Calculation of the temperature and the purity dependence of sound attenuation in superconducting Nb

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(Received 25 June 1973)

Recent experimental results on the sound attenuation, α_s, in the superconducting state of high-purity Nb are studied. By including the electron-phonon interaction in the BCS theory according to Eliashberg, as suggested by Carsey, Kegiwada, Levy, and Maki, we show that α_s/α_n decreases much faster than that limited by impurity scattering, where α_n is the sound attenuation in the normal state. The results deviate from the experimental data by approximately 40%, which is a substantial improvement over the impurity-limited BCS theory. If an energy gap is used to fit the data, it is found that the empirical value deviated from the BCS energy gap by 25%. In order to obtain the correct temperature dependence of α_n in comparison with experimental data, we have neglected the vertex correction in our calculation. In addition to the one-band model, we also examine the two-band model. Our results indicate that there is little difference between these two models for temperatures near the transition temperature; however, the two-band model predicts a smaller α_s in the lower-temperature region, in better agreement with the experimental data.

I. INTRODUCTION

Recent experiments[1-3] concerning the ultrasonic attenuation in normal and superconducting Nb[4,5] of high purity show a large deviation from the BCS theory. The deviations reported in these experiments are for samples with resistivity ratio $r \geq 10^3$. For $r \leq 200$, earlier ultrasonic-attenuation experiments show essentially BCS results. Since Nb is not a strong-coupling superconductor, the band-structure effect is expected to be small.[1,6] Furthermore, how purity changes the properties of the strong-coupling superconductors is not clear from the literature and we doubt that this discrepancy in Nb can be completely explained by considering Nb as a strong-coupling superconductor.

It is reasonable to expect that the explanation, as advanced by Carsey, Kegiwada, Levy, and Maki,[1] is in the relative role played by the electron-phonon interaction compared to electron-impurity scattering. As pointed out by Carsey *et al.*, the lifetime $\Gamma(\omega)$ of quasiparticles depends on the energy ω and energy gap Δ of the quasiparticle above the Fermi surface through the density of states $N(\omega)$. Consequently, the electron mean free path for superconducting Nb is smaller than what is obtained in the BCS theory when it is assumed that the impurity scattering dominates Γ. This effect theoretically predicts that $\alpha_s/\alpha_n < (\alpha_s/\alpha_n)_{\rm imp}$ around the transition temperature T_c, where α_n and α_s are the sound attenuation in the normal and superconducting states; consequently, the deviation between the theory and the experiment is reduced. In Ref. 1 only the first order in $\Delta(T)/T$ is taken and the calculation applies only for $|1 - T/T_c| \leq 0.02$, since $\Delta(T)$ is a rapidly increasing function of $t \equiv T/T_c$. Furthermore, according to Ref. 1, $\Gamma_n(\omega) \propto T^{-3}$ in the normal state and $\Gamma_s(\omega) \propto e^{+\Delta/T}$ in the superconducting state[7]; the ratio α_s/α_n, which is proportional to Γ_s/Γ_n, will be larger than $(\alpha_s/\alpha_n)_{\rm imp}$ in the low-T region. The main reason for this difficulty is that Carsey *et al.* take the value of $\Gamma(\omega)$ from Eliashberg[8] at $\omega = 0$, but in a more realistic calculation a complete function of Γ through the entire range of ω is needed.

Although the deficiency of Ref. 1 in the analysis of the experimental data can be improved by using the $\Gamma(\omega)$ calculated by Eliashberg,[8] we have even more serious problems in calculating the transport properties of transition metals. A brief review is given below.

Mott[9] has shown the T^3 dependence of the resistivity in transition metals by assuming the dominance of the interband scattering. The validity of this assumption was recently confirmed by Webb[10] in his measurement of the resistivity of Nb. However, Mott's assumption that $m_d^*/m_s^* \gg 1$, where m_d^* and m_s^* are the effective masses of d and s electrons, is not consistent with band-structure calculation[11] and cyclotron-resonance experiments.[12] It should be noted, however, that $m_d^*/m_s^* \gg 1$ is not necessary to prove the importance of the interband scattering or the T^3 dependence of the resistivity.

