

lattice constant). When an atom is removed, the volume available to the electrons on the remaining atom in the unit cell is doubled. It is assumed that in this region, four valence electrons occupy a volume of $\frac{1}{4}a^3$. The interaction energy is determined from formulas for the free-electron gas, containing direct, exchange, and correlation terms.¹⁵ Suppose n electrons occupy uniformly a volume $\frac{4}{3}\pi r_s^3$ (this quantity being set equal either to $\frac{1}{8}a^3$ or $\frac{1}{4}a^3$), then their interaction energy is (in Ry)¹⁴

$$E_I = \frac{1.2n^2}{r_s} - \frac{0.916n^{4/3}}{r_s} - nE_c \frac{r_s}{n^{1/3}}. \quad (33)$$

Here, E_c is the correlation function. We employ the formula of Pines¹⁶

$$E_c = -0.115 + 0.031 \ln r_s. \quad (34)$$

However, the contribution from the correlation term

is quite small compared to the direct and exchange terms, so that uncertainties in E_c do not contribute significantly to the uncertainty in the final result.

The decrease in the electron interaction energy computed in this way amounts to 0.83 Ry (11.3 eV). This is quite close to half of the contribution from the one-electron energies. It is quite probably an overestimate, since the electrons are not uniformly spread through the available volume but are partially confined to covalent bonds. The change in energy associated with the formation of a vacancy is thus estimated as 0.84 Ry. This is not, however, the observed formation energy, as the displaced atom must be deposited somewhere (either as an interstitial, or on the surface). Much of this energy is recovered in that process, and a calculation of the formation energy of a vacancy, or of a vacancy-interstitial pair cannot be completed without such considerations. We hope to return to this problem in a future paper.

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Impurity Lifetime Broadening on Noble-Metal Fermi Surfaces*

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A simple theory of lifetime broadening due to scattering from isolated impurities in noble-metal hosts is presented and used to calculate the Dingle temperature observed in de Haas-van Alphen experiments. Details of the scattering anisotropy are easily calculated when the impurity is a transition metal. Numerical estimates of the Dingle temperatures for three extremal orbits are in good agreement with experiments on CuNi and CuZn.

INTRODUCTION

Accurate de Haas-van Alphen measurements of lifetime broadening in dilute alloys¹ now provide a very specific measure of the strength and anisotropy

of electron impurity scattering at the Fermi surface of noble metals. Difficulties in constructing an impurity potential have so far deterred theoretical calculations in the cases where the impurity is of different valence or a transition metal. This

paper presents a simple low-concentration scattering theory, appealing primarily to the atomic properties of the impurities. For transition-metal impurities, the anisotropy of the lifetime broadening over the Fermi surface is easily calculated. A good account of the experimental observations in CuNi and CuZn is obtained.

From the decay envelope of a de Haas-van Alphen signal one observes an effective temperature increase, or "Dingle temperature,"² X , related to the lifetime broadening of a Landau level by

$$X = \Gamma(E_F)/\pi\kappa, \quad (1)$$

where κ is the Boltzmann constant, and Γ , as Brailsford³ has shown, is the imaginary part of the electron self-energy in the presence of impurities, calculated at zero field and suitably averaged over an extremal orbit. Thus the Dingle temperature is a direct experimental measure of the scattering of a quasiparticle by impurities, unlike the resistivity and other transport properties, whose interpretation requires the solution of transport equations. Dingle temperatures have usually been evaluated⁴ from the total cross section for single impurity scattering. However, that approach is merely equivalent to (1) by the optical theorem⁵ in the low-concentration limit, and the form (1) is more general.

THEORY

For a sufficiently low impurity concentration c , the independent scattering approximation⁶ will be valid, and $\Gamma(\vec{k})$, for a state ψ_k on the Fermi surface, is given by

$$\Gamma(\vec{k}) = (c \operatorname{Im} \sum_i \langle \psi_k | T | i \rangle \langle i | T | \psi_k \rangle) / (E_k - E_i + i\epsilon), \quad (2)$$

where the $|i\rangle$ are intermediate states and T is the t matrix which describes exactly the scattering by one impurity.

