed and the appropriate forms of the transition matrix are presented. In Sec. III, impurity scattering in a relativistic host is considered. Relativistic and nonrelativistic analyses of Dingle-temperature data for dilute alloys of gold are presented and compared. In Sec. IV, scattering by a relativistic impurity in a nonrelativistic host is considered. Analyses of both conduction-electron spin-resonance relaxation rates and Dingle-temperature anisotropies are presented and discussed, with reference to dilute alloys in a copper host. The results and conclusions of this work are discussed in Sec. V.

II. REVIEW OF THEORY

The transition matrix $T^{\theta'\theta}_{\vec{k}'\vec{k}}(E)$ describes the rate of change of the probability amplitude for finding an electron in the Bloch state $\Psi_E^{(0)\theta'}(\vec{k}', \vec{r})$ under the influence of the perturbing impurity potential, given that it was initially in the Bloch state $\Psi_E^{(0)\theta}(\vec{k}, \vec{r})$. Relativistic expressions for the T matrices appropriate for a single substitution impurity in an otherwise perfect lattice of muffin-tin potentials were derived in Ref. 3, following earlier nonrelativistic treatments of Dupree,[9] Morgan,[10] Harris,[11] Coleridge,[12] and Coleridge and Lee.[1]

The relativistic T matrix can be written as a sum of partial-wave double-point-group components in the form

$$T^{\theta'\theta}_{\vec{k}'\vec{k}}(E) = -\sum_{\substack{lj\tilde{\Gamma}\tilde{\gamma} \\ l'j'}} \tilde{f}^{\theta'*}_{lj\tilde{\Gamma}\tilde{\gamma}}(\vec{k}', E)(\tilde{\xi} - \tilde{\chi}^{\tilde{\Gamma}})^{-1}_{lj,l'j'}\tilde{f}^{\theta}_{l'j'\tilde{\Gamma}\tilde{\gamma}}(\vec{k}, E) \ . \tag{2}$$

Here we have introduced a tilde notation to distinguish relativistic functions from their nonrelativistic counterparts. The kernel of this expression contains two terms. Information about the impurity phase shifts is contained in the diagonal phase-shift matrix $\tilde{\xi}$, whose elements are

$$\tilde{\xi}_{lj}(E) = [\cot \eta^h_{lj}(E) - \cot \eta^i_{lj}(E)]^{-1} \ . \tag{3}$$

$\tilde{\chi}^{\tilde{\Gamma}}$ is the integral over the volume $[(2\pi)^3/\Omega]$ of the Brillouin zone of the inverse of the KKR secular matrix $\tilde{M}(\vec{k}, E)$[6,3]:

$$\tilde{\chi}^{\tilde{\Gamma}}_{lj,l'j'}(E) = \frac{\Omega}{(2\pi)^3}\int_{BZ} d^3\vec{k}[\tilde{M}(\vec{k}, E)]^{-1}_{lj\tilde{\Gamma}\tilde{\gamma},l'j'\tilde{\Gamma}\tilde{\gamma}} \ . \tag{4}$$

The basis functions $\tilde{f}^{\theta}_{lj\tilde{\Gamma}\tilde{\gamma}}(\vec{k}, E)$ are proportional to the Bloch-wave amplitudes $\tilde{V}^{\theta}_{lj\tilde{\Gamma}\tilde{\gamma}}(\vec{k}, E)$, which are components of the normalized eigenvector of $\tilde{M}(\vec{k}, E)$ that corresponds to its zero eigenvalue $\tilde{\lambda}(\vec{k}, E) = 0$:

$$\tilde{f}^{\theta}_{lj\tilde{\Gamma}\tilde{\gamma}}(\vec{k}, E) = \exp(i\vec{k}\cdot\vec{R}_I)\tilde{V}^{\theta}_{lj\tilde{\Gamma}\tilde{\gamma}}(\vec{k}, E) \times\left(-\frac{\partial\tilde{\lambda}(\vec{k}, E)}{\partial E}\right)^{-1/2} \ . \tag{5}$$

It was shown in Ref. 3 that the sum over partial-wave indices l, j in Eq. (2) may be truncated at the lowest angular momentum for which the corresponding host phase shift is negligible. In the present Fermi-surface studies of noble-metal hosts, host phase shifts $\eta^h_{lj}(E_F)$ are included for $l \leq 2$. The corresponding single- and double-point-group representations which enter the analysis are listed in Table I. It will be seen that the relativistic kernel $(\tilde{\xi} - \tilde{\chi}^{\tilde{\Gamma}})^{-1}$ is diagonal for all representations, except for the representation Γ_8^+ for which it is a two by two matrix in partial-wave indices lj and $l'j'$ equal to 2, $\frac{3}{2}$ and 2, $\frac{5}{2}$. It is convenient to describe the k dependence of the diagonal part of the T matrix by defining a set of partial-wave factors

TABLE I. Single- and double-point-group representation for $l \leq 2$.

l	Single-point-group representations Γ	j	Double-point-group representations $\tilde{\Gamma}$
0	Γ_1	$\frac{1}{2}$	Γ_6^+
1	Γ_{15}	$\frac{1}{2}$	Γ_6^-
		$\frac{3}{2}$	Γ_8^-
2	Γ_{12}	$\frac{3}{2}$	Γ_8^+
		$\frac{5}{2}$	Γ_8^+
2	$\Gamma_{25'}$	$\frac{3}{2}$	Γ_8^+
		$\frac{5}{2}$	$\Gamma_8^+,\ \Gamma_7^+$

$$\tilde{G}^{\tilde{\Gamma}}_{lj,l'j'}(\vec{k},\ E) \equiv \sum_{\tilde{\gamma}} \tilde{f}^{\theta *}_{lj\tilde{\Gamma}\tilde{\gamma}}(\vec{k},\ E)\tilde{f}^{\theta}_{l'j'\tilde{\Gamma}\tilde{\gamma}}(\vec{k},\ E)\ . \quad (6)$$

