# Empirical electron-phonon coupling constants and anisotropic electrical resistivity in hcp metals

B. A. Sanborn and P. B. Allen

*Department of Physics, State University of New York, Stony Brook, New York 11794-3800*

D. A. Papaconstantopoulos

*Complex Systems Theory Branch, Naval Research Laboratory, Washington, D.C. 20375-5000*

(Received 8 May 1989)

The Fermi-surface density of states $N(0)$ and Drude-plasma-frequency tensor $(\Omega_p^2)_{\alpha\beta} = 4\pi e^2 N(0)\langle v_\alpha v_\beta \rangle$ are calculated for 14 metallic elements with hcp structures. By comparison with measured anisotropic resistivity components $\rho_\perp$ and $\rho_\parallel$, electron-phonon coupling constants are extracted. The resulting values of $\lambda_{tr}$ compare reasonably well with $\lambda$ from $T_c$ for the ten superconducting elements and provide new information on electron-phonon coupling for the four that are not. In particular, $\lambda_{tr}$ for Mg is sufficiently low as to discourage a further search for superconductivity, whereas $\lambda_{tr}$ for Sc and Y is sufficiently high (0.5–0.6) to require spin-fluctuation suppression of $T_c$ and motivate a low-$T$ search for exotic superconductivity. Co is found to have very weak electron-phonon coupling in the majority-spin band and much stronger specific-heat enhancement in the minority-spin band. The anisotropy $\rho_{zz}/\rho_{xx} = \rho_\parallel/\rho_\perp$ is moderately well accounted for by the anisotropy of the Drude plasma frequency $(\Omega_p^2)_{xx}/(\Omega_p^2)_{zz} = \langle v_x^2 \rangle / \langle v_z^2 \rangle$, except for the $sp$ elements, which have significant scattering anisotropy ($\lambda_{zz}/\lambda_{xx} \neq 1$). A systematic onset of "resistivity saturation" (signifying a breakdown of Boltzmann theory) is found when the mean free path $l \lesssim 10$ Å. The onset occurs at a variable value $40 < \rho < 160$ $\mu\Omega$ cm.

## I. INTRODUCTION

Transport properties of hexagonal-close-packed (hcp) metals are interesting because the noncubic symmetry of this structure requires that quantities such as resistivity be anisotropic. Angular correlations may be possible which are not seen in the scalar quantities associated with materials of cubic symmetry. Also, deviation of the hcp lattice constants from the ideal $c/a$ ratio of $(\frac{8}{3})^{1/2}$ is reflected in nonspherical charge densities at atomic sites,[1,2] which could affect the scattering properties of these centers in significant ways. The additional considerations necessary to account for the anisotropic nature of transport in these materials may be viewed as a test for methods which have proved to be successful for analyzing the dc resistivity of cubic metals.

One useful method for understanding the room-temperature dc resistivity of metals was proposed by Chakraborty, Pickett, and Allen[3] and has been carried out[4] for 25 cubic metals. This approach makes use of the fact that the electron-phonon interaction determines both conventional (BCS-type) superconductivity and normal-state resistivity at high temperature. The electrical resistivity $\rho$ of a crystalline metal is related to the quasiparticle transport scattering rate $1/\tau$ of the material and the Drude plasma frequency $\Omega_p$ according to the relation

$$\rho = 4\pi/\Omega_p^2\tau .\qquad (1)$$

Consider $\rho$ in Eq. (1) to stand for the resistivity of a metal after the residual resistivity due to impurities is subtracted off. $1/\tau$ is then related to $\lambda_{tr}$, the electron-phonon

coupling parameter for transport properties, through the high-temperature expansion[3] of the lowest-order variational solution to the Bloch-Boltzmann equation:

$$\hbar/\tau = 2\pi\lambda_{tr}k_B T(1 - \hbar^2\langle\omega^2\rangle_{tr}/12k_B^2 T^2 + \cdots ) ,\qquad (2)$$

where $\langle\omega^2\rangle_{tr}$ is a weighted mean-square phonon frequency of the metal. The electron-phonon mass enhancement $\lambda$, which determines the transition temperature of conventional superconductors, is closely related to $\lambda_{tr}$. However, they are not necessarily equal, and it is one of our goals to study their relative magnitudes. The approach of Ref. 3 is to calculate $\Omega_p$ from energy-band theory and to combine this result with an experimental value for $\rho$ according to Eqs. (1) and (2) to obtain an empirical value for $\lambda_{tr}$. If the metal is superconducting, this number may then be compared to a value for $\lambda$ obtained from an experimental value for $T_c$ according to the McMillan equation,[5]

$$T_c = \frac{\Theta_D}{1.45}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right] .\qquad (3)$$

Here, $\Theta_D$ denotes the Debye temperature of the material and $\mu^*$ represents a repulsive electron-electron interaction.

The validity of this empirical method for finding a value for $\lambda_{tr}$ has been confirmed by detailed microscopic calculations[6] (using the rigid muffin-tin model) of $\lambda_{tr}$ for Cu, Nb, Ta, and Pd. The close agreement between $\lambda_{tr}^{emp}$ and $\lambda_{tr}^{calc}$ suggests that the role of the electron-phonon interaction in the dc resistivity of these metals is well un-

derstood and demonstrates the accuracy of the empirical method of finding $\lambda_{tr}$. In contrast, the empirical values of $\lambda$ found for Nb and Ta from the McMillan equation show greater differences from the values obtained through theoretical calculations.[6] $(\lambda_{calc}-\lambda_{McM})/\lambda_{calc}$ is 27% for Nb and 26% for Ta. Also, from these calculations one finds that $|\lambda_{calc}-\lambda_{tr\ calc}|/\lambda_{calc} < 10\%$ for Cu, Pd, and Nb, whereas for Ta the value is 35%. We know of no published theoretical calculations of transport properties for hcp transition metals. There have been calculations for hcp metals like Mg, Zn, and Cd with only $s$ or $p$ electrons at $\varepsilon_F$. Of these, the most complete is by Tomlinson[7,8] for Zn.

Another value for $\lambda$ may be obtained from an experimental value for the electronic specific-heat coefficient $\gamma$ and a band-theoretical value for the quasiparticle density of states at the Fermi energy, $N(0)$. $\gamma$ is proportional to the true quasiparticle density of states at the Fermi energy, $N_\gamma(0)$:

$$\gamma = \pi^2 k_B^2 N_\gamma(0)/3 ,\qquad (4)$$

and many-body effects make $N_\gamma(0)$ larger than $N(0)$:

$$1+\lambda_\gamma \equiv N_\gamma(0)/N(0) .\qquad (5)$$

$\lambda_\gamma$ is equal to $\lambda$ provided $N(0)$ is calculated from an exact quasiparticle band structure which includes all many-body effects except electron-phonon interaction.[9] The estimated reliability of the empirical values for $\lambda_{tr}$ and $1+\lambda_\gamma$ is about 10–20 %, so that, for small $\lambda$, $\lambda_\gamma$ is a much less accurate number.