In the superconducting state, earlier attempts[13] to explain the thermal conductivity in a transition metal assumed that s electrons must have a nonvanishing density of states starting from Δ_d, the energy gap of the d band. This is not justifiable in

the case of pure metals. In order to show that the d electrons dominate the transport properties, Chow[14] recently argued that n_s and n_d in the Lorentz formula for the conductivity σ,[15,16]

$$\sigma = \frac{n_s e^2}{m_s^*}\Gamma_s + \frac{n_d e^2}{m_d^*}\Gamma_d \quad , \tag{1}$$

should have the relationship $n_d/n_s \approx 10^2$ on the basis that $n_{s(d)} = (P_{Fs(d)})^3/2\pi^2$ and the assumption that the Fermi momenta P_{Fd}, P_{Fs} satisfy $P_{Fd} \gg P_{Fs}$. This argument cannot be accepted because n_s and n_d in Eq. (1) are simply the number of s and d electrons per unit volume, and $n_d/n_s = 4$ exactly in Nb. We question the procedure of fitting one experimental result at the expense of denying the fact that Nb has four d electrons and one s electron. In contrast to Chow, Kumar and Gupta[16] show that, within the same theoretical frame of Chow, the recent low-temperature thermal-conductivity data by Anderson *et al.*[17] can be explained by assuming that s electrons are the current carriers. These two examples help to demonstrate the present need of introducing an excessive number of parameters into calculations in order to obtain agreement with experimental data. The results of such studies show that we do not have a realistic physical picture of the transport properties in the transition metals. Despite a considerable effect in theoretical work, there is not even an agreement as to the physical mechanism for the transport properties in the superconducting transition metals.

In this paper we examine the one-band and two-band models in the calculation of α_n and α_s. Since there is no complete theoretical frame within which to calculate the transport properties by including the band structure, we use two isotropic Fermi surfaces to characterize the d and s bands. In Sec. II a review of the models and an estimate of the value of the parameters used is given; next, in Sec. III, α_n and α_s in each of these two models are computed. In Sec. IV we discuss our calculation and conclusions, after making a detailed comparison with recent experimental data.

II. MODELS

Since we are only interested in the imaginary part of the self-energy, all the effect of electron-electron and electron-phonon interactions on the real part of the self-energy is included in the effective masses, m_s^* and m_d^*. The unperturbed Hamiltonian is H_0,[18]

$$H_0 = \sum_{\vec{k},\sigma} \frac{k^2}{2m_s^*}\, s^\dagger_{\vec{k},\sigma} s_{\vec{k},\sigma} + \sum_{\vec{k},\sigma} \frac{k^2}{2m_d^*}\, d^\dagger_{\vec{k},\sigma} d_{\vec{k},\sigma} \quad . \tag{2}$$

The interaction between electrons and phonons is

$$H' = \sum_{\vec{p},\vec{k},\sigma}\left(g_{sd}\frac{\omega(p)}{\sqrt{2}}\, d^\dagger_{\vec{k},\sigma} s_{\vec{k}+\vec{p},\sigma} b^\dagger_{\vec{p}} + g_d \frac{\omega(p)}{\sqrt{2}}\, d^\dagger_{\vec{k},\sigma} d_{\vec{k}+\vec{p},\sigma} b^\dagger_{\vec{p}} + g_s \frac{\omega(p)}{\sqrt{2}}\, s^\dagger_{\vec{k},\sigma} s_{\vec{k}+\vec{p},\sigma} b^\dagger_{\vec{p}} + \text{H. c.}\right) \quad , \tag{3}$$

where $d^\dagger_{k\sigma}$ ($s^\dagger_{k\sigma}$) is the creation operator of d (s) electrons. Here, $\omega(k) = sk$, where s is the velocity of sound, and g_s, g_d, and g_{sd} are the coupling constants. $b^\dagger_{\vec{p}}$ is the phonon creation operation.

The interaction between electrons and impurities is H'',

$$H'' = \sum_{\vec{p},\vec{k},\sigma}\left[U_s(k)\, s^\dagger_{\vec{k}+\vec{p},\sigma} s_{\vec{p},\sigma} + U_d(k)\, d^\dagger_{\vec{k}+\vec{p},\sigma} d_{\vec{p},\sigma} + U_{sd}(k)\, s^\dagger_{\vec{k}+\vec{p},\sigma} d_{\vec{p},\sigma} + \text{H. c.}\right] \quad , \tag{4}$$

where U_s, U_d, and U_{sd} are the potentials between electrons and impurities.