The double group representations $\tilde{\Gamma}\tilde{\gamma}$ are formed from direct products of representations $\Gamma\gamma$ of the single-point group of the lattice and the two dimensional representation of electron spin $m_s = \pm\frac{1}{2}$. For cubic symmetry the unitary transformation $U^{lj\tilde{\Gamma}\tilde{\gamma}}_{l\Gamma\gamma m_s}$ between double-point-group and single-point-group lattice harmonics has been worked out by Onodera and Okazaki.[13] In order to study the scattering properties of a relativistic impurity in a nonrelativistic host, it is convenient to express the nonrelativistic host parameters in terms of the double-point-group representations. The transformation of the amplitude factors takes the form (with $\theta \equiv m_s$):

$$\tilde{f}^{m_s}_{lj\tilde{\Gamma}\tilde{\gamma}}(\vec{k},\ E) = \sum_{\Gamma\gamma} (U^{lj\tilde{\Gamma}\tilde{\gamma}}_{l\Gamma\gamma m_s})^* f_{l\Gamma\gamma}(\vec{k},\ E)\ . \quad (7)$$

Similarly, the Brillouin-zone integrals for the nonrelativistic host can be transformed to the double-point-group representation:

$$\tilde{\chi}^{\tilde{\Gamma}}_{lj,l'j'}(E) = \sum_{\Gamma\gamma m_s} U^{lj\tilde{\Gamma}\tilde{\gamma}}_{l\Gamma\gamma m_s}(U^{l'j'\tilde{\Gamma}\tilde{\gamma}}_{l'\Gamma\gamma m_s})^*\ \chi^{\Gamma}_{ll'}(E)\ . \quad (8)$$

The coefficients for the transformation of the Brillouin-zone integral Eq. (8) and for the analogous transformation of the partial-wave factors defined by Eq. (6) are given for $l \leq 2$ in Table II.

The impurity wave function can be described in terms of a set of Friedel phase shifts. The Friedel phase shift $\tilde{\phi}_{\nu\tilde{\Gamma}}(E)$ is related to the eigenvalue $\exp[2i\tilde{\phi}_{\nu\tilde{\Gamma}}(E)]$ of the kernel of the scattering matrix[3]:

$$[(\tilde{\xi} - \tilde{\chi}^{\tilde{\Gamma}*})(\tilde{\xi} - \tilde{\chi}^{\tilde{\Gamma}})^{-1}]\ . \quad (9)$$

Here $\tilde{\chi}^{\tilde{\Gamma}*}$ denotes the complex conjugate of the matrix $\tilde{\chi}^{\tilde{\Gamma}}$. The Friedel phase shifts evaluated at the Fermi level E_F describe the displacement of conduction charge in the vicinity of the impurity, which, according to the Friedel sum rule,[15] depends upon the valence difference Z between the impurity and host atoms according to

$$\mathfrak{F}(E_F) \equiv \frac{1}{\pi} \sum_{\nu\tilde{\Gamma}} d(\tilde{\Gamma})\ \tilde{\phi}_{\nu\tilde{\Gamma}}(E_F) = Z\ , \quad (10)$$

where $d(\tilde{\Gamma})$ is the degeneracy of the double-point-group representation $\tilde{\Gamma}$.

Assuming incoherent scattering from a finite atomic fraction C_I of impurities, the T matrix, evaluated at the host Fermi level E_F, may be applied to the analysis of several types of experimental data on dilute alloys. The experiments considered here measure Dingle-temperature anisotropies and longitudinal relaxation rates for conduction-electron spin resonance.

The Dingle temperature $X(\omega)$ is a measure of the damping of de Haas–van Alphen oscillations for orbit ω.[16] The damping due to impurity scattering of electrons at the Fermi level may be approximated by the orbital average of the inverse lifetime of each Bloch state $\Psi^{(0)\theta}_{E_F}(\vec{k},\ \vec{r})$ included in the orbit, evaluated in zero magnetic field. Expressing this inverse lifetime in terms of the imaginary part of the diagonal element of the T matrix calculated for incoherent impurity scattering, the Dingle temperature is given by

$$X(\omega) = \frac{\hbar}{2\pi k_B}\ \frac{\hbar^2}{2\pi m_c(\omega)} \oint_{\omega} \frac{d\psi\, k_\perp}{\hbar V_{E_F}(\vec{k}) \cdot \hat{k}_\perp} \times \left(-\frac{2C_I}{\hbar}\ \mathrm{Im} T^{\uparrow\uparrow}_{\vec{k}\vec{k}}(E_F) \right)\ . \quad (11)$$

Here $m_c(\omega)$ is the experimental cyclotron mass of the orbit, k_B is Boltzmann's constant; $\vec{k}_\perp$, with polar coordinates $(k_\perp, \psi)$, is the component of the wave vector $\vec{k}$ in the plane of the orbit, measured with respect to the center of the orbit; and the notation $\hat{k}_\perp$ denotes a unit vector. The evaluation of this expression for a nonrelativistic impurity in a relativistic host and for a relativistic impurity in a nonrelativistic host will be discussed in Secs.

TABLE II. Expressions for double-point-group representations (Ref. 13) of host lattice coefficients in terms of single-point-group representations (Ref. 14) in absence of host spin-orbit interaction.

l	j	l'	j'	$\tilde{\Gamma}$	Brillouin-zone integrals $\tilde{\chi}^{\tilde{\Gamma}}_{lj,l'j'}$	Partial-wave factors $G^{\tilde{\Gamma}}_{lj,l'j'}$
0	$\frac{1}{2}$	0	$\frac{1}{2}$	Γ_6^+	$\chi_{00}^{\Gamma_1}$	$G_{00}^{\Gamma_1}$
1	$\frac{1}{2}$	1	$\frac{1}{2}$	Γ_6^-	$\chi_{11}^{\Gamma_{15}}$	$\frac{1}{3}G_{11}^{\Gamma_{15}}$
1	$\frac{3}{2}$	1	$\frac{3}{2}$	Γ_8^-	$\chi_{11}^{\Gamma_{15}}$	$\frac{2}{3}G_{11}^{\Gamma_{15}}$
2	$\frac{3}{2}$	2	$\frac{3}{2}$	Γ_8^+	$\frac{1}{5}(2\chi_{22}^{\Gamma_{12}} + 3\chi_{22}^{\Gamma_{25'}})$	$\frac{2}{5}(G_{22}^{\Gamma_{12}} + G_{22}^{\Gamma_{25'}})$
2	$\frac{5}{2}$	2	$\frac{5}{2}$	Γ_8^+	$\frac{1}{5}(3\chi_{22}^{\Gamma_{12}} + 2\chi_{22}^{\Gamma_{25'}})$	$\frac{1}{15}(9G_{22}^{\Gamma_{12}} + 4G_{22}^{\Gamma_{25'}})$
2	$\frac{3}{2}$	2	$\frac{5}{2}$	Γ_8^+	$-(\sqrt{6}/5)(\chi_{22}^{\Gamma_{12}} - \chi_{22}^{\Gamma_{25'}})$	$-(\sqrt{6}/5)(G_{22}^{\Gamma_{12}} - \frac{2}{3}G_{22}^{\Gamma_{25'}})$
2	$\frac{5}{2}$	2	$\frac{5}{2}$	Γ_7^+	$\chi_{22}^{\Gamma_{25'}}$	$\frac{1}{3}G_{22}^{\Gamma_{25'}}$

III and IV, respectively.