In this paper we report empirical values of $\lambda_{tr}$ and $\lambda_\gamma$ for 14 hcp metals calculated by means of the method of Ref. 3 generalized for noncubic materials. There are three reasons for extending the calculation to these materials. First, an exact calculation of the Drude plasma frequency $\Omega_p$ for any metal requires true quasiparticle (QP) energy bands, whereas only density-functional (DF) bands are available. Therefore, we may learn whether low-lying QP excitation energies differ from DF eigenvalues by examining transport properties using values of $\Omega_p$ calculated with the DF bands and comparing with experiment. Second, many of the hcp elements are transition metals, among which there is evidence for interesting differences between $\lambda_{tr}$, $\lambda$ from $T_c$, and $\lambda_\gamma$, especially in the case of elements at the ends of this series where spin fluctuations may be important in suppressing $T_c$.[10] Finally, hcp metals provide an opportunity to study anisotropic transport. For noncubic materials, the conductivity $\sigma$ is an invertible second-rank tensor,

$$\sigma_{\alpha\beta} = \partial j_\alpha/\partial E_\beta = (\Omega_p^2 \tau)_{\alpha\beta}/4\pi .\qquad (6)$$

$\Omega_p^2$ is also an invertible second-rank tensor in this case and is defined by the relation

$$(\Omega_p^2)_{\alpha\beta} \equiv (4\pi e^2/V_{cell})\sum_k v_{k\alpha}v_{k\beta}\delta(\varepsilon_k)$$

$$\equiv 4\pi e^2 N(0)\langle v_{k\alpha}v_{k\beta}\rangle ,\qquad (7)$$

where $v_{k\alpha}$ is the group velocity $\partial\varepsilon_k/\partial(\hbar k_\alpha)$ of the QP state $k$, and the label $k$ is short for wave vector $k$ and

band index $n$. The symmetry properties of the hcp structure require that $\sigma$ and $\Omega_p^2$ be diagonal in the Cartesian basis when the $z$ axis coincides with the $c$ axis of the crystal. Therefore, $\tau$ must have the form of a diagonal second-rank tensor in this basis:

$$(1/\tau)_{\alpha\alpha} = (\Omega_p^2)_{\alpha\alpha}\rho_{\alpha\alpha}/4\pi .\qquad (8)$$

Similarly, Eqs. (1) and (2) are generalized and combined to find an expression for $\lambda_{tr}$ with its Cartesian decomposition made explicit:

$$\lambda_{\alpha\alpha\ tr} = \hbar(\Omega_p^2)_{\alpha\alpha}\rho_{\alpha\alpha}F/8\pi^2 k_B T ,$$

$$F = [1-(0.68\Theta_D)^2/12T^2]^{-1} .\qquad (9)$$

The mean-square phonon energy $\hbar^2\langle\omega^2\rangle_{tr}$ has been approximated by $(0.68 k_B\Theta_D)^2$. We have determined values of $\lambda_{tr\ \alpha\alpha}$ with this expression using experimental values for $\rho_{\alpha\alpha}$ along with values of $(\Omega_p^2)_{\alpha\alpha}$ calculated according to Eq. (7). In this work, $\rho_{xx}$ $(\rho_{zz})$ denotes the resistivity measured in the direction perpendicular (parallel) to the $c$ axis. hcp symmetry requires that $\rho_{xx}=\rho_{yy}$. If the anisotropy in the resistivity of hcp metals was fully accounted for by the anisotropy in $\Omega_p^2$, we should find that $\lambda_{tr\ xx}$ does not differ from $\lambda_{tr\ zz}$. From the lowest-order variational calculation[11] for $\rho_{\alpha\alpha}$ at high temperature, the formula for $\lambda_{tr\ \alpha\alpha}$ is obtained:

$$\lambda_{tr\ \alpha\alpha} = \frac{\sum_{k,k'}(v_{k\alpha}-v_{k'\alpha})^2\lambda_{kk'}\delta(\varepsilon_k)\delta(\varepsilon_{k'})}{\sum_{k,k'}(v_{k\alpha}-v_{k'\alpha})^2\delta(\varepsilon_k)\delta(\varepsilon_{k'})} ,\qquad (10)$$

$$\lambda_{kk'} = N(0)|M(k,k')|^2(\hbar\omega_{k-k'})^{-1} ,\qquad (11)$$

where $M(k,k')$ is the electron-phonon matrix element. The mass enhancement $\lambda$ has a similar definition, except that the weight factors $(v_{k\alpha}-v_{k'\alpha})^2$ in Eq. (10) are replaced by 1. Note that if the velocity differences $(v_{k\alpha}-v_{k'\alpha})^2$ vary with $k,k'$ in a way uncorrelated with the $k,k'$ variation of $\lambda_{kk'}$, then $\lambda$, $\lambda_{tr\ xx}$, and $\lambda_{tr\ zz}$ will all be equal. In order for $\lambda_{tr\ xx}$ to differ from $\lambda_{tr\ zz}$, the $x$ components of $v_k$ must have a different correlation with $\lambda_{kk'}$ than the $z$ components. It is a reasonable guess that $\lambda_{tr\ xx}$ and $\lambda_{tr\ zz}$ should not differ much, and both should be similar to $\lambda$.

## II. DESCRIPTION OF THE CALCULATION

In order to calculate $N(0)$ and $(\Omega_p^2)_{\alpha\alpha}$, we used Slater-Koster fits[12,13] to first-principles band-structure calculations. One of us[13] has calculated the hcp energy bands using augmented-plane-wave (APW) codes and self-consistent scalar-relativistic (without spin-orbit) potentials. Only muffin-tin terms were included in the potentials. Blaha et al.[2] found that non-muffin-tin corrections had only a small effect on energy bands or densities of states of most hcp metals.

Slater-Koster parameters for nonorthogonal $s$, $p$, and $d$ orbitals were fitted using 67 adjustable matrix elements to the lowest 12 bands on a uniform mesh of 23 $k$ points in the irreducible $(\frac{1}{24})$ Brillouin zone. The two-center approximation was used and interactions out to third neigh-

bor were included. Typical rms error for the first six bands of hcp transition metals is 3–4 mRy. The higher bands, seventh through ninth, do not fit as well because these bands contain $f$ character, which was not included in the basis set.