Our model is almost equivalent to the free-electron model used in the literature, and we summarize as follows: (a) The Debye phonon energy spectrum is used. The energy ϵ_k of the s and d electrons is $k^2/2m_s^*$ and $k^2/2m_d^*$, respectively. (b) At present only g_d can be inferred accurately from T_c,[6] and both g_s and g_{sd} are unknown. g_s/g_d and g_{sd}/g_d should be small if we believe that the specific-heat data of Nb at low T are related to a small energy gap, Δ_s.[19] (c) Our model differs from the free-eleectron model in not using the free-electron density of states $N_{s(d)}(0) = m^*_{s(d)} P_{Fs(d)}/2\pi^2$. Instead we write

$$\int \frac{d^3p}{(2\pi)^3} = \int d\epsilon_p \int \frac{dS}{v} \equiv N(0)\int d\epsilon_p \quad , \tag{5}$$

where $N(0)$ is the reciprocal velocity averaged over the Fermi surface of the s or d band. We will use $N_{s(d)}(0)$ as parameters.

The following estimations are made on the basis of present experimental and theoretical understanding: (a) $P_{Fs} \cong P_{Fd} \cong P$, which is consistent with the free-electron model $(P_{Fd}/P_{Fs})^3 = 4$ and the fact that the two bands must overlap at some point in order to obtain T^3 dependence in the resistivity.[9] (b) $m_d^*/m_s^* \approx 1$ to 2, in accordance with a recent calculation.[11] (c) $N_d(0)/N_s(0)$ should be large, but its magnitude varies with crystalline direction.[12] (d) g_d is known, and g_s and g_{sd} should be relatively small.

In the following calculation of the transport lifetime, the one-band and two-band models are used without the vertex correction. This allows us to take the mean lifetime as the transport lifetime. Such a procedure is justified in the one-band model by the empirical observation that $\Gamma_n \propto T^{-3}$, which is obtained only by neglecting the vertex correction. We should emphasize that there is no theoretical reason to neglect the vertex correction in the one-band model. The mean lifetime is used for the transport time in order to have the right temperature dependence for α_n. Although the calculation

of the vertex correction is given in Ref. 1, the result which gives $\Gamma_n \propto T^{-5}$ is not used in their discussion of their experimental results.

In the two-band model, it can be shown that the interband scattering has negligible vertex correction.[20] Here again we appeal to the empirical fact and assume that the interband scattering must dominate the mean lifetime of s or d electrons. In other words, the omission of the vertex correction is justified if the interband scattering dominates the intraband scattering. We want to emphasize again that this approximation is carried out not for mathematical convenience but rather for physical necessity in order to obtain the correct T dependence of both α_n and the electrical resistivity.

III. SOUND ATTENUATION

A. One-band model

The renormalized Green's function G and F are given by[1,8]

$$G(\vec{p}, \omega_n) = \frac{\tilde{\omega}_n + \tilde{\epsilon}_p}{\tilde{\omega}_n^2 - \tilde{\epsilon}_p^2 - \tilde{\Delta}^2} \tag{6}$$

and

$$F(\vec{p}, \omega_n) = \frac{\tilde{\Delta}}{\tilde{\omega}_n^2 - \tilde{\epsilon}_p^2 - \tilde{\Delta}^2} \quad , \tag{7}$$

where $\tilde{\epsilon}_p = \epsilon_p - \mu$, with μ being the chemical potential, and

$$\tilde{\omega} = \omega + i\omega_1 \quad , \tag{8}$$

$$\tilde{\Delta} = \Delta + i\Delta_1 \quad , \tag{9}$$

with ω_1 and Δ_1 being the imaginary part of the self-energy Σ_1 and Σ_2, respectively. We write the self-energy terms as

$$\Sigma_1(\vec{p}, \omega_n) = \frac{Tg_{dd}^2}{(2\pi)^3} \sum_{n'} \int d^3p_1 G(\vec{p}_1, \omega_n') D(\vec{p} - \vec{p}_1, \omega_n - \omega_{n'}), \tag{10}$$

$$\Sigma_2(\vec{p}, \omega_n) = \frac{Tg_{dd}^2}{(2\pi)^3} \sum_{n'} \int d^3p_1 F(\vec{p}_1, \omega_n') D(\vec{p} - \vec{p}_1, \omega_n - \omega_{n'}), \tag{11}$$

where $D(p, \omega)$ is the phonon propagator. Both ω_1 and Δ_1 have been calculated in Ref. 8, with the results