The longitudinal relaxation time T_1 observed in conduction-electron spin resonance is the time constant for the exponential decay of conduction-electron magnetization when the magnetic field is switched off. Its inverse can be calculated from the Fermi-surface average of the spin-flip scattering rate[3,17]:

$$\frac{1}{T_1} = \frac{4\pi}{\hbar}\,\frac{C_I}{\mathfrak{D}(E_F)}\left(\frac{\Omega}{(2\pi)^3}\right)^2 \times \iint \frac{dS_{\vec{k}}}{|\hbar V_{E_F}(\vec{k})|}\,\frac{dS_{\vec{k}'}}{|\hbar V_{E_F}(\vec{k}')|}\,|T^{\uparrow\downarrow}_{\vec{k}',\vec{k}}(E_F)|^2 \,. \tag{12}$$

Here $dS_{\vec{k}}$ denotes integration over the Fermi surface. $\mathfrak{D}(E_F)$ denotes the number of states of given spin per unit energy of the host metal at the Fermi level, normalized to the volume of a unit cell Ω:

$$\mathfrak{D}(E_F) \equiv \frac{\Omega}{(2\pi)^3}\int \frac{dS_{\vec{k}}}{|\hbar V_{E_F}(\vec{k})|} \,. \tag{13}$$

$1/T_1$ will be evaluated for a relativistic impurity in a nonrelativistic host in Sec. IV.

III. IMPURITY SCATTERING IN A RELATIVISTIC HOST

Of the three noble-metal hosts, spin-orbit effects are expected to be largest in gold. Although a nonrelativistic analysis of Dingle-temperature anisotropies can be carried out for dilute gold alloys,[2,4] a relativistic analysis is expected to better approximate the physical situation. In particular, one would expect the relativistic treatment to give more reliable values for the impurity phase shifts.

In order to proceed with an analysis of Dingle-temperature data, the atomic phase shifts at the Fermi level of the host metal must first be determined. This is conveniently achieved by fitting[18] a model Fermi surface generated by a KKR band-structure calculation[6] to the experimental Fermi-surface areas determined by de Haas–van Alphen measurements. Lee and Heine[19] have shown that equally accurate fits to de Haas–van Alphen data may be obtained for a wide range of values of the Fermi energy parameter E_F, and that these correspond to different forms of the muffin-tin potential. In the present work, the Fermi energy parameter was chosen to be $E_F = 0.53$ Ry, equal to that determined in an *ab initio* band-structure calculation by Christensen.[20] The experimental de Haas–van Alphen frequencies for six symmetry orbits of gold were taken from the data of Coleridge and Templeton,[21] and the lattice constant a was that quoted by Halse.[22] The error in the experimental parameters is dominated by the uncertainty in the lattice constant, and amounts to a few parts in 10^4.

Setting the spin-orbit parameters Δ_1^h and Δ_2^h equal to zero, and considering only partial waves for $l \leq 2$, the best nonrelativistic fit to the three Fermi-surface areas N_{111}, B_{111}, and B_{100}, resulted in average fractional errors in the hole and turning-point orbits of 14 parts in 10^4. A relativistic model Fermi-surface, however, could be found within the experimental error. Starting from the spin-orbit parameters calculated from the potential of Christensen,[20] we found that, by making small adjustments to the spin-orbit parameters, the average fractional error in the fit to the hole and turning-point orbits could be reduced to less than 2 parts in 10^4. In this way, estimates of the spin-orbit parameters in gold were obtained. Unfortunately, the sensitivity of the shape of the gold Fermi surface to the spin-orbit parameters is weak, presumably because no degeneracy of the energy bands close to the Fermi level is split by the spin-orbit interaction. A more thorough investigation of the sensitivity of the shape of the gold Fermi surface to the spin-orbit parameters will be warrented only when more accurate data become available. It will then be necessary to consider also the effects of f wave contributions to the anisotropy of the Fermi surface.

The relativistic T matrix Eq. (2) must be used to evaluate the impurity-induced Dingle temperature in a relativistic host from Eq. (11). The resulting expression for the Dingle temperature may be written

$$X(\omega) = \frac{\hbar^2}{2m_c(\omega)\,a^2}\,\frac{C_I}{k_B} \times \sum_{ij\Gamma;\,i'j'} \tilde{W}^{\tilde{\Gamma}}_{ij,\,i'j'}(\omega)\,\mathrm{Im}[(\tilde{\xi} - \tilde{\chi}^{\tilde{\Gamma}})^{-1}_{ij,\,i'j'}] \,, \tag{14}$$

where the dimensionless "host orbital parameters" $\tilde{W}^{\tilde{\Gamma}}(\omega)$ are orbital averages of the partial-wave factors $\tilde{G}^{\tilde{\Gamma}}(k, E_F)$ of Eq. (6), and are defined by

$$\tilde{W}^{\tilde{\Gamma}}_{ij,\,i'j'}(\omega) \equiv \left(\frac{a}{\pi}\right)^2 \oint_\omega \frac{d\psi\, k_\perp}{[\nabla_{\vec{k}}(E)]_{E_F}\cdot\hat{\epsilon}}\,\tilde{G}^{\tilde{\Gamma}}_{ij,\,i'j'}(\vec{k}, E_F) \,. \tag{15}$$

In order to carry out a phase-shift analysis of Dingle-temperature anisotropies, the host orbital parameters $\tilde{W}^{\tilde{\Gamma}}$ defined in Eq. (15) and the Brillouin-zone integrals $\tilde{\chi}^{\tilde{\Gamma}}$ defined in Eq. (4) were evaluated numerically for gold as described in Ref. 4. The results are presented in Tables III and IV for the nonrelativistic and for the relativistic Fermi-surface parametrizations, respectively.[2,4] The relationship between the present notation and the notation of previous papers for nonrelativistic host orbital parameters $W^{\Gamma}(\omega)$ is discussed in Appendix A.

Once these host parameters are known, the im-

TABLE III. Nonrelativistic host parameters for Au ($E_F = 0.53$ Ry, $a = 7.682115$ bohr).