We used the tetrahedron method[14] to calculate $N(\varepsilon)$ and $N(\varepsilon)\langle v_\alpha^2 \rangle_\varepsilon$ from the Slater-Koster eigenvalues $\varepsilon_k$ and the group-velocity components $v_{k\alpha}$. Here the notation $\langle \ \rangle_\varepsilon$ means an average over the surface of energy $\varepsilon$. This method is used to compute energy surface integrals of the form

$$F(\varepsilon) = \sum_k A(k)\delta(\varepsilon - \varepsilon_k) \ . \tag{12}$$

For $F(\varepsilon) = N(\varepsilon)$, $A(k) = 1$. For $F(\varepsilon) = N(\varepsilon)\langle v_{k\alpha}^2 \rangle_\varepsilon$, $A(k) = v_{k\alpha}^2$. We used a mesh of 3078 $k$ points in the $\frac{1}{24}$ wedge of the Brillouin zone for all of the elements studied except Cd and Zn. Because of the convergence difficulties discussed below, we used 7200 $k$ points for the latter two cases. The integration region was divided into space-filling tetrahedra with corners at the mesh points. The functions $v_{k\alpha}^2$ and $\varepsilon_k$ were approximated within each tetrahedron by linear interpolation from the corner-point values, and the integrals represented in Eq. (12) were tabulated at energy intervals of 0.001 Ry. For illustration, in Fig. 1 we show $N(\varepsilon)$, $N(\varepsilon)\langle v_{kx}^2 \rangle$, and $N(\varepsilon)\langle v_{kz}^2 \rangle$ plot-

ted as a function of energy for the case of scandium. The Fermi energy was found by integrating the density of states. The values found for $N(0)$ by this method differ in some cases from the ones shown in Ref. 13 since, in the latter case, a less accurate histogram method was used on the Slater-Koster (SK) eigenvalues to find $N(0)$.

In order to judge the degree of convergence of the results, we tried the calculations for various numbers, $N$, of $k$ points in the irreducible Brillouin zone ranging from 405 to 3078. Good convergence [no more than 6% deviation of $N(0)$ from the final value as $N$ increased from 405] was seen for all cases except Zr and Zn. The reason for the difficulty in converging $N(0)$ for these two metals is that $N(\varepsilon)$ varies sharply at the Fermi level. Generally, $(\Omega_p^2)_{\alpha\alpha}$ converges more smoothly than $N(0)$, even for the problem cases.

To find empirical values of $\lambda_{\mathrm{tr}\,\alpha\alpha}$ from our calculated $(\Omega_p^2)_{\alpha\alpha}$ values, we used experimental single-crystal resistivity data compiled by Bass.[15] Our computed values of $N(0)$ and $(\Omega_p^2)_{\alpha\alpha}$ and extracted values of $\lambda_{\mathrm{tr}\,\alpha\alpha}$ are tabulated for 14 elements in Table I, which gives isotropic properties, and in Table II, which gives anisotropic properties. Be is omitted because a sufficiently accurate SK fit has not been obtained. Also shown in Table I are values of $N(0)$ found by Blaha et al.[2] The generally good agreement between these independent calculations confirms the accuracy of our procedures.
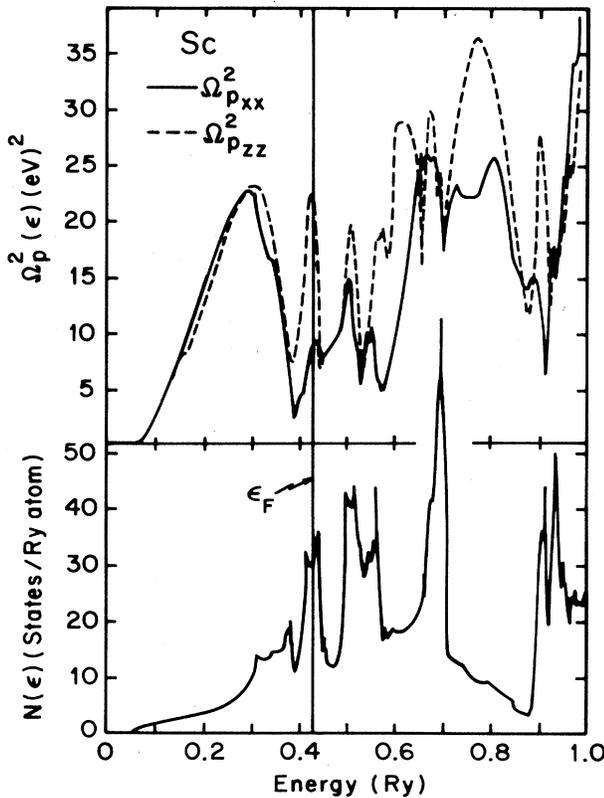


FIG. 1. Lower curve: density of states $N(\varepsilon)$ vs energy for scandium. Upper curves: Drude plasma frequencies for $E$ fields in the $xy$ plane (solid curve) and along the $z$ axis (dashed curve).

## III. DISCUSSION

### A. Ti, Zr, and Hf

These elements are low-$T_c$ superconductors ($T_c \simeq 0.4$, 0.5, and 0.1 K). McMillan[5] deduced values of $\lambda$ (0.4, 0.4, and 0.3) assuming $\mu^* = 0.13$. Our values of $\lambda_{\mathrm{tr}}$ (Table I) are somewhat higher (0.5, 0.5, and 0.45) than the $\lambda$ values. Some of this discrepancy can be assigned to uncertainties in $\lambda$; for low-$T_c$ materials, McMillan's $\lambda$ is especially sensitive to the choice of $\mu^*$ and $\Theta_D$. Even allowing for this, it seems likely that $\lambda_{\mathrm{tr}}$ is larger than $\lambda$ for these metals, implying that $\lambda_{kk'}$ varies significantly around the Fermi surface. This permits (but does not require) $\lambda_{\mathrm{tr}\,xx}$ and $\lambda_{\mathrm{tr}\,zz}$ to differ. We find (Table II) that $(\Omega_p^2)_{\alpha\alpha}$ and $\lambda_{\mathrm{tr}\,\alpha\alpha}$ are quite isotropic. There are no single-crystal measurements of $\rho_{\alpha\alpha}$ for Zr, but Hf and Ti have isotropic values of $\rho_{\alpha\alpha}$. For Ti, experimental single-crystal measurements have yielded contradictory results for the sign of the (small) resistivity anisotropy, $\rho_{zz} - \rho_{xx}$.[16] We have listed values derived from both sets of measurements in our tables. The specific-heat values $\lambda_\gamma$ for Ti and Hf agree well with $\lambda_{\mathrm{tr}}$. In Zr it is impossible to derive a reliable $\lambda_\gamma$ because the Fermi level lies in an almost vertical step of $N(\varepsilon)$, making $N(0)$ highly uncertain. However, $\Omega_p^2(\varepsilon)$ is less singular and $\Omega_p^2(0)$ was relatively stable as the sampling mesh changed. A theoretical calculation of $\eta$ for Zr was carried out by Chatterjee[17] from non-self-consistent energy bands, yielding an estimate of $\lambda = \eta/M\langle\omega^2\rangle \sim 0.37$, which is closer to McMillan's $\lambda$ value than to our value of $\lambda_{\mathrm{tr}}$. For Hf, $\eta$ was calculated by John et al.[18] They give an estimate of