For heterovalent impurities with no d orbitals near the Fermi surface, the $|i\rangle$ are states on the Fermi surface and the sum over intermediate states is difficult to carry out in practice. Therefore we replace the sum by an average over the Fermi surface, and use as an estimate of the matrix element the average diagonal element $\langle \langle \psi_k | T | \psi_k \rangle \rangle_{\text{av}} = \Delta E_{\text{OPW}}$. Here ΔE_{OPW} is just the average energy shift of a state at the Fermi surface, and can be estimated from atomic considerations. The energy denominators, when averaged, give an imaginary contribution of $\pi\rho_{\text{host}}(E_F)$, where $\rho_{\text{host}}(E_F)$ is the host density of states at the Fermi surface.

With these simplifications, Γ_{OPW} for OPW's scattered by heterovalent impurities is given by

$$\Gamma_{\text{OPW}} = c\pi\rho_{\text{host}}(E_F)(\Delta E_{\text{OPW}})^2. \quad (3)$$

When the impurity is a transition metal, there is

a second contribution to Γ in which the intermediate state $|i\rangle$ is an impurity d orbital, and not T but the impurity Hartree-Fock potential V enters the matrix element. Because each d orbital is broadened into a virtual level by mixing with the host conduction band, we replace E_i in (2) by $E_d + i\Delta_d(E_F)$, and obtain

$$\Gamma_{sd}(\vec{k}) = (c \operatorname{Im} \sum_d \langle \psi_k | V | d \rangle \langle d | V | \psi_k \rangle) / (E_k - E_d - i\Delta_d(E_F)). \quad (4)$$

We shall assume that E_d and $\Delta_d(E_F)$ are the same for all five d orbitals, and treat the imaginary part of $(E_k - E_d - i\Delta_d(E_F))^{-1}$ as a common density of d states, $\rho_d(E_F)$, per impurity atom. This is reasonable because crystal field splitting is negligible in the transition metals, and the differences between the d -band partial densities of states associated with different orbital symmetries in pure Ni⁷ are due primarily to d - d overlap, which is absent in the low-concentration limit. This approximation yields

$$\Gamma_{sd} = c\pi\rho_d(E_F) \sum_d |\langle \psi_k | V | d \rangle|^2. \quad (5)$$

Impurity scattering was first treated in this way by Anderson.⁸ Heine has shown⁹ that the orbitals $|d\rangle$ in (5) are in fact the atomic orbitals one would use in constructing a tight-binding wave function, and Hubbard¹⁰ has established the equivalence between this description and that of resonant d -wave scattering.

To evaluate (5), we expand ψ_k in a basis of OPW's

$$\psi_k = \sum_i \alpha_i(\vec{k}) |\vec{k} - \vec{Q}_i\rangle, \quad (6)$$

where the \vec{Q}_i are reciprocal lattice vectors, and $\sum_i |\alpha_i|^2 = 1$. The matrix elements may be factored into radial and angular integrals, and the sum over d states carried out, with the result

$$\Gamma_{sd} = \pi c \rho_d(E_F) V_{sd}^2(k_F) \Theta(\vec{k}), \quad (7)$$

in which only the angular part,

$$\Theta(\vec{k}) = 1 + \sum_{i \neq j} \alpha_i^*(\vec{k}) \alpha_j(\vec{k}) P_2(\cos \phi_{ij}), \quad (8)$$

depends upon the direction of \vec{k} . In (8), $P_2(x) = \frac{1}{2}(3x^2 - 1)$, and ϕ_{ij} is the angle between $\vec{k} - \vec{Q}_i$ and $\vec{k} - \vec{Q}_j$. The radial part $V_{sd}(k)$ depends only weakly on the magnitude of k .⁹ Since the states which will be of interest are well represented by a few OPW's of nearly equal length, we have approximated $V_{sd}(k - Q)$ by $V_{sd}(k_F)$, and taken it outside the sum over reciprocal lattice vectors in (8). It should be noted that, in deriving (3) and (7), direct effects of the host d bands have been neglected. These lie several volts below E_F , and contribute only a small admixture to the states at the Fermi surface.