$l\Gamma$	$0\Gamma_1$	$1\Gamma_{15}$	$2\Gamma_{12}$	$2\Gamma_{25'}$
$\eta_l^{\hbar}(E_F)$ (rad)	0.249562	0.063150	−0.242562	
$\mathrm{Re}[\chi_{ll}^{\Gamma}(E_F)]$	0.291731	0.062153	−0.314925	−0.303971
$\mathrm{Im}[\chi_{ll}^{\Gamma}(E_F)]$	0.041666	0.002100	0.051887	0.073557
$W_{ll}^{\Gamma}(\omega)$[a]				
N_{111}	0	0.010052	0.066888	0.073561
B_{111}	0.159872	0.015584	0.401440	0.853738
B_{100}	0.172353	0.020809	0.333425	0.746617
T_{110}	0.145213	0.018204	0.329724	0.759363
D_{110}	0.104120	0.022511	0.280056	0.547697
R_{110}	0.120548	0.019635	0.366281	0.703482
T_{100}	0.153467	0.019094	0.321453	0.729645

[a] The notation for the orbits is as follows: N_{111} and B_{111} refer to neck and belly orbits, respectively, perpendicular to the [111] axis. B_{100} and R_{100} refer to belly and rosette orbits, respectively, perpendicular to the [100] axis. D_{110} is the dog's bone orbit perpendicular to the [110] axis. There are two turning-point orbits T_{110} and T_{100} in the (110) and (100) zones, respectively. The host orbital parameters defined in Eq. (15) are related to those in Table II of Ref. 2 according to

$$|\partial A(\omega)/\partial\eta_l^{\hbar}| = (\pi/12)^{2/3}(\pi \sin^2\eta_l^{\hbar})^{-1} \sum_{\Gamma} W_{ll}^{\Gamma}(\omega).$$

purity phase shifts $\eta_{lj}^{i}(E_F)$ can be determined from least-squares fits to experimental Dingle temperature $X(\omega)$ and cyclotron mass $m_c(\omega)$ data, according to Eq. (14). In the analysis presented here we have assumed for simplicity that the impurity spin-orbit parameters $\Delta_l^i(E_F)$ are negligible so that $\eta_{lj}^{i}(E_F) = \eta_l^i(E_F)$. This is a reasonable assumption for the dilute alloys considered here except, perhaps, for Au(Ag). With this assumption, the impurity atom is characterized by three phase shifts, $\eta_0^i(E_F)$, $\eta_1^i(E_F)$, and $\eta_2^i(E_F)$, which were determined by fitting the data to Eq. (14) using a nonlinear least-squares-fitting procedure described by Bevington.[23]

The analysis of Dingle-temperature data alone does not generally lead to a unique set of impurity phase shifts.[2,4] The earlier nonrelativistic analysis (Ref. 4) resolved this ambiguity by fitting the Dingle-temperature data with the constraint that the calculated residual resistivity of the alloy should agree with the experimental value. In the present work, the impurity phase shifts were deduced from the fits to the Dingle-temperature data by requiring consistency of the corresponding Friedel phase shifts with those determined in the earlier work.[4,24] We have carried out relativistic and nonrelativistic analyses of experimental Dingle-temperature anisotropies in dilute alloys of Au(Ag), Au(Cu), and Au(Zn), as measured by Lowndes, Miller, Poulsen, and Springford.[25] Only Dingle-temperature data for the five symmetry orbits that were measured were included in the fit, since these data are not complicated by phase smearing due to sensitivity to small crystalline misorientation.[25]

The results of the phase-shift analyses are given in Table V. For each of the three gold alloys, the best fit to the data involved discrepancies substantially larger than the quoted experimental errors, the largest fractional error occurring for one of the hole orbits, either R_{100} or D_{110}. This result suggests that the quoted errors of the experimental data may underestimate the actual errors for these orbits. The following comparisons can be made between the relativistic and the nonrelativistic analyses. First, the fit to the data in the relativistic analysis is marginally better than that in the nonrelativistic analysis, even though the number of fitting parameters is the same. However, the inferred impurity phase shifts $\eta_l^i(E_F)$ differ between the two analyses by as much as 30%. For Cu and Zn impurities, the relativistic analysis yields a Friedel sum which

TABLE IV. Relativistic host parameters for Au [$E_F = 0.53$ Ry, $a = 7.682115$ bohr].

$\Gamma lj, l'j'$	$\Gamma_6^+ 0\frac{1}{2}, 0\frac{1}{2}$	$\Gamma_6^- 1\frac{1}{2}, 1\frac{1}{2}$	$\Gamma_8^- 1\frac{3}{2}, 1\frac{3}{2}$	$\Gamma_8^+ 2\frac{3}{2}, 2\frac{3}{2}$	$\Gamma_8^+ 2\frac{5}{2}, 2\frac{5}{2}$	$\Gamma_8^+ 2\frac{3}{2}, 2\frac{5}{2}$	$\Gamma_7^+ 2\frac{5}{2}, 2\frac{5}{2}$
$\eta_{lj}^{\hbar}(E_F)$ (rad)	0.266985	0.168650	0.014420	−0.206771	−0.267214	···	−0.267214
$\mathrm{Re}(\tilde{\chi}_{lj,l'j'}^{\tilde{\Gamma}})$	0.317356	0.162035	0.014366	−0.261584	−0.345423	0.003847	−0.325963
$\mathrm{Im}(\tilde{\chi}_{lj,l'j'}^{\tilde{\Gamma}})$	0.048624	0.012422	($\times 10^2$)[b]	0.042218	0.083520	0.012052	0.092460
$\tilde{W}_{lj,l'j'}^{\tilde{\Gamma}}$[a]			0.011834 ($\times 10^2$)[b]				
N_{111}	0.000503	0.021308	0.036586	0.042082	0.083198	−0.002343	0.018242
B_{111}	0.187258	0.028491	0.060350	0.338565	0.629233	0.091302	0.345889
B_{100}	0.200900	0.042072	0.077705	0.274474	0.554585	0.089518	0.326006
T_{110}	0.169064	0.035023	0.068726	0.277510	0.555233	0.092610	0.328659
D_{110}	0.121645	0.046118	0.083401	0.216063	0.438733	0.052856	0.224972
R_{100}	0.141628	0.038259	0.074342	0.297186	0.542856	0.063450	0.268450

[a] See footnote of Table III for orbital notation.