TABLE I. Calculated and derived isotropic properties of hcp metals.

| | $\bar{\rho}_{\rm expt}$[a] $(\mu\Omega\,{\rm cm})$ (273.2 K) | $\hbar\Omega_p$[b] (eV) | $N(0)$ (states/atom Ry) (both spins) | $N(0)$ (states/atom Ry) (both spins) (Ref. 2) | $\lambda_\gamma$[c] | $\lambda_{\rm tr}$[d] | $\lambda_{\rm McM}$ (Ref. 5) | $\langle v^2\rangle^{1/2}$ $(10^8$ cm/s) | $l(273.2\,{\rm K})$[j] (Å) |
|---|---|---|---|---|---|---|---|---|---|
| Sc | 50.5 | 3.7 | 30.5 | 29.5 | 1.02 | 0.51 | | 0.24 | 18 |
| Y | 53.6 | 3.8 | 30.4 | 27.35 | 0.94 | 0.62 | | 0.29 | 21 |
| Ti | 44.7, 46.1[e] | 3.6 | 12.0 | 11.9 | 0.61 | 0.53, 0.54[e] | 0.38 | 0.32 | 25 |
| Zr | 38.6 | 3.8–3.9 | 12.1–15.3 | 13.0 | 0.05–0.33 | 0.48–0.50 | 0.41 | 0.35–0.38 | 29–34 |
| Hf | 32.2 | 4.0 | 8.6 | | 0.46 | 0.45 | 0.34 | 0.47 | 46 |
| Tc | 16.7 | 8.0 | 12.7 | 12.3 | 0.96 | 0.99 | 0.68[f] | 0.61 | 25 |
| Re | 16.0 | 7.4 | 10.0 | | 0.33 | 0.76 | 0.46 | 0.65 | 37 |
| Ru | 6.12 | 8.9 | 11.0 | 11.0 | 0.73 | 0.45 | 0.38 | 0.71 | 65 |
| Os | 7.9 | 8.7 | 8.4 | | 0.66 | 0.54 | 0.39 | 0.81 | 64 |
| Co↑ | 6.4 | 5.1[g] | 2.2[h] | 2.2[h] | | 0.15 | | 0.82 | 245 |
| Co↓ | | 3.7[g] | 9.9[h] | 10.4[h] | ~1.2 | | | 0.28 | |
| Mg | 3.95 | 7.6 | 5.7 | 5.9 | 0.31 | 0.20 | | 1.11 | 231 |
| Zn | 5.46 | 9.4–10.3 | 2.8–5.0 | 2.7 | −0.26–0.34 | 0.42–0.50 | 0.38 | 1.30–1.62 | 117–171 |
| Cd | 6.80 | 7.9 | 5.7 | 3.05 | −0.31 | 0.37 | 0.38 | 1.10 | 138 |
| Tl | ≃15 | 9.1 | 5.3 | | 0.60 | 1.11 | 0.71[i] | 1.53 | 63 |

[a]$\bar{\rho}_{\rm expt}\equiv\frac{1}{3}(\rho_{zz}+2\rho_{xx})$, where values for $\rho_{zz}=\rho_\parallel$ and $\rho_{xx}=\rho_\perp$ were obtained from Ref. 15. For Zr and Tc, values for $\rho_{zz}$ and $\rho_{xx}$ were not available and polycrystalline measurements of $\rho$ were used in these cases.
[b]$\Omega_p\equiv(\bar{\Omega}_p^2)^{1/2}=[\frac{1}{3}(\Omega_p^2)_{zz}+\frac{2}{3}(\Omega_p^2)_{xx}]^{1/2}$.
[c]Values for $\gamma$ are from C. Kittel, *Introduction to Solid State Physics*, 6th ed. (Wiley, New York, 1976), except in the case of Tc the value is from R. J. Trainor and M. B. Brodsky, Phys. Rev. B **12**, 4867 (1975).
[d]$\lambda_{\rm tr}\equiv\frac{1}{3}(2\lambda_{\rm tr\,xx}+\lambda_{\rm tr\,zz})$, except in the cases of Zr and Tc, where we use $\lambda_{\rm tr}=\frac{1}{3}\rho_{\rm poly}(hF/8\pi^2 k_B T)[(2\Omega_p^2)_{xx}+(\Omega_p^2)_{zz}]$.
[e]First entry assumes values for $\rho_\perp,\rho_\parallel$ given by Darnell, whereas the second entry assumes those of Wasilewski. See Ref. 16.
[f]A. F. Guillermet and G. Grimvall, J. Less-Common Met. **147**, 195 (1989).
[g]We define for each spin species $\Omega_{p\sigma}^2=4\pi e^2 N_\sigma(0)\langle v_\sigma^2\rangle$, so that $\Omega_p^2=\Omega_{p\uparrow}^2+\Omega_{p\downarrow}^2$, contrary to Ref. 4.
[h]Value for $N(0)$ is for single spin.
[i]Tunneling gives a value 0.78 (see Ref. 27).
[j]$l\equiv(2\langle v_x^2\rangle\tau_x^2+\langle v_z^2\rangle\tau_z^2)^{1/2}$, except in the cases of Zr and Tc, where $l\equiv(\langle v^2\rangle)^{1/2}\tau$ since no information on $\rho_{xx}$ and $\rho_{zz}$ is available for these elements.

TABLE II. Calculated and derived anisotropic properties of hcp metals.

| | $(c/a)/(c/a)_{\rm ideal}$ | $\rho_{zz}/\rho_{xx}$ | $(\Omega_p^2)_{xx}/(\Omega_p^2)_{zz}$ | $\lambda_{\rm tr\,zz}/\lambda_{\rm tr\,xx}$ |
|---|---|---|---|---|
| Sc | 0.976 | 0.37 | 0.39 | 0.95 |
| Y | 0.962 | 0.47 | 0.63 | 0.75 |
| Ti | 0.972 | 0.90, 1.05[a] | 1.08 | 0.84, 0.97[a] |
| Zr | 0.975 | | 1.01–1.10 | |
| Hf | 0.969 | 1.02 | 1.01 | 1.02 |
| Tc | 0.983 | | 0.76 | |
| Re | 0.989 | 0.72 | 0.78 | 0.92 |
| Ru | 0.970 | 0.78 | 0.87 | 0.90 |
| Os | 0.967 | 0.63 | 0.85 | 0.74 |
| Co | 0.994 | 1.84 | 1.18 | 1.56 |
| Mg | 0.994 | 0.83 | 0.74 | 1.12 |
| Zn | 1.14 | 1.04 | 0.60–0.64 | 1.63–1.72 |
| Cd | 1.15 | 1.24 | 0.69 | 1.79 |
| Tl | 0.979 | ~1.3 | 0.66 | 1.95 |

[a]See footnote e of Table I.