$$\omega_1 = \frac{\pi\lambda_d}{\omega_0^2}\left[\int_{\Delta_d}^{\omega} d\omega' \frac{\omega'}{(\omega'^2 - \Delta_d^2)^{1/2}}\left((\omega - \omega')^2 + \frac{4\omega\omega'}{e^{\omega'/T}+1} + \frac{(\omega-\omega')^2}{e^{(\omega-\omega')/T}-1} + \frac{(\omega+\omega')^2}{e^{(\omega+\omega')/T}+1}\right)\right.$$

$$\left. + \int_{\omega}^{\infty} d\omega' \frac{\omega'}{(\omega'^2 - \Delta_d^2)^{1/2}}\left(\frac{2(\omega^2+\omega'^2)}{e^{\omega'/T}+1} + \frac{(\omega-\omega')^2}{e^{(\omega'-\omega)/T}-1} + \frac{(\omega+\omega')^2}{e^{(\omega+\omega')/T}+1}\right)\right] \equiv \frac{\pi\lambda_d}{\omega_0^2} T^3 h^0(\omega) \tag{12}$$

and

$$\Delta_1 = \frac{\pi\lambda_d}{\omega_0^2}\left[\int_{\Delta_d}^{\omega} d\omega' \frac{\Delta_d}{(\omega'^2 - \Delta_d^2)^{1/2}}\left((\omega - \omega')^2 - \frac{2(\omega^2+\omega'^2)}{e^{\omega'/T}+1} + \frac{(\omega-\omega')^2}{e^{(\omega-\omega')/T}-1} - \frac{(\omega+\omega')^2}{e^{(\omega+\omega')/T}+1}\right)\right.$$

$$\left. + \int_{\omega}^{\infty} d\omega' \frac{\Delta_d}{(\omega'^2 - \Delta_d^2)^{1/2}}\left(-\frac{4\omega\omega'}{e^{\omega'/T}+1} + \frac{(\omega-\omega')^2}{e^{(\omega'-\omega)/T}-1} - \frac{(\omega+\omega')^2}{e^{(\omega+\omega')/T}+1}\right)\right] \equiv \frac{\pi\lambda_d}{\omega_0^2} T^3 h^1(\omega) \quad , \tag{13}$$

where $\lambda_d = g_{dd}^2 N_d(0)$ and $\omega_0 = 2sP_{Fd}$. We have assumed that the phonon energy is given by $\omega = sk$ and that the renormalization effect from the self-energy can be ignored. These approximations cause the minor differences between Eqs. (12), (13) and Ref. 8.

The mean lifetime due to the electron-phonon interaction is Γ_{ph}, where

$$\Gamma_{ph}^{-1} = 2\mathrm{Im}(\tilde{\omega}^2 - \tilde{\Delta}^2)^{1/2} = \frac{\omega}{(\omega^2 - \Delta_d^2)^{1/2}} \times\left(\omega_1 - \frac{\Delta\Delta_1}{\omega}\right)\theta(\omega - \Delta_d). \tag{14}$$

The mean free path $l_s(\omega)$ in the superconducting state is given by

$$l_s(\omega) = V_F\Gamma_s \equiv V_F(\Gamma_{imp}^{-1} + \Gamma_{ph}^{-1})^{-1} \quad , \tag{15}$$

where V_F is the Fermi velocity, and Γ_{imp} is the mean lifetime due to impurity scattering,

$$\Gamma_{imp}^{-1} = n\pi N_d(0) \int |U_d(\theta)|^2 d\Omega \quad , \tag{16}$$

with n being the impurity density. $l_n(\omega)$, the mean free path in the normal state, is given by $l_s(\omega)$ with $\Delta = 0$.

For each impurity concentration n, the relative importance of Γ_{imp} and Γ_{ph}, characterized by introducing x into Eq. (15), is

$$l_{s(n)}(\omega) = l_{imp}\left[1 + x\left(\frac{T}{T_c}\right)^3\left(h_{s(n)}^0(\omega) - \frac{\Delta}{\omega} h_{s(n)}^1(\omega)\right) \times \frac{\omega}{(\omega^2 - \Delta_d^2)^{1/2}}\theta(\omega - \Delta_d)\right] \quad ; \tag{17}$$

l_{imp} is defined by $V_F\Gamma_{imp}$, and $h_{s(n)}$ are the integrals in the large parentheses of Eqs. (12) and (13) with a change of variables $\omega/T \to \omega$, $\omega'/T \to \omega'$, and

$\Delta/T \to \Delta$. The ratio α_s/α_n is given by[1]

$$\alpha_s/\alpha_n = \int_{\Delta_d}^{\infty} \frac{d\omega}{2T} \frac{\Gamma_s(\omega)}{\cosh^2(\omega/2T)} \Big/ \int_0^{\infty} \frac{d\omega}{2T} \frac{\Gamma_n(\omega)}{\cosh^2(\omega/2T)} \quad . \tag{18}$$

The difference between this work and Ref. 1 is that we have used the complete expression for ω_1 and Δ_1, while ω_1 is taken to be a constant proportional to T^3 in Ref. 1. Note that the vertex correction, calculated in Ref. 1, was never used because it gives the undesirable T^5 dependence as explained before. Also the implicit assumption is made that $ql_{s(n)} \ll 1$, where q is the wave number of the sound wave. This condition may not be satisfied when T is sufficiently low.