[b] For convenience the numbers quoted below are 100 times the coefficient.

TABLE V. Phase-shift analyses of Dingle-temperature data for dilute gold alloys. Impurity phase shifts $[\eta^i(E_F)]$ listed correspond most closely to those determined in Ref. 4 to be consistent with residual resistivity measurements.

	Au(Cu)			Au(Zn)			Au(Ag)		
	Experiment[a]	Nonrelativistic fit[b]	Relativistic fit[c]	Experiment[a]	Nonrelativistic fit[b]	Relativistic fit[c]	Experiment[a]	Nonrelativistic fit[b]	Relativistic fit[c]
Orbit[d]				Dingle temperatures (°K/at.%)					
N_{111}	4.53(2)	4.53	4.53	24.5(15)	25.66	25.67	2.83(3)	2.83	2.83
B_{111}	10.10(9)	10.14	10.14	38.7(15)	40.23	40.33	9.27(10)	9.39	9.40
B_{100}	9.16(22)	9.98	9.93	35.6(15)	37.10	37.02	9.82(55)	9.89	9.85
T_{110}		9.37	9.43		36.96	37.36		8.78	8.70
D_{110}	8.59(11)	8.22	8.22	36.3(15)	33.53	33.63	7.62(18)	7.57	7.53
R_{100}	9.82(100)	9.22	9.18	39.8(15)	38.41	38.30	9.03(24)	8.21	8.23
T_{100}		9.53			36.57			9.21	
				Impurity phase shifts (rad)					
$\eta_l^i(E_F)$									
$l=0$		−0.20	−0.14		0.51	0.45		−0.36	−0.35
$l=1$		0.22	0.19		0.42	0.39		−0.077	−0.065
$l=2$		−0.15	−0.16		0.064	0.070		−0.21	−0.26
				Friedel sum [Eq. (10)]					
$\mathfrak{F}(E_F)$		0.30	0.29		1.28	1.24		−0.23	−0.36

[a]Reference 25.
[b]Using host parameters of Tables III.
[c]Using host parameters of Tables IV.
[d]See footnote of Table III for orbital notation.

is in slightly better agreement with the Friedel sum rule [Eq. (10)]. In Au(Cu) and Au(Zn), the impurity phase shifts are quite comparable to those predicted for the same atoms in a copper environment at a similar Fermi energy ($E_F = 0.55$ Ry), as will be discussed in Sec. IV below. The impurity phase shifts for Au(Ag) determined by the present analysis are comparable to the phase shifts for a pure silver lattice evaluated at the same value of the Fermi energy parameter.[26] In fact, they are uniformly smaller than the pure silver phase shifts, indicating that the effective silver potential for Au(Ag) is less attractive than that for Ag(Ag), as expected owing to the stronger binding of the conduction electrons in gold. However, the sum of the corresponding Friedel phase shifts is in rather poor agreement with the sum rule [Eq. (10)] both in the nonrelativistic and in the relativistic analyses. In order to check whether this might be due to our having neglected spin-orbit interaction on the impurity atom, the calculation was repeated assuming spin-orbit parameters $\Delta_l^i(E_F)$ calculated from Christensen's silver potential.[20] We find that agreement with the Friedel sum rule is not improved. The discrepancy is surprising because the lattice constants of pure Ag and pure Au differ by only 0.2%, which suggests that distortion of the lattice by the impurity should be negligible, and if this is so the Friedel sum rule should be accurately satisfied.

IV. IMPURITY SCATTERING BY A RELATIVISTIC IMPURITY IN A NONRELATIVISTIC HOST

The evaluation of the T matrix for a relativistic impurity in a nonrelativistic host is most easily accomplished by using the unitary transformations [Eq. (7)] to express the relativistic host parameters in terms of the single-point-group representations. Using the transformations listed in Table II, the explicit expression for the Dingle temperature (including only partial waves for $l \leq 2$) is

$$X(\omega) = \frac{\hbar^2 C_I}{2 m_c(\omega)\, a^2 k_B} \left(W_{00}^{\Gamma_1}(\omega)\, \mathrm{Im}(\xi_{0,1/2} - \chi_{00}^{\Gamma_1})^{-1} + W_{11}^{\Gamma_{15}}(\omega)\, \mathrm{Im}\left[\tfrac{1}{3}(\xi_{1,1/2} - \chi_{11}^{\Gamma_{15}})^{-1} + \tfrac{2}{3}(\xi_{1,3/2} - \chi_{11}^{\Gamma_{15}})^{-1}\right] \right.$$
$$+ W_{22}^{\Gamma_{12}}(\omega)\, \mathrm{Im}\left\{\left[\xi_{2,5/2} - \chi_{22}^{\Gamma_{25'}} - \tfrac{3}{5}(\xi_{2,5/2} - \xi_{2,3/2})\right]/D\right\} + W_{22}^{\Gamma_{25'}}(\omega)\, \mathrm{Im}\left\{\tfrac{1}{3}(\xi_{2,5/2} - \chi_{22}^{\Gamma_{25'}})^{-1}\right.$$
$$\left. \left. + \tfrac{2}{3}\left[\xi_{2,3/2} - \chi_{22}^{\Gamma_{12}} + \tfrac{3}{5}(\xi_{2,5/2} - \xi_{2,3/2})\right]/D\right\} \right), \tag{16}$$

where

$$D \equiv \left[(\xi_{2,3/2} - \chi_{22}^{\Gamma_{12}})(\xi_{2,5/2} - \chi_{22}^{\Gamma_{25'}}) - \tfrac{3}{5}(\xi_{2,5/2} - \xi_{2,3/2})(\chi_{22}^{\Gamma_{25'}} - \chi_{22}^{\Gamma_{12}})\right] \tag{17}$$

is the determinant of the 2×2 matrix $(\xi - \tilde{\chi}^{\Gamma_8^+})$. The orbital variation of the Dingle temperature associated with p-wave scattering involves only a single term, and is therefore independent of the spin-orbit parameter $\Delta_1^i(E_F)$. Physically, this is because the p-like partial waves are not split by either the single- or the double-point-group symmetries of the cubic crystal field. The d-like partial waves, are however, split by the crystal field into single-point-group representation Γ_{12} and $\Gamma_{25'}$, which characterize the host wave functions, and into double-point-group representations Γ_7^+ and Γ_8^+ which characterize the impurity wave functions. The recombination of the outgoing scattered wave with the backscattered waves characterized by different symmetry groups causes the orbital variation of the d wave contribution to the Dingle temperature to be weakly dependent on the d wave spin-orbit parameter $\Delta_2^i(E_F)$. Since the Dingle temperature is a measure of the total scattering rate, including spin-flip as well as no spin-flip processes, it is not surprising that it is generally only weakly dependent upon the impurity spin-orbit parameters $\Delta_l^i(E_F)$.