$\lambda \sim 0.47$, which agrees well with our $\lambda_{tr}$ and $\lambda_\gamma$, but exceeds McMillan's $\lambda$.

## B. Tc, Re, Ru, and Os

These metals are also superconducting, with higher values of $T_c$ (7.8, 1.4, 0.5, and 0.7 K). Again, the $\lambda_{tr}$ values are larger than McMillan's values of $\lambda$. The experimental resistivities are anisotropic ($\rho_{zz}/\rho_{xx} \sim 0.7$), while $\lambda_{tr}$ seems to be more isotropic ($\lambda_{tr\ zz}/\lambda_{tr\ xx} \sim 0.9$). Much of the anisotropy of $\rho$ is accounted for as anisotropy in $\Omega_p^2$. The value of $\lambda_\gamma$ for Re is anomalously small, but our value of $N(0)$ agrees well with Mattheiss.[19] For Ru and Os, $\lambda_\gamma$ is larger than $\lambda_{tr}$, while, for Tc, $\lambda_\gamma$ and $\lambda_{tr}$ agree. Theoretical estimates of $\lambda$ (from $\eta$) for Re and Os were made by John et al.,[18] who find $\lambda \sim 0.58$ for Re and 0.21 for Os. The latter value seems too small.

For Tc, $\eta$ was calculated from non-self-consistent energy levels by Asokamani and Iyakutti[20] and by Chatterjee.[21] The latter calculation gives an estimated $\lambda \sim 0.60$–0.87, which agrees better with McMillan's value 0.68 than does our empirical $\lambda_{tr}$. However, Chatterjee's value of $N(0)$ does not agree closely with ours or that of Blaha et al.,[2] so we do not feel this calculation adds much support to McMillan's.

## C. Sc and Y

Sc and Y have the highest values for the density of states at the Fermi energy, $N(0)$, and the highest average resistivities $\bar{\rho} = \frac{1}{3}\rho_{zz} + \frac{2}{3}\rho_{xx}$ of all the materials studied, yet lack any sign of superconductivity at atmospheric pressure. This is believed[10] to be the result of long-lived spin fluctuations which suppress Cooper pairing. The magnetic susceptibility of Sc and Y is also strongly enhanced, and has almost a Curie-law increase as $T$ decreases.[22] These observations apply equally to Pd, and it is commonly accepted[10] that spin fluctuations are most important at both ends of the transition-metal series, where the correlation between $T_c$ and $\gamma$ found in the transition metals breaks down. The resistivity of Sc and Y has an ordinary Bloch-Boltzmann–like $T$ dependence up to 300 K, and gives fairly large values of $\lambda_{tr} = (0.51, 0.62)$ for (Sc,Y) (larger, for example, than for Pd). Thus superconducting $T_c$'s would have been higher than 2 K if spin fluctuations had not suppressed superconductivity. Further experimental searches for phase transitions in higher-purity material at lower $T$ would be valuable. Very little information about $\lambda$ has previously been available in these materials. Knapp and Jones[23] found $\lambda \sim 0.3$ by comparing electronic specific heat at low $T$ and at high $T$. The accuracy of this procedure is limited by the lack of a clean separation between electronic and lattice (anharmonic) specific heat at high $T$.

## D. Co

Co is the only ferromagnetic hcp transition element. The Stoner picture of ferromagnetism in the band model is incomplete at best, so there is less reason to trust the ingredients like $N_\sigma(0)$ and $\Omega_{p\sigma}^2$ than in nonmagnetic metals. The majority-spin $d$ band is filled, giving a low

$N_\uparrow(0) = 2.2$ states/spin atom Ry, while the minority-spin Fermi level lies well within the $d$ bands, giving $N_\downarrow(0) = 9.9$. These agree nicely with the values of Blaha et al.,[2] and are also close to the values $N_\uparrow(0) = 2.3$ and $N_\downarrow(0) = 9.0$ found by Jarlborg and Peter.[24] There is no way to extract both up- and down-spin electron-phonon coupling constants $\lambda_{\sigma\ tr}$ from the measured $\sigma = \rho^{-1} = (\Omega_{p\uparrow}^2 \tau_\uparrow + \Omega_{p\downarrow}^2 \tau_\downarrow)/4\pi$. Our calculated Drude plasma frequencies are $\Omega_{pxx\uparrow} = 5.2$ eV, $\Omega_{pxx\downarrow} = 3.3$, $\Omega_{pzz\uparrow} = 4.8$, and $\Omega_{pzz\downarrow} = 4.3$. Notice the $\uparrow$-spin band dominates $\sigma$, both because $\Omega_{p\uparrow}^2$ is larger by about 2 than $\Omega_{p\downarrow}^2$, and because we expect $\tau_\uparrow$ to exceed $\tau_\downarrow$ based on the much larger density of states $N_\downarrow(0)$ for down spins to scatter into. Therefore we assume that only $\uparrow$ spins contribute ($\sigma = \Omega_{p\uparrow}^2 \tau_\uparrow/4\pi$) and Tables I and II show the up-spin values of $\lambda_{tr}$. Our value $\lambda_{tr\uparrow} = 0.15$ should be considered an upper limit, because the $\rho(T)$ data for Co show an upward curvature at 300 K, suggesting that additional scattering is coming from spin waves. Similarly, the down-spin contribution to specific heat $\gamma$ exceeds the up-spin contribution; thus in a first approximation, $\lambda_\gamma$ in Table I is associated with down spins. The electron-phonon coupling for $\uparrow$ spins is weak ($\lambda_{tr} \sim 0.15$, similar to Cu), while down spins have $\lambda_\gamma \sim 1.2$. No doubt, this large value contains other many-body effects besides electron-phonon interactions. Our analysis agrees qualitatively with Jarlborg and Peter,[24] who find $\lambda_\uparrow = 0.07$ and $\lambda_\downarrow = 0.44$ from $\eta$ calculations. They also find evidence for additional enhancement in $\gamma$. The resistivity of cobalt is quite anisotropic, whereas $\Omega_p^2$ for $\uparrow$ spins is less anisotropic, requiring a large anisotropy $\lambda_{tr\ zz}/\lambda_{tr\ xx} \sim 1.6$.