ANISOTROPY

The anisotropy in $\Gamma_{sd}(\vec{k})$, a quantity of experimental interest, is now given by $\Theta(\vec{k})$. If ψ_k is a single OPW, $\Theta(\vec{k})=1$, but on the Fermi surface of Cu, sketched in Fig. 1, this is seldom true. The Fermi surface lies everywhere close to the zone boundary, touching it at "necks" along the $\langle 111 \rangle$ axes. Thus at least two OPW's contribute to ψ_k at every point of the Fermi surface, and there will be interference terms in $\Theta(\vec{k})$. To characterize the resulting anisotropy we have calculated $\Theta(\vec{k})$ at several points which lie on the three well-studied orbits shown in Fig. 1: the "neck" orbit and two inequivalent "belly" orbits.

For \vec{k} on the neck, $\psi_k = (|\vec{k}\rangle - |\vec{k} - \vec{L}\rangle)/\sqrt{2}$, and $\Theta(k)$ is given by

$$\Theta_{\text{neck}} = 6k_N^2 |L|^2 / (k_N^2 + |L|^2)^2, \quad (9)$$

where k_N is the radius of the neck, and $|L|$ is the length of the wave vector $\vec{L} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. The total cross section for scattering of the neck states from the d resonance is seen in (9) to be very sensitive to the size of the neck radius. If k_N were zero, then ψ_k would be antisymmetric, and would not scatter at all. Using the Cu Fermi surface dimensions summarized by Lee,¹¹ one finds that $\Theta_{\text{neck}} = 0.165$.

States on the belly of the Cu Fermi surface are commonly thought of as free-electron-like, yet Θ was found to vary widely over the two belly orbits. In calculating Θ , we have used wave functions obtained by perturbation theory with values of the pseudopotential coefficients taken from an interpolation scheme calculation of the Cu band structure.⁷ At the points (A), where the $[111]$ belly orbit passes beneath the line from L to U (BSW¹² notation), and (C), on the $\Delta[100]$ axis, two OPW's

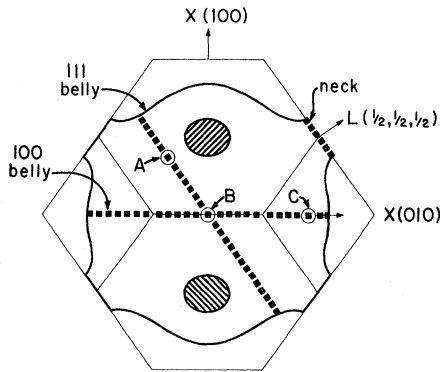


FIG. 1. Cu Fermi surface, viewed down the $[110]$ axis. The light lines indicate the Brillouin zone boundaries, while the wide dashed lines denote de Haas-van Alphen orbits discussed in the text. The anisotropy factor Θ for s - d scattering was calculated at the points A, B, and C on the Fermi surface.

dominate ψ_k . In both cases, interference reduces Θ significantly to $\Theta_A = 0.50$, $\Theta_C = 0.45$. The point (B), however, at the intersection of the $\Sigma[110]$ axis with the Fermi surface, lies beneath the intersection of two zone faces, so three OPW's contribute to ψ_k . We find that $\Theta_B = 0.99$, with a cross term between the two higher plane waves acting to enhance the s - d scattering.

We can use these values of Θ to obtain estimates of the relative magnitudes of the s - d contributions to the Dingle temperatures of the three orbits considered in Fig. 1. The Γ which appears in (1) is obtained from the $\Gamma(\vec{k})$ on a given orbit by taking a weighted average in which the inverse of the group velocity v_k is the weight factor. Since v_k varies little over the $[111]$ belly orbit, we estimate the weighted average of Θ as $\frac{1}{2}(\Theta_A + \Theta_B)$, or $\Theta_{[111]\text{belly}} = 0.75$. The states beneath the $[100]$ zone face have slightly greater velocities than average, so the portions of the $[100]$ belly orbit lying beneath the intersection of the two hexagonal zone faces will tend to dominate the average. The enhancement seen in Θ_B will affect all the states along these portions of the orbit, so we conclude that

$$0.99 \geq \Theta_{[100]\text{belly}} > \Theta_{[111]\text{belly}} \approx 0.75.$$

There is experimental evidence¹³ that impurity scattering is indeed stronger on the $[100]$ belly orbit than on the $[111]$ belly.