B. Two-band model

In this model, we take the interband scattering only. The self-energy $\Sigma^{s(d)}$ of $s(d)$ electrons is given by

$$\Sigma_1^{s(d)} = \frac{Tg_{sd}^2}{(2\pi)^3} \sum_{n'} \int d^3p_1 G_{d(s)}(\vec{p}_1, \omega_n') D(\vec{p} - \vec{p}_1, \omega_n - \omega_{n'}) \quad . \tag{19}$$

Similar changes are to be made in $\Sigma_2^{s(d)}$. Since $\omega_1^{s(d)}$ and $\Delta_1^{s(d)}$ are very similar, we write down only ω_1^d explicitly,

$$\omega_1^d = \frac{\pi\lambda_{sd}^s}{\omega_0^2}\left[\int_{\Delta_s}^{\omega} d\omega' \frac{\omega'}{(\omega'^2-\Delta_s^2)^{1/2}}\left((\omega-\omega')^2 + \frac{4\omega\omega'}{e^{\omega'/T}-1} + \frac{(\omega-\omega')^2}{e^{(\omega-\omega')/T}-1} + \frac{(\omega+\omega')^2}{e^{(\omega+\omega')/T}+1}\right)\right.$$
$$\left. + \int_{\omega}^{\infty} d\omega' \frac{\omega'}{(\omega'^2-\Delta_s^2)^{1/2}}\left(\frac{2(\omega^2+\omega'^2)}{e^{\omega'/T}+1} + \frac{(\omega-\omega')^2}{e^{(\omega'-\omega)/T}+1} + \frac{(\omega+\omega')^2}{e^{(\omega+\omega')/T}+1}\right)\right] \quad , \tag{20}$$

where $\lambda_{sd}^s = g_{sd}^2 N_s(0)$.

Again for the low-ql limit and assuming that the sound attenuation from the two bands are additive, one obtains

$$\frac{\alpha_s}{\alpha_n} = \left(m_s^* n_s V_{Fs}^2 \int_{\Delta_s}^{\infty} \frac{d\omega}{2T} \frac{\Gamma_s^s}{\cosh^2(\omega/2T)} + m_d^* n_d V_{Fd}^2 \int_{\Delta_d}^{\infty} \frac{d\omega}{2T} \frac{\Gamma_s^d}{\cosh^2(\omega/2T)}\right) \Big/$$
$$\left(m_s^* n_s V_{Fs}^2 \int_0^{\infty} \frac{d\omega}{2T} \frac{\Gamma_n^s}{\cosh^2(\omega/2T)} + m_d^* n_d V_{Fd}^2 \int_0^{\infty} \frac{d\omega}{2T} \frac{\Gamma_n^d}{\cosh^2(\omega/2T)}\right) \quad , \tag{21}$$

where

$$(\Gamma_s^{s(d)})^{-1} = (\Gamma_{\text{imp}}^{s(d)})^{-1} + \frac{\omega}{(\omega^2-\Delta_{s(d)}^2)^{1/2}}\left(\omega_1^{s(d)} - \Delta_1^{s(d)}\right)\theta(\omega - \Delta_{s(d)}) \tag{22}$$

and

$$(\Gamma_{\text{imp}}^{s(d)})^{-1} = n\pi N_{d(s)}(0) \int |U_{sd}(\theta)|^2 d\Omega \quad . \tag{23}$$

IV. CALCULATIONS AND DISCUSSION

A. α_n

All experimental results on samples of different purity indicate α_n, as a function of T, is proportional to

$$\int_0^{\infty} \frac{d\omega}{2T} \frac{\Gamma_n(\omega)}{\cosh^2(\omega/2T)}$$

with a proper choice of x, which measures the relative importance of Γ_{imp} and Γ_{ph}. α_n for various values of x is given in Fig. 1. Aside from determining x from α_n, there are no adjustable parameters in our theory.