## E. Mg, Zn, Cd, and Tl

These are the only non-transition-metal elements we studied. Zn, Cd, and Tl are superconducting ($T_c \simeq 0.9$, 0.6, and 2.4 K), whereas Mg has not been observed to superconduct above 0.002 K.[25] We find a value of 180 $\mu$K for the $T_c$ of Mg from the McMillan equation using $\mu^* = 0.1$ and our empirical $\lambda_{tr}$ value of 0.20 for $\lambda$, contradicting an earlier theoretical result by one of us[26] which indicated that Mg should superconduct at temperatures as high as 0.012 K. However, our value of 0.31 for $\lambda_\gamma$ of Mg agrees well with the earlier result[26] of $\lambda_\gamma = 0.33$. For Cd, $N(0)$ values were fairly well converged and not far from those of Ref. 13, but yielded unphysical negative $\lambda_\gamma$ values. The value given by Blaha et al.[2] yields a much more realistic value of $\lambda_\gamma = 0.30$. They suggest that the non-muffin-tin terms which they include in their potential (but we do not) may be important for obtaining the correct band structure for Cd. Another possible source of discrepancy derives from small differences between the true local-density-approximation (LDA) bands and the SK fits. The rms fitting error is small for most transition elements, but larger for the non-transition-metal elements. Our $\lambda_{tr}$ value for Cd agrees well with McMillan's value. On the other hand, our $\lambda_{tr}$ values exceed McMillan's $\lambda$ values for Zn and especially Tl, following the trend seen in the transition metals. For Tl, Dynes[27] has obtained a value of $\lambda_{tun} = 0.78$ from the measured

tunneling density of states, which agrees more closely with McMillan's $\lambda$ than our $\lambda_{tr}$. Our $\lambda_\gamma$ value of 0.60 for Tl seems low. Ament and Vroom[28] and Holtham et al.[29] have carried out non-self-consistent band-structure calculations for Tl and determined values for $\lambda_\gamma$ of 0.70 and 0.67, respectively. Spin-orbit–interaction effects, which were not included in the band structures we used, might be significant for Tl, which is the heaviest element we studied. For Zn, our computed values of $N(0)$ did not converge, as the number of sampled $k$ points was increased. As in the case of Zr, the Fermi level of Zn lies in a steep section of the $N(\varepsilon)$-versus-$\varepsilon$ curve, making $N(0)$ and $\lambda_\gamma$ difficult to determine. Our range of $\lambda_{tr}$ values for Zn compares well with Auluck's[30] $\lambda_\gamma$ of 0.40 and $\lambda_{cr}$ (from cyclotron resonance) of 0.51, which he obtained by comparing pseudopotential band masses averaged over cyclotron orbits with experimentally determined cyclotron masses. Tomlinson and Swihart[8] calculated $\lambda_{cr}$ from first principles and obtained a value of 0.41. Yanson[31] has measured the nonlinear current-voltage characteristics of point contacts to determine $\lambda_p$ values of 0.13 for both Cd and Zn. These metals show greater discrepancies between $\lambda_p$ values and $\lambda$, $\lambda_{tr}$, or $\lambda_\gamma$ values than for other simple metals studied with point-contact spectroscopy.[32] Several theoretical calculations of both isotropic and anisotropic effects of the electron-phonon interaction have been carried out for the nontransition hcp metals.[33] Truant and Carbotte[34] calculated a value of $\lambda=0.425$ for zinc using realistic phonon spectra and electron-phonon interactions, but neglecting any departure from free-electron behavior of the conduction electrons. Tomlinson and Swihart[8] did a more complete calculation of $\lambda$, taking into account all important sources of anisotropy, obtaining 0.36 for $\lambda$. We find that Zn, Cd, and Tl have the most anisotropic $\lambda_{tr\ \alpha\alpha}$ values of all the metals studied. For Zn and Cd this anisotropy may be correlated with their large deviations from the ideal $c/a$ ratio, their highly nonspherical charge densities,[2] and their extremely large electric-field-gradient values.[1] However, a more detailed calculation than we have attempted would be necessary to understand how these properties are related to $\lambda_{tr\ zz}/\lambda_{tr\ xx}$. Tomlinson[7] studied the anisotropic transport properties of zinc by solving the Boltzmann equation by the variational method. He found that $\rho_{\alpha\alpha}$ is very isotropic at high temperatures, in agreement with experiment. This is a remarkable result since he calculated driving-force and scattering-operator terms for the Boltzmann equation which, separately, are quite anisotropic. This result agrees with our finding that band-theoretical $(\Omega_p^2)_{\alpha\alpha}$ values and empirical $\lambda_{tr\ \alpha\alpha}$ values are both highly anisotropic, each in opposite directions.

## IV. CONCLUSIONS

The two principal issues addressed in this paper are (1) whether values of $\Omega_p^2$ from LDA band structures are close enough to the true QP values of $\Omega_p^2$ to permit the coupling constant $\lambda_{tr}$ to be extracted, and (2) whether anisotropy in $\sigma_{\alpha\alpha}$ can be accounted for by anisotropy in $(\Omega_p^2)_{\alpha\alpha}$. Unambiguous answers are not possible. The main test of question (1) is by comparison by $\lambda_{tr}$ extracted

from experiment and LDA bands with $\lambda$ extracted from superconductivity. This is graphically illustrated in Fig. 2. The vertical axis, according to McMillan's equation[5] [Eq. (3)] is $-0.37-1.04(1+\lambda)/[\lambda-\mu^*(1+0.62\lambda)]$, which is plotted as the hatched region for values of $\mu^*$ in the interval (0.10,0.15). The experimental points would all lie in this region if standard McMillan theory worked perfectly and if $\lambda_{tr}$ were identical to $\lambda$. Instead, we see a tendency for $\lambda_{tr}$ to exceed $\lambda$. Three types of explanations are possible.

(a) The intrinsic difference between $\lambda_{tr}$ and $\lambda$ may be the cause. This seems unlikely, since of the four metals[6] in which we have good simultaneous calculations of $\lambda$ and $\lambda_{tr}$, the only one with a $|\lambda_{tr}-\lambda|$ exceeding 10% was Ta, and there $\lambda_{tr}$ was smaller than $\lambda$. We know of no intrinsic reason why $\lambda_{tr}$ should exceed $\lambda$.

(b) The LDA values of $\Omega_p^2$ are systematically high, compared to QP theory. This seems reasonable, since there is indeed evidence, both from experiment[35] and theory,[36] that the LDA bandwidth exceeds the QP values. If the LDA bands were stretched uniformly relative to QP's, then the ratio of $\Omega_p^2$ in the two theories would equal the bandwidth ratio. It is easy to believe that a systematic effect of $\leq 10\%$ exists. The extreme case of Ni is sometimes cited as evidence for a large disagreement between LDA and QP theories in transition metals. Williams and Von Barth[37] argue that Ni is "the exception rather than the rule."