The form (4) is easily generalized to the case where the impurity atoms have a magnetic moment, but the host remains paramagnetic.¹⁴ Thus the discussion of the anisotropy as given by $\Theta(\vec{k})$ remains valid for Kondo systems, such as CuFe. Templeton *et al.*¹ have measured Dingle temperatures for the neck and $[111]$ belly orbits in CuNi, CuCo, and CuFe. They find that $X_{\text{neck}} = (25 \pm 1)$, 70, and 100 deg/at.%, while $X_{\text{neck}}/X_{\text{belly}} = 0.5$, 0.4, and 0.3. We argue below that Γ_{OPW} should be roughly constant for the three systems, so the observed $X_{\text{neck}}/X_{\text{belly}}$ ratios in these three cases appear to approach a value characteristic of s - d scattering. Our calculated anisotropy $\Theta_{\text{neck}}/\Theta_{[111]\text{belly}} \approx 0.22$ agrees very well with this limit.

When Ag, instead of Cu, is the host, the s - d contribution to the impurity-scattering lifetime broadening will be still more anisotropic. The Fermi surface shrinks in going from Cu to Ag, and the necks become about 30% narrower.¹⁵ Consequently, $\Theta_{\text{neck}} = 0.09$ in Ag, about half the value found in Cu. At the same time the states on the bellies will contain a smaller admixture of higher OPW's, so that Θ_{belly} will be closer to unity. The resulting ratio of the s - d scattering strength on the belly to that on the neck will be more than twice as great in Ag hosts as in Cu. Unfortunately, there appears to be no published de Haas-van Alphen data on Ag-host alloys with transition-metal impurities against

which to check this prediction. Data on classical transport properties sensitive to scattering anisotropy such as the Hall coefficient are available, but their interpretation requires more elaborate calculations, for which the simple perturbation-theory wave functions used in estimating $\Theta(\vec{k})$ are not adequate.

QUANTITATIVE RESULTS

To evaluate the remaining parameters of (3) and (7), we assume only that an impurity cell, once screened to preserve local charge neutrality, will contain essentially the potential found in a pure crystal of the same substance. For Fe, Co, Ni, and Cu, Hartree-Fock potentials associated with the $3d^7 4s^1$ configuration all give physically reasonable band structures.¹⁶ Using such potentials, Watson, Ehrenreich, and Hodges¹⁷ have studied the relative position of the bottom of the conduction band in these materials, taking into account crudely the effects of screening at metallic densities. Comparing Cu with Ni, they find a shift of 0.5 eV. We shall use this value as an estimate of the matrix element ΔE_{OPW} needed in (3) for the case of CuNi. The same argument gives $\Delta E_{OPW} = 1.0 - 1.4$ eV for CuZn, where we have taken the shift of the 4s levels calculated by Hermann and Skillman¹⁸ for isolated atoms, and the uncertainty is an estimate of the greater effect of metallic screening on the two 4s electrons of Zn.

With these parameters, and the value $\rho_{\text{host}}(E_F) = 0.18$ estimated for Cu by Hodges *et al.*,⁷ we obtain for the CuZn Dingle temperature $X = 27 \pm 9$ deg/at.%. This is in reasonable agreement with, although somewhat greater than, the most recent experimental value $(21 \pm 1)^\circ$ at the necks, obtained by Templeton *et al.*¹ In CuNi we obtain $X_{OPW} \approx 4$ deg/at.%. The similarity of the $3d^7 4s^1$ potentials associated with the other transition metal impurities suggests that X_{OPW} will not be much greater in CuFe, for example, than in CuNi.

$V_{sd}(k_F)$ can be evaluated from the hybridization splitting of the two Δ_1 bands, as suggested by Heine.⁹ The result is $V_{sd} = 3.6$ eV. We find $\rho_d(E_F) = 0.08$ by assuming that ρ_d is a Lorentzian with the half-width 0.7 eV observed by Seib and Spicer,¹⁹ then placing it with respect to the Fermi level by the requirement that there be 9.4 d states per impurity atom, as in pure Ni.⁷ This value of $\rho_d(E_F)$ is probably an underestimate, since including the effects of energy dependence of Δ_d can be shown to modify $\rho_d(E)$ in such a way that $\rho_d(E_F)$ increases.