B. Deviation of α_s/α_n from $(\alpha_s/\alpha_n)_{\text{imp}}$ at T_c

This is emphasized in Ref. 1. It was shown that $(\alpha_s/\alpha_n)/(\alpha_s/\alpha_n)_{\text{imp}} \equiv f(x) \to \pi/2$ as $x \to \infty$. We also

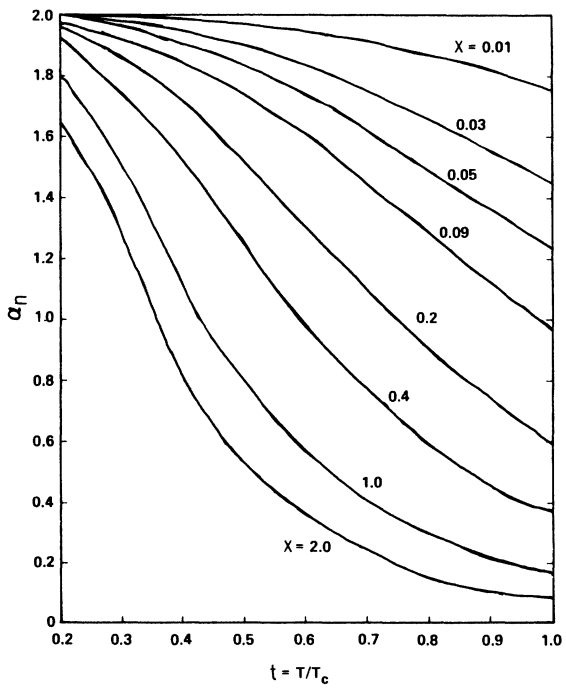

FIG. 1. α_n vs T/T_c. Note that α_n at $T/T_c = 1$ is arbitrary.

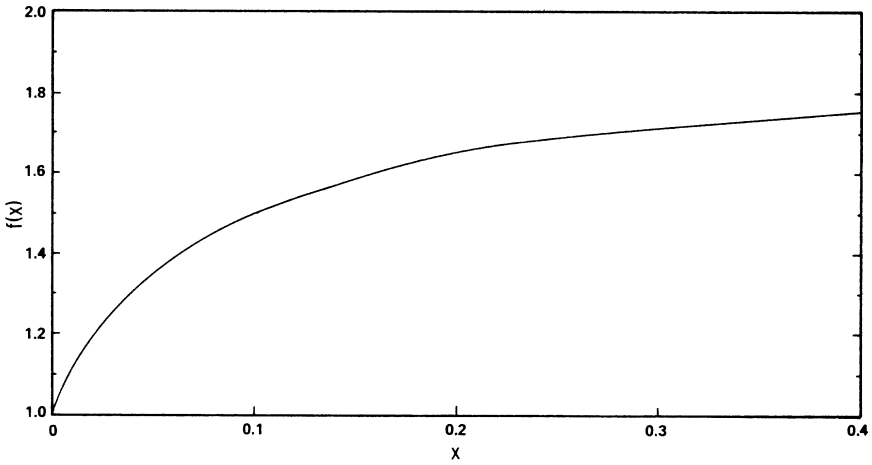

FIG. 2. $f(x)$ vs x.

compute $f(x)$ as plotted in Fig. 2, and find $f(x) \to 2$ approximately as $x \to \infty$. The difference is caused by the negligence of the ω dependence in Γ_n in Ref. 1. Including the ω dependence does not affect the temperature dependence of α_n but enhances its magnitude. Note that x of this work and that in Ref. 1 are proportional, but not equal.

C. Experimental data (Ref. 21)

The experimental data on α_s/α_n for $t \gtrsim 0.5$ are given in Refs. 1–3. Unfortunately, there is some confusion about the data in $t \lesssim 0.3$. Almond[22] shows that α_s/α_n behaves according to $(\alpha_s/\alpha_n)_{\text{imp}}$ at $t \lesssim 0.3$. However, thermal-conductivity data[17] for the low-T region show a deviation from the impurity-limited BCS theory. We also note that the data from Ref. 22 are inferred from some theoretical expressions whose validity might be challenged. In summary, it is believed that, for the purpose of understanding the true contribution of the electron-phonon interaction, no useful discussion of the theory can be made by fitting the data in the very-low-T region. Thus we concentrate on the region $t \geq 0.4$.