(c) Of equal or larger significance are two problems in applying McMillan theory. First, the "prefactor" $\Theta_D$ in McMillan's equation should be[38] $\hbar\omega_{log}/k_B$ and can only be found by quasiparticle tunneling or a detailed microscopic theory. In particular, values of $\Theta_D$ from elastic constants or low-$T$ specific heat tend to overestimate $\omega_{log}$ and thus yield overly small values of $\lambda$. We have used values of $\Theta_D$ fitted[39] to high-$T$ specific heat in estimating the correction factor $F$ of Eq. (9) and in plotting Fig. 2.
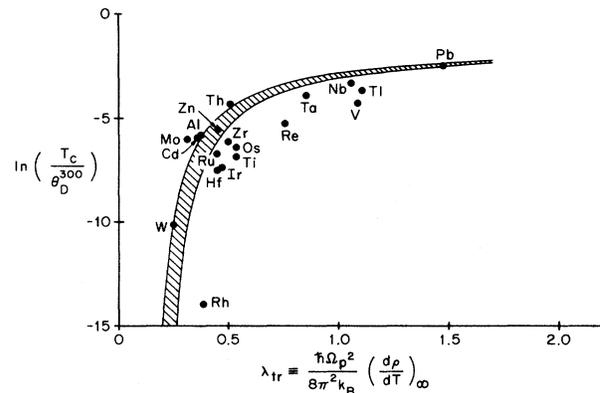


FIG. 2. Empirical $T_c/\Theta_D$ (using the high-$T$ $\Theta_D$ values of Ref. 39) plotted logarithmically against the semiempirical $\lambda_{tr}$ extracted from resistivity. The values of $\lambda_{tr}$ for 10 hcp elements are from the present paper, while nine cubic elements come from Ref. 4. The McMillan equation [Eq. (3)] predicts the hatched range provided $\lambda=\lambda_{tr}$ and $0.10<\mu^*<0.15$.

Tunneling experiments have confirmed a systematic trend for $\lambda$ to exceed the values extracted by McMillan from $T_c$. Second, the Coulomb interaction parameter $\mu^*$ may be outside the range (0.10,0.15). When spin-fluctuation effects are important, for example, this is approximately equivalent to an enhanced value of $\mu^*$, which will suppress $T_c$, or else require a compensating increase in $\lambda$. Rietschel and Winter[40] have argued that this effect is more widespread than has been "commonly assumed." Perhaps it is not a coincidence that the two transition metals Mo and W, which do not have $\lambda_{tr} > \lambda$ in Fig. 2, have the lowest values of $N(0)$ and, thus, the least phase space for Coulomb scattering of all transition elements. Therefore, it is not possible to be sure that $\Omega_p^2$ has been overestimated by LDA theory. We can surely say that the LDA value of $\Omega_p^2$ provides a good guide to reality, in the absence of a value from QP theory.

On the issue of anisotropy of $\sigma$, Table II shows that for all transition elements, especially Sc and Y (which have the largest anisotropy in $\sigma$), a significant part of the anisotropy of $\sigma$ comes from anisotropy of $\Omega_p^2$. Nevertheless, we are left with some ambiguity about how complete the effect is, largely because we do not know what accuracy to assign to the experimental $\rho_{zz}/\rho_{xx}$. Therefore, we do not know how much error to assign to the extracted value of $\lambda_{tr\,zz}/\lambda_{tr\,xx}$. The largest anisotropies of $\lambda_{tr}$ in Table II occur for nontransition metals. There is relatively little direct experimental evidence about the relative anisotropies of different metals. Allen and Mitrović[41] estimated the rms anisotropy of $\lambda_k$ in Zn to be $\sim 20\%$, whereas in most metals there is no evidence for an effect this large. The evidence suggests that the electron-phonon interaction is more isotropic in transition elements than in $sp$ elements.

Finally, our work enables us to make a comment on the validity of the Boltzmann equation. The last column of Table I shows extracted values of the mean free path (MFP) $l = v_F \tau$ at 273 K. The criterion for validity is usually stated as $k_F l \gg 1$, or, equivalently, $\varepsilon_F \tau / \hbar \ll 1$, although we prefer $l \gg a$, or else $N(0)\hbar/\tau \ll 1$ since $k_F$ and $\varepsilon_F$ are not well defined for transition metals. Consider, first, Ru, Os, Mg, Zn, Cd, and Tl, which all have $l > 60$ Å, implying that Boltzmann theory is completely safe. All except Os show a small upward curvature $(d^2\rho/dT^2 > 0)$ at $T > 300$ K, while Os has a small downward curvature. The simple Bloch-Grüneisen theory[42] predicts a small downward curvature that disappears rapidly as $T$ increases, but this neglects thermal expansion and anharmonicity, which normally cause phonon fre-

quencies to diminish and $\lambda$ and $\rho$ to increase as $T$ increases. Thus a small upward curvature, more pronounced at high $T$, is characteristic of most good Boltzmann metals. Next, consider Sc and Y with the smallest values, $l \sim 20$ Å. These materials show typical Boltzmann behavior for $T \leq 300$ K. [A good signature is that the tangent to $\rho(T)$ at 300 K intersects the residual resistivity $\rho(0)$ at $T = 0$.] However, for $T \geq 600$ K, there is very noticeable downward curvature (more pronounced than in Os). This is the signature of resistivity "saturation," a familiar phenomenon[43,44] in $d$-band compounds with $\rho \geq 100$ $\mu\Omega$ cm and $l < 10$ Å. This behavior lies outside Boltzmann theory and its interpretation is still controversial. However, it is remarkably regular, and occurs almost without fail at $T \geq 300$ K if $l \leq 10$ Å. To estimate where the onset of saturation should occur, we calculate the temperature at which Boltzmann theory predicts $l = 10$ Å. This is easily done using the values of $l$ at 273 K from Table I and the Boltzmann result that $l \propto T^{-1}$. For Sc and Y, onset is predicted to happen at $\sim 500$ and $\sim 600$ K, respectively, agreeing completely with the measured onset temperature, where $\rho$ has become $\sim 110$ and 140 $\mu\Omega$ cm, respectively. Table I then allows us to predict 700 K as the onset of saturation in Ti and Tc, 900 K for Zr, 1000 K for Re, and 1300 K for Hf. The actual onsets [determined with the help of a ruler from the $\rho(T)$ curves in Ref. 15] are $(T = 700$ K, $\rho = 135$ $\mu\Omega$ cm) in Ti, $(T = 700$ K, $\rho = 40$ $\mu\Omega$ cm) in Tc, $(T = 900$ K, $\rho = 130$ $\mu\Omega$ cm) in Zr, $(T = 900$ K, $\rho = 60$ $\mu\Omega$ cm) in Re, and $(T = 1400$ K, $\rho = 160$ $\mu\Omega$ cm) in Hf. The value of $\rho$ at which onset is first seen is surprisingly variable, with 40 $\mu\Omega$ cm in Tc being remarkably low (comparable to Pd). Extrapolating to very high temperatures gives 80 $\leq \rho_{max} \leq 100$ $\mu\Omega$ cm as the fully saturated value of $\rho$ for Tc. In summary, the criterion $l \simeq 10$ Å is a remarkably accurate predictor (using our procedure to extract $\tau$). These results support the argument of Gurvitch and Fiory,[45] who associate the linear resistivity of high-$T_c$ superconductors with a mean free path $l > 10$ Å.