On the other hand, the rate of spin-flip scattering induced by the spin-orbit interaction depends strongly on the spin-orbit parameters. The longitudinal relaxation rate for conduction-electron spin resonance [Eq. (12)] may be evaluated in terms of the unitary transformations [Eq. (7)][13]:

$$\frac{1}{T_1} = \frac{4C_I}{\pi\hbar\mathfrak{D}(E_F)} \sum_{\substack{l\Gamma;l_1\\ l'\Gamma';l_1'}} \operatorname{Im}\chi^{\Gamma}_{ll_1}\operatorname{Im}\chi^{\Gamma'}_{l'l_1'} \times\left(\sum_{\substack{j\tilde{\Gamma}\tilde{\gamma};j'\\ j_1\tilde{\Gamma}_1\tilde{\gamma}_1;j_1'}}\sum_{\gamma\gamma'} U^{lj\tilde{\Gamma}\tilde{\gamma}}_{l\Gamma\gamma\iota}(U^{l'j'\tilde{\Gamma}\tilde{\gamma}}_{l'\Gamma'\gamma'\iota})^*(U^{l_1j_1\tilde{\Gamma}_1\tilde{\gamma}_1}_{l_1\Gamma\gamma\iota})^* U^{l_1'j_1'\tilde{\Gamma}_1\tilde{\gamma}_1}_{l_1'\Gamma'\gamma'\iota}(\tilde{\xi}-\tilde{\chi}^{\tilde{\Gamma}})^{-1}_{lj,l'j'}(\tilde{\xi}-\tilde{\chi}^{\tilde{\Gamma}_1*})^{-1}_{l_1j_1,l_1'j_1'}\right). \tag{18}$$

Evaluating this expression for partial waves $l\leq 2$, the explicit form of the spin relaxation rate is

$$\frac{1}{T_1} = \frac{4C_I}{\pi\hbar\mathfrak{D}(E_F)}\left[\frac{4}{9}\frac{(\xi_{1,3/2}-\xi_{1,1/2})^2(\operatorname{Im}\chi_{11}^{\Gamma_{15}})^2}{|\xi_{1,3/2}-\chi_{11}^{\Gamma_{15}}|^2\,|\xi_{1,1/2}-\chi_{11}^{\Gamma_{15}}|^2} + \frac{4}{25}\frac{(\xi_{2,5/2}-\xi_{2,3/2})^2}{|D|^2}\left((\operatorname{Im}\chi_{22}^{\Gamma_{25'}})^2\left|\frac{\xi_{2,5/2}-\chi_{22}^{\Gamma_{12}}}{\xi_{2,5/2}-\chi_{22}^{\Gamma_{25'}}}\right|^2 + 4\operatorname{Im}\chi_{22}^{\Gamma_{12}}\operatorname{Im}\chi_{22}^{\Gamma_{25'}}\right)\right]. \tag{19}$$

It is evident that the spin relaxation rate is directly dependent upon the impurity spin-orbit parameters $\Delta_l^i(E_F)$ through the factors $(\xi_{1,3/2}-\xi_{1,1/2})^2$ and $(\xi_{2,5/2}-\xi_{2,3/2})^2$. The d-wave term has an additional contribution due to crystal-field splittings. In the absence of backscattering by the host lattice, this expression for $1/T_1$ reduces to that derived for a free-electron model of the host lattice[17]:

$$1/T_1^f = [4C_I/\pi\hbar\mathfrak{D}(E_F)]\left[\tfrac{4}{9}\sin^2(\eta^i_{1,3/2}-\eta^i_{1,1/2}) + \tfrac{4}{5}\sin^2(\eta^i_{2,5/2}-\eta^i_{2,3/2})\right]. \tag{20}$$

In order to estimate the magnitudes of spin-orbit effects in a series of copper alloys, we have constructed approximate muffin-tin potentials for substitutional Ni, Zn, Ga, and Ge impurities in copper lattices by superposition of atomic potentials.[4] The potentials were adjusted, by a small constant shift to represent screening effects, so that the Friedel sum rule [Eq. (10)] was satisfied. The relativistic impurity phase shifts $\eta^i_{lj}(E_F)$ for these potentials were calculated by numerical integration of the Dirac equation,[27] as briefly discussed in Appendix B. The results in Table VI show clearly the anticipated increase in the magnitude of the spin-orbit effects across a single row of the periodic table.[7] From these estimates of the impurity phase shifts, and the known host parameters of copper,[2] reproduced for convenience

TABLE VI. Calculated relativistic phase shifts for substitutional impurities in Cu ($E_F = 0.55$ Ry): neighbors of Cu in 4th row of periodic table.[7]

	$\eta^i_{lj}(E_F)$ in radians				
Impurity configuration	Ni ($3d^9 4s^1$)	Cu[a] ($3d^{10}4s^1$)	Zn ($4s^2$)	Ga ($4s^2 4p^1$)	Ge ($4s^2 4p^2$)
$\eta^i_{0,1/2}$	−0.173	−0.076	0.616	1.010	1.251
$\eta^i_{1,1/2}$	0.040	0.130	0.418	0.917	1.457
$\eta^i_{1,3/2}$	0.028	0.130	0.386	0.856	1.381
$\eta^i_{2,3/2}$	−0.273	−0.119	0.009	0.032	0.051
$\eta^i_{2,5/2}$	−0.336	−0.119	0.008	0.031	0.051
$\mathfrak{s}\,(E_F)$[b]	−1.1		1.0	2.0	3.1

[a]Cu phase shifts fitted to Fermi-surface data of pure Cu, Refs. 18 and 28 (see Table VII).

[b]Equation (10).

TABLE VII. Nonrelativistic host parameters for Cu ($E_F = 0.55$ Ry, $a = 6.8087$ bohr).