D. One-band model

The calculation is straightforward. The value of x for the Nb samples in Refs. 1 and 2 was determined by comparing the α_n data with the results of Fig. 1. After obtaining x, α_s/α_n was computed numerically. The results are given in Figs. 3 and 4. The general features of the theoretical curves can be explained as follows: While $\Gamma_s(\omega)$ becomes large as $T \to 0$ for $\omega \approx 0$, the contribution to α_s from higher values of ω becomes increasingly more important. The neglected term in Ref. 1, $(\omega - \omega')^2$ in Eq. (12), which comes from the emission of

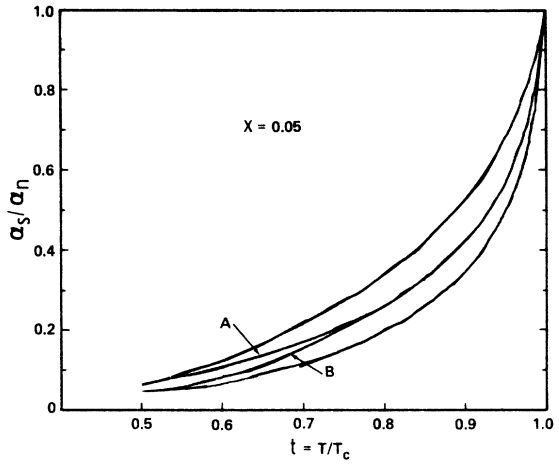

FIG. 3. α_s/α_n vs T/T_c for $x = 0.05$. The upper curve is for $(\alpha_s/\alpha_n)_{\text{imp}}$. Curves A and B are calculated from the one-band and two-band models, respectively. The lowest curve is the experimental data from Ref. 1.

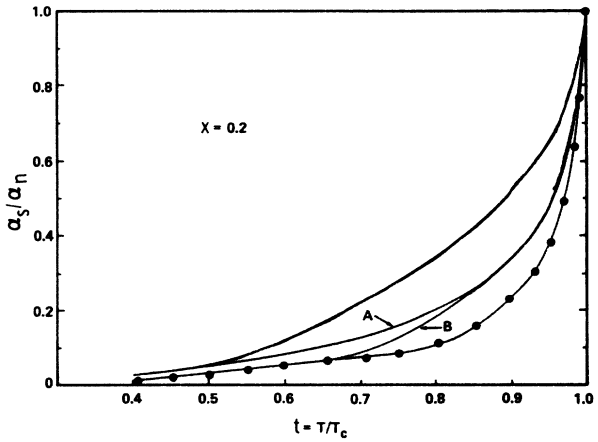

FIG. 4. α_s/α_n vs T/T_c for $x = 0.2$. Curves A and B are obtained from the one-band and the two-band models, respectively. The points are the experimental data, from Ref. 2.

phonons by the quasiparticles, is very important at smaller t; however, Γ_{ph} becomes ineffective because of the cancellation between $\omega\omega_1$ and $\Delta\Delta_1$ in Eq. (14). This explains why $\alpha_s/\alpha_n \to (\alpha_s/\alpha_n)_{imp}$ for $t \lesssim 0.5$.

The discrepancy between the calculated α_s/α_n and the experimental data for both $x = 0.05$ and $x = 0.2$ is about 50% around $T/T_c \approx 0.8$.

E. Two-band model

In order to avoid any parameters, let $\Delta_s \approx 0$ in Eq. (20), hence $\Delta_1^d \approx 0$, since it is generally believed that $\Delta_s/\Delta_d \leq \frac{1}{10}$. This approximation is used for numerical convenience. Next note that $n_d/n_s = 4$ and $m_d^* V_d^2/m_s^* V_s^2 \approx 1$, but $\Gamma_{ph}^s/\Gamma_{ph}^d \simeq N_s(0)/N_d(0)$, according to Eqs. (20) and (22).

Now we discuss the s component and d component separately. If one assumes the d band alone in Eq. (21), α_s/α_n is not much different from the one-band model at $t \gtrsim 0.8$, but at a lower t, α_s/α_n decreases faster than $(\alpha_s/\alpha_n)_{imp}$ or (α_s/α_n) in the one-band model, as shown in Figs. 3 and 4. The reason is due to the vanishing Δ_1^d in the calculation of Γ_{ph}. When the s band alone in Eq. (21) is taken, α_s/α_n is almost a constant.