Measurements of the electronic specific heat of moderately dilute CuNi alloys²⁰ provide a rough upper bound to $\rho_d(E_F)$, and consequently furnish a check on the above estimate. If we assume that the increase in the linear term γT in the electronic

specific heat is solely due to an extra density of states $c \rho_d(E_F)$ at the Fermi level, and extrapolate the data reported in Ref. 20 to low concentrations, we obtain $\rho_d(E_F) \approx 3 \cdot \rho_{\text{host}}(E_F)$ or $\rho_d(E_F) \approx 0.5$. This value is too high by a factor of 2 or 3, as it ignores the spin-fluctuation enhancement known to be significant at higher concentrations.²⁰ Consequently, for CuNi the estimate of the preceding paragraph [$\rho_d(E_F) = 0.08$] should not be in error by more than a factor of 2 or 3. Using it, we obtain $X_{sd} = 17$ deg/at.%. The total Dingle temperature calculated for CuNi, $X = 21^\circ$, is to be compared with the experimental result¹ that $X = 25 \pm 1$ deg/at.%.

CONCLUSIONS

The agreement obtained between the experimental and calculated values of X for both CuZn and CuNi is encouraging, since the expressions (3) and (7) depend on only a few physical parameters, most of them well known. This suggests that experimental study of Dingle temperatures, and especially of the strongly anisotropic s - d contributions, can provide information about the less certain parameters. In particular, measurement of the temperature dependence of the anisotropy in the lifetime broadening in Kondo systems whose moment is just stable enough to overcome magnetic field quenching²¹ (perhaps CuCr or CuFe) will provide a direct measure of the effective scattering strength of the impurity.

Calculations are being undertaken to put this work on a fully quantitative footing by using accurate Cu wave functions¹¹ to carry out the Fermi-surface integral in (2) and improve the estimates of Θ reported above. In this way a complete description of lifetime broadening on the Fermi surface is obtained in terms of a few physically understood parameters: two pseudopotential coefficients and a single s - d scattering strength. This description also permits straightforward calculation of conventional transport properties in dilute transition-metal-host alloys.

After this paper was completed, a paper by Lowndes, Miller, and Springford²² reached us in which a heuristic model of the variation of the lifetime broadening is proposed, and fitted to the Dingle temperatures measured over five orbits of high symmetry in Au-host alloys. Their results are in general quite consistent with the predictions of (3) and (7). For example, in AuFe they find somewhat stronger scattering on the [100] belly orbit than on the [111] belly, with the consequence, in their model, that strong scattering is predicted over the region of the Fermi surface lying beneath the intersection of the two hexagonal zone faces, as was suggested above in the discussion of Θ_B . From the value of $X_{\text{neck}}/X_{[111]\text{belly}} \approx 0.6$, which they obtain

for AuFe, we conclude that the s - d and other scattering contributions are of equal magnitude. However, the variation of $\Gamma(\vec{k})$ over the various belly orbits obtained from their model is greater than we predict from consideration of the s - d term Γ_{sd} alone. Since the model of Ref. 22 is purely heuristic, we cannot resolve this discrepancy, without further study of the anisotropy contained in the

ordinary scattering, as described in (2).

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Optical Anisotropy of Silicon Single Crystals*

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The birefringence of Si single crystal was measured for He-Ne laser light of wavelength $\lambda = 1.15 \mu$ propagating along $\langle 110 \rangle$ directions, and found to be $\Delta n = n_{\langle 110 \rangle} - n_{\langle 100 \rangle} = (5.04 \pm 0.12) \times 10^{-6}$. For $\langle 100 \rangle$ and $\langle 111 \rangle$ directions of propagation, no birefringence was observed. The magnitude and symmetry of the observed optical response as well as the spectral dependence of birefringence are in good agreement with the theory of spatial dispersion in cubic crystals.

INTRODUCTION

According to classical crystal optics which neglects spatial dispersion and takes into account only dipole-type transitions, cubic crystals should be optically isotropic.¹ Lorentz indicated the possibility of optical anisotropy in cubic crystals if one considers the polarization in a given point to be dependent not only on the value of the local field at that point but also on its value in the close neigh-

borhood, i. e., polarization being not only frequency but also wave vector dependent. On the Lorentz calculation, the birefringence is a maximum for the cubic crystal for light propagation along $\langle 110 \rangle$ directions and takes the value²

$$\Delta n = 0.44\pi\bar{n}(\bar{n}^2 - 1)^2(a/\lambda)^2, \quad (1)$$

where a is the characteristic dimension of the order of the molecule size or interatomic distance, λ is the wavelength, and \bar{n} is the mean of the mea-