$l\Gamma$	$0\Gamma_1$	$1\Gamma_{15}$	$2\Gamma_{12}$	$2\Gamma_{25'}$
$\eta_l^{\Gamma}(E_F)$ (rad)	0.075 529	0.129 800	−0.118 591	
$\mathrm{Re}[\chi_l^{\Gamma}(E_F)]$	0.076 069	0.124 118	−0.132 327	−0.128 621
$\mathrm{Im}[\chi_l^{\Gamma}(E_F)]$	0.003 183	0.013 922	0.015 023	0.015 637
$W_{ll}^{\Gamma}(\omega)$[a]				
N_{111}	0	0.073 960	0.020 204	0.018 715
B_{111}	0.011 437	0.109 983	0.106 946	0.186 669
B_{100}	0.013 169	0.121 561	0.099 387	0.145 394
T_{110}	0.012 115	0.116 146	0.098 356	0.158 150
D_{110}	0.008 165	0.142 338	0.083 011	0.115 622
R_{100}	0.007 986	0.133 708	0.091 557	0.147 468
T_{100}	0.012 579	0.118 148	0.098 458	0.151 229

[a] See footnote of Table III for orbital notation.

in Table VII,[28] the spin relaxation rates $1/T_1$ have been calculated for these alloys. The total density of electronic states $2\mathfrak{D}(E_F)$ was estimated from specific-heat data of Martin.[29] The results are presented in Table VIII, where they are compared with the corresponding relaxation rates calculated from the free-electron formula [Eq. (20)], and with the experimental relaxation rates measured by Monod.[30] It is interesting to note that the value of the spin-flip relaxation rate calculated from Eq. (19) differs significantly from the value calculated in the free-electron approximation from Eq. (20), indicating that host lattice backscattering contributes significantly to conduction-electron spin relaxation. When backscattering effects are included, our results agree well with the experimental data for Ga and Ge. This agreement is independent of small shifts in the impurity potentials. The agreement between calculation and experiment is understandably poorer for Ni and Zn. First, we have neglected spin-orbit interactions in the Cu host. The estimated spin-orbit parameters for copper are significantly smaller than those of Ga and Ge, but comparable in magnitude to those of Zn. Second, the spin-orbit interaction of Ni is mainly of d-wave character. Strong exchange interactions among the d electrons are responsible for the magnetic properties of pure Ni. Even if there is no local-moment formation in Cu(Ni), one might suspect that j is no longer a good quantum number inside the Ni muffin-tin sphere. It has been shown by Yafet[31] that the spin-flip scattering rate due to spin-orbit interaction can be enhanced in the presence of a local moment. Whether the spin-flip scattering rate can also be enhanced by an incipient local moment, or by electron-electron correlations in general, is an interesting problem for further investigation. For comparison with these fourth row impurities, we have estimated the inverse spin-flip relaxation time $1/T_1$ for Cu(Au), approximating the relativistic phase shifts by those of pure Au. Our results suggest that the scattering rate in Cu(Au) is roughly an order of magnitude larger than in Cu(Ga) and Cu(Ge) (Table VIII).

The construction of accurate effective impurity potentials was not the focus of the present work. The spin-orbit interaction is strongest in the spatial region of the atomic core, where the potential is well described by any reasonable atomic potential, and we therefore expect that our calculated spin-flip scattering rates should be rather insensitive to inaccuracies in the constructed potentials. On the other hand, Dingle-temperature anisotropies are expected to be sensitive to the details of the effective impurity potentials. Ideally, one would like to analyze Dingle-temperature anisotropy and spin-flip scattering data simultaneously in order to infer the relativistic impurity phase shifts, thereby obtaining the greatest possible amount of information about the impurity potential. This we have done for Cu(Ge), using the Dingle-temperature data of Poulsen, Randles, and Springford[32] and the spin-flip scattering data of Monod,[30] as well as for Cu(Au) using the Dingle-temperature data of Poulsen *et al.*[32] and the spin-flip rate estimated as described above. Our results are given in Table IX. We find that the Dingle-temperature and the spin-flip scattering data can be fit simultaneously to give reasonable values of both the impurity spin-orbit parameters and impurity phase shifts. We find that the quality of the fits to the Dingle-temperature anisotropy data is only very weakly, if at all, affected by the inclusion of spin-orbit effects in the analysis. Both the relativistic and the nonrelativistic analyses of Cu(Ge) data imply an s-wave phase shift $\eta_{0,1/2}^{i}(E_F)$ which is considerably smaller than that calculated from the constructed impurity potential for this alloy (Table VI). It may be that the experimental Dingle temperature anisotropy includes contributions from lattice-strain effects. The impurity phase shifts for

TABLE VIII. Spin-orbit induced spin-lattice relaxation rate for conduction electron spin resonance.

	$1/T_1$ ($10^{10}\,\mathrm{sec}^{-1}/\mathrm{at.}\,\%$)		
Alloy	Present calculation[a]	Free electron calculation[b]	Experiment[c]
Cu(Ni)	24.9	10.4	44.9 ± 3.5
Cu(Zn)	0.8	1.4	1.5 ± 0.2
Cu(Ga)	3.0	5.5	3.3 ± 0.4
Cu(Ge)	7.1	8.4	6.9 ± 0.7
Cu(Au)	50 ± 10	50 ± 10	···

[a] Equation (19).
[b] Equation (20).
[c] Philippe Monod, Ref. 30.

TABLE IX. Phase-shift analyses of Dingle-temperature and spin-flip scattering data for Cu(Ge) and Cu(Au).

	Cu(Ge)			Cu(Au)		
	Experiment	Nonrelativistic fit[b]	Relativistic fit	Experiment	Nonrelativistic fit[b]	Relativistic fit
Orbit		Dingle temperatures (°K/at.%)[a]				
N_{111}	118(18)	184	185	7.9(9)	7.6	7.6
B_{111}	114(11)	110	104	15.1(11)	13.8	13.1
B_{100}	109(8)	116	112	13.2(10)	13.3	13.7
T_{110}	119(12)	116	110	13.9(14)	13.5	13.5
D_{110}	161(18)	137	134	12.4(9)	11.6	11.6
R_{100}	119(7)	130	126	10.2(8)	12.3	11.7
T_{100}	100(13)	116	111	12.9(14)	13.4	13.6
		Spin-flip scattering rate (10^{10} sec^{-1}/at.%)				
$1/T_1$	6.9(7)[c]	0	6.9	...	0	50
$\eta^i_{lj}(E_F)$		Impurity phase shifts (rad)				
$0\frac{1}{2}$		0.232	0.135		0.403	0.493
$1\frac{1}{2}$		1.106	1.176		0.008	0.065
$1\frac{3}{2}$		1.106	1.090		0.008	−0.095
$2\frac{3}{2}$		0.126	0.082		−0.228	−0.149
$2\frac{5}{2}$		0.126	0.069		−0.228	−0.219
		Friedel sum [Eq. (10)]				
$\mathfrak{F}(E_F)$		2.1	2.0		−0.5	−0.3

[a]Experimental values quoted from Ref. 32; see footnote of Table III for explanation of orbital notation.