The 50% difference between our calculation and the experimental data could possibly be accounted for by assuming a 20% increase in $\Delta(T)$. In Fig. 5 we have shown that if the BCS energy gap of curve B is increased to the value indicated in curve A then the remaining discrepancy could be accounted for. The theoretical curve of Fig. 5 is obtained by using the two-band model as described in Sec. IV E. If we used the one-band model in Sec. IV D, then the BCS energy gap would have to be selectively increased by ~25%. The discrepancy between the energy gap of A and B, which is perhaps larger than what is usually observed in weak-coupling superconductors,[23] remains to be studied. In summary, we have used the formalism given by Eliashberg[8] to include the electron-phonon interaction in the calculation of $\alpha_n(T)$ and $\alpha_s(T)$ for all values of purity and T. Whether or not one can attribute the discrepancy between the empirical Δ and the BCS Δ to an anisotropic or a band-structure effect requires more detailed calculations.

F. Discussion and conclusion

(i) Despite the apparent better agreement between the experimental data and the results of the two-band model at lower T over the one-band model, it should be pointed out that this agreement may be fortuitous, since we have assumed $N_s(0)/N_d(0) \ll 1$ in Eq. (21). Is the contribution of the s electrons really very small? Is it indistinguishable from the constant background contribution since both are insensitive to temperature? We have not tried to answer these questions. We also have not tried to achieve an agreement between theory and experiment by assigning an arbitrary number of m_d^*, P_{Fd}, P_{Fs}, and so on. Instead, we have shown that approximately $\frac{2}{3}$ of the anomalous temperature dependence of α_s/α_n can be accounted for by the BCS theory, when the electron-phonon interaction is included.

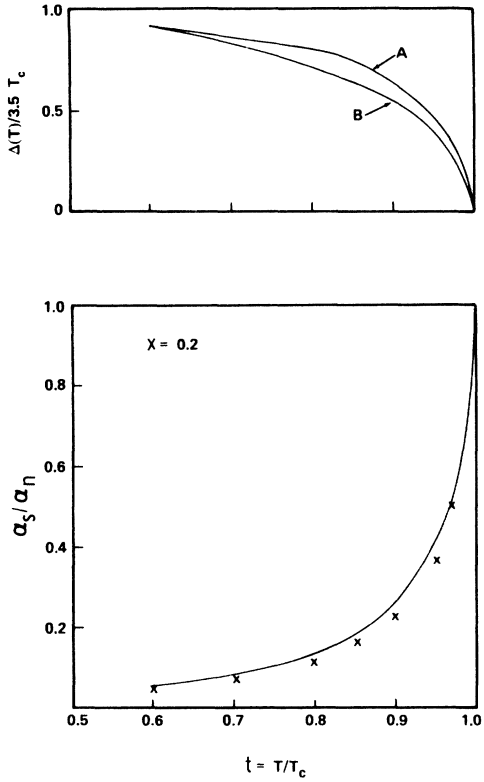

FIG. 5. α_s/α_n vs T/T_s assuming an empirical energy gap. The curve is calculated by using $\Delta_s \cong 0$ and Δ_d in curve A, which is to be compared with the Δ(BCS) of curve B. The points (×) are the data from Ref. 2.

(ii) It is shown that the electron-phonon interaction does reduce α_s/α_n substantially. Since this interaction exists in other metals, the same feature should also appear in other very pure superconductors. This effect should be taken into account in the analysis of ultrasonic-attenuation data in terms of an energy gap.

(iii) Considering the results obtained in the two-band model, we are forced to conclude that the d electron plays a dominating role in the transport properties of superconducting transition metals. This conclusion is reasonable on the basis of $\Gamma_{ph}^d/\Gamma_{ph}^s = N^d/N^s \gg 1$. To draw this conclusion, we have to assume dominance of the interband scattering at low T. Whether or not this picture is consistent with other physical quantities remains to be studied.

*Work supported in part by NASA Grant under Contract No. NGL-01-008-001.

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[18]A few words on the notations are in order here. In the one-band model, we assume the d band is the only band, and all physical quantities carry subscript d, which is dropped for clarity. In the two-band model all quantities without subscript apply to both bands. We also write $(\alpha_s/\alpha_n)_{\text{imp}}$ as the theoretical value of α_s/α_n obtained in the BCS theory without the correction for the electron-phonon interaction.

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[21]In our theory it is assumed that $ql < 1$. This condition is not generally satisfied in Ref. 3, where the frequency dependence of α_s/α_n is discussed. Hence, our discussion is confined to the data from the lower frequency region. An extension of this work to $ql > 1$ is straightforward.

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