[1]P. Blaha, K. Schwarz, and P. H. Dederichs, Phys. Rev. B 37, 2792 (1988).

[2]P. Blaha, K. Schwarz, and P. H. Dederichs, Phys. Rev. B 38, 9368 (1988).

[3]B. Chakraborty, W. E. Pickett, and P. B. Allen, Phys. Rev. B 14, 3227 (1976).

[4]P. B. Allen, Phys. Rev. B 36, 2920 (1987).

[5]W. L. McMillan, Phys. Rev. 167, 331 (1968).

[6]P. B. Allen, T. P. Beaulac, F. S. Khan, W. H. Butler, F. J. Pin-

ski, and J. C. Swihart, Phys. Rev. B 34, 4331 (1986).

[7]P. G. Tomlinson, Phys. Rev. B 19, 1893 (1979).

[8]P. G. Tomlinson and J. C. Swihart, Phys. Rev. B 19, 1867 (1979).

[9]D. J. Scalapino, in *Superconductivity*, edited by R. D. Parks (Dekker, New York, 1969), Vol. I, p. 449.

[10]G. Gladstone, M. A. Jensen, and J. R. Schrieffer, in *Superconductivity*, edited by R. D. Parks (Dekker, New York, 1969), Vol. II, p. 665; N. F. Berk and J. R. Schrieffer, Phys. Rev.

Lett. **17**, 433 (1966); M. A. Jensen and J. P. Maita, Phys. Rev. **149**, 409 (1966); M. A. Jensen and J. P. Maita, *ibid.* **149**, 409 (1966); K. Andres and M. A. Jensen, *ibid.* **165**, 533 (1968); M. A. Jensen and K. Andres, *ibid.* **165**, 545 (1968).

[11]P. B. Allen, Phys. Rev. B **3**, 305 (1971); **17**, 3725 (1978).

[12]J. C. Slater and G. F. Koster, Phys. Rev. **94**, 1498 (1954).

[13]D. A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986).

[14]G. Lehmann and M. Taut, Phys. Status Solidi B **54**, 469 (1972); **57**, 815 (1973).

[15]J. Bass, in *Landolt-Börnstein, Metals: Electronic Transport Phenomena,* edited by K. H. Hellwege and J. L. Olsen (Springer-Verlag, Berlin, 1982), Gp. 3, Vol. 15, Pt. a, Sec. 1.2.1.

[16]F. J. Darnell, Trans. Met. Soc. AIME **212**, 356 (1958); R. J. Wasilewski, *ibid.* **224**, 13 (1962).

[17]P. Chatterjee, J. Phys. F **14**, 2027 (1984).

[18]W. John *et al.,* Phys. Status Solidi B **121**, 233 (1984).

[19]L. F. Mattheiss, Phys. Rev. **151**, 450 (1966).

[20]R. Asokamani and K. Iyakutti, J. Phys. F **10**, 1157 (1980).

[21]P. Chatterjee, Phys. Rev. B **27**, 4722 (1983).

[22]W. E. Gardner and J. Penfold, Philos. Mag. **11**, 549 (1965); V. I. Chechernikov *et al.,* Zh. Eksp. Teor. Fiz. **44**, 1826 (1963) [Sov. Phys.—JETP **17**, 1228 (1963)]; J. W. Ross *et al.,* Phys. Rev. **183**, 645 (1969).

[23]G. S. Knapp and R. W. Jones, Phys. Rev. B **6**, 1761 (1972).

[24]T. Jarlborg and M. Peter, J. Magn. Magn. Mater. **42**, 89 (1984).

[25]R. A. Buhrman and W. P. Halperin, J. Low Temp. Phys. **16**, 409 (1974).

[26]P. B. Allen and M. L. Cohen, Phys. Rev. **187**, 525 (1969); Solid State Commun. **7**, 677 (1969).

[27]R. C. Dynes, Phys. Rev. B **2**, 644 (1970).

[28]M. A. Ament and A. R. Vroom, J. Phys. F **7**, 97 (1977).

[29]P. M. Holtham, J. P. Jan, and H. L. Skriver, J. Phys. F **7**, 635 (1977).

[30]S. Auluck, J. Low Temp. Phys. **12**, 601 (1973).

[31]T. K. Yanson, Fiz. Nizk. Temp. **3**, 1516 (1977) [Sov. J. Low Temp. Phys. **3**, 726 (1977)].

[32]A. G. M. Jansen, A. P. van Gelder, and P. Wyder, J. Phys. C **13**, 6073 (1980).

[33]The early calculations are reviewed in Ref. 8.

[34]P. T. Truant and J. P. Carbotte, Can. J. Phys. **51**, 922 (1973); Solid State Commun. **11**, 443 (1972).

[35]E. Jensen and E. W. Plummer, Phys. Rev. Lett. **55**, 1918 (1985).

[36]J. E. Northrup, M. S. Hybertsen, and S. G. Louie, Phys. Rev. Lett. **59**, 819 (1987); P. Horsch, W. vonder Linden, and W.-D. Lukas, Solid State Commun. **62**, 359 (1987).

[37]A. R. Williams and U. von Barth, in *Theory of the Inhomogeneous Electron GaS,* edited by S. Lundqvist and N. H. March (Plenum, New York, 1983), p. 189.

[38]P. B. Allen and R. C. Dynes, Phys. Rev. B **12**, 905 (1975).

[39]K. A. Gschneidner, in *Solid State Physics,* edited by F. Seitz and D. Turnbull (Academic, New York, 1964), Vol. 16, p. 275.

[40]H. Rietschel and H. Winter, Phys. Rev. Lett. **43**, 1256 (1979).

[41]P. B. Allen and B. Mitrović, in *Solid State Physics,* edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1982), Vol. 37, p. 1.

[42]A. H. Wilson, *The Theory of Metals,* 2nd ed. (Cambridge University Press, Cambridge, 1965).

[43]Z. Fisk and G. W. Webb, Phys. Rev. Lett. **36**, 1084 (1976).

[44]P. B. Allen, in *Superconductivity in d- and f-Band Metals,* edited by H. Suhl and M. B. Maple (Academic, New York, 1980), p. 291.

[45]M. Gurvitch and A. T. Fiory, Phys. Rev. Lett. **59**, 1337 (1987).