[b]Reference 4.

[c]Reference 30.

Cu(Au) are close to the phase shifts for pure gold that correspond to the same value of the Fermi energy parameter. The relativistic impurity phase shifts for Cu(Au) are tentative because they are based on our estimate of $1/T_1$; there being, to our knowledge, no experimental measurements of $1/T_1$ for this alloy.

V. CONCLUSIONS

It has been shown that relativistic effects can be easily incorporated into a phase shift analysis of Fermi-surface anisotropies and impurity scattering in noble metals and their dilute alloys. In these metals, in contrast to the divalent hexagonal metals and many transition metals, the spin-orbit interaction does not produce qualitative changes in the shape of the Fermi-surface or the Dingle-temperature anisotropy. We have shown that the effect of the spin-orbit interaction upon these properties is small, and that it is close to the limit of what is experimentally observable at the present time. Spin-flip scattering rates, on the other hand, depend strongly upon the magnitude of the spin-orbit interaction and can be used, together with Dingle-temperature anisotropy data, to determine the relativistic phase shifts for an impurity in a nonrelativistic host. The possibility of wider application of such analyses depends upon experimental measurements being made of $1/T_1$ for dilute copper alloys such as Cu(Au).

Experimental observations of impurity scattering may be influenced by lattice distortion in the vicinity of the impurity site. The effects of departures from a uniform lattice are neglected in the expressions derived above on the basis of an ideal muffin-tin lattice. Lattice distortion can contribute both to the primary scattering, by altering the effective potential on the impurity site, and to the backscattering, by locally altering the host structure factor. Consequently, lattice distortion can contribute to the scattering parameters determined by fitting Dingle-temperature data. It seems likely that the failure of the Friedel phase shifts, determined from analysis of Dingle-temperature data, to satisfy the Friedel sum rule in certain alloys can be attributed to the effects of lattice distortion. Lattice distortion is expected to contribute less strongly to spin-orbit induced spin relaxation, since in this case the primary scattering is caused by the strong potential gradient at the impurity nucleus, which is only weakly influenced by the local lattice structure. This argu-

ment suggests that the calculated impurity phase shifts from which spin-flip relaxation times are derived, can be taken to satisfy the Friedel sum rule, as we have done. A quantitative study of electron scattering in a distorted lattice is needed to clarify this point.

In discussing spin-flip scattering, we have judiciously avoided consideration of spin-orbit effects in the host metal. Host spin-orbit effects cause difficulty in interpreting experimental data to yield a measurement of $1/T_1$, by introducing additional mechanisms which contribute to the experimental linewidth.[33] In addition, the inclusion of host spin-orbit interactions involves the interesting theoretical problem of how to determine the effective spin-up ($\uparrow$) and spin-down ($\downarrow$) states in a weak magnetic field. From both the experimental and the theoretical points of view, a general treatment of spin-flip scattering due to spin-orbit interaction requires further investigation.

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APPENDIX A: SUMMARY OF RESULTS CONCERNING NONRELATIVISTIC IMPURITY SCATTERING

The nonrelativistic expression for the T matrix is most conveniently written as a sum of partial-wave single-point-group components:

$$T^{\theta'\theta}_{\vec{k}'\vec{k}}(E) = -\sum_{l\Gamma\gamma;\,l'} f^{*}_{l\Gamma\gamma}(\vec{k}',\,E)(\xi - \chi^{\Gamma})^{-1}_{ll'} f_{l'\Gamma\gamma}(\vec{k},\,E)\delta_{\theta'\theta}\,. \tag{A1}$$

Since the nonrelativistic T matrix is diagonal in the electron-spin polarization, the indices θ, θ' are usually omitted from the nonrelativistic expression. The notation used here differs from the notation of Refs. 2 and 4. For $l \leq 2$, the nonrelativistic kernel of the T matrix (A1) is diagonal and is related to the scattering parameter $S_{l\Gamma}$ introduced in Ref. 2 according to

$$S_{l\Gamma} = \sin^2\eta^h_l(\xi_l - \chi^{\Gamma}_{ll})^{-1}\,. \tag{A2}$$

The partial-scattering rate $t^{l\Gamma}_k$ introduced in Ref. 2 is related to the diagonal nonrelativistic partial-wave factor (6) of the present notation by

$$t^{l\Gamma}_{\vec{k}} \equiv (1/\sin^2\eta^h_l)\, G^{\Gamma}_{ll}(\vec{k},\,E_F)\,. \tag{A3}$$

APPENDIX B: CALCULATION OF PHASE SHIFTS $\eta^{(a)}_{lj}(E)$ FROM SOLUTIONS OF THE RADIAL DIRAC EQUATION

Loucks[27] has shown how the radial Dirac equation can be written as a pair of coupled first-order differential equations for the upper $[g_{lj}(r)]$ and lower $[f_{lj}(r)]$ wave function components. For a given electronic energy E (total relativistic energy minus rest energy) the amplitudes of these components at the muffin-tin radius s can be determined by numerical integration. The quantity $L_{lj}(E) = cf_{lj}(s)/g_{lj}(s)$ (where c is the velocity of light) is analogous to the logarithmic derivative of the solution to the radial Schrödinger equation in a nonrelativistic treatment. $L_{lj}(E)$ is related to the phase shifts $\eta_{lj}(E)$ according to

$$\tan\eta_{lj}(E) = \frac{L_{lj}(E)\,j_l(\kappa s) + Kj_{l+1}(\kappa s)}{L_{lj}(E)\,n_l(\kappa s) + Kj_{l+1}(\kappa s)} \quad \text{for } j = l + \tfrac{1}{2}\,, \tag{B1}$$

and by

$$\tan\eta_{lj}(E) = \frac{L_{lj}(E)j_l(\kappa s) - Kj_{l-1}(\kappa s)}{L_{lj}(E)n_l(\kappa s) - Kn_{l-1}(\kappa s)} \quad \text{for } j = l - \tfrac{1}{2}. \tag{B2}$$

Here κ is the scalar wave vector $\hbar\kappa = [2mE + (E/c)^2]^{1/2}$, $K = E/\hbar\kappa$, and j_l and n_l are spherical Bessel and Neumann functions, respectively.

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