the first definitive measurement of a more peaked distribution function. It should be pointed out however, that as Δ becomes small, it may be impossible to keep the tunnel-junction injection voltage sufficiently near 2Δ to obtain the peaked f necessary for the instabilities.

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Maximum Superconducting Transition Temperatures in *A*15 Compounds?

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Strong electron-phonon scattering results in a smearing of the peak structure in the electronic density of states in high-T_c *A*15 materials. This smearing may impose limits on the highest T_c achievable for these and similar materials. Numerical estimates are made using band structure and electrical resistivity data.

A high superconducting-transition temperature (T_c) is the most spectacular manifestation of strong electron-phonon coupling. The dependence of T_c on the electron-phonon coupling constant λ has been closely studied, and many of the important features of $T_c(\lambda)$ have been established. For small λ, $T_c \sim \omega e^{-1/\lambda}$, as shown by Bardeen, Cooper, and Schrieffer[1] and by McMillan[2] (here ω is a typical phonon frequency, and we have neglected the electron-electron Coulomb interaction). For very large λ, Allen and Dynes[3] have established that $T_c \sim \omega\lambda^{1/2}$, thus increasing idefinitely as λ is increased. For intermediate λ, the behavior is more complicated but generally the T_c-vs-λ curve has been found to be monotonically increasing. In this paper we establish that in certain high-T_c *A*15 compounds and most likely in some other systems, there may occur an intermediate region in which T_c actually *decreases* with increasing λ. Furthermore, this behavior may act as an effective limit for T_c within a given class of materials.

The large resistivities of high-T_c materials are a direct consequence of strong scattering of electrons by phonons. A related, but often overlooked, consequence is the broadening of electronic energy levels by an amount $\sim\hbar/\tau$, where τ is the electron-phonon contribution to the electron scattering time, as required by the uncertainty principle. This broadening effectively smears any fine structure in the density of states $N(E)$ over an energy width $\hbar/\tau$. In cases where the Fermi energy E_F lies in (or near) a peak in $N(E)$, a broadening will lower the effective value of $N(E_F)$ at a temperature $T>0$. Since τ^{-1} increases strongly with temperature, this smearing results in $\lambda(T_c)$ (which is that value calculated with the band structure at T_c) being significantly

lower than $\lambda(T=0)\equiv\lambda$, and hence causes new difficulties in attaining high T_c. Thus we have a situation where the very mechanism which raises T_c would scatter electrons so strongly that the resultant smearing of $N(E)$ limits T_c.

We have recently completed self-consistent psuedopotential band-structure calculations[4] for Nb_3Ge ($T_c\simeq 23$°K) and Nb_3Al ($T_c\simeq 18.5$°K). Allen *et al.*[5] have used the results of these calculations and estimates of λ from T_c values to calculate the lattice resistivity ρ_L, the mean free path l, and the energy broadening $\hbar/\tau$ at room temperature. For both materials the calculated values of ρ_L agree well with the experimental values (using the "saturation" hypothesis[6]), and $l\sim 5$–6 Å is of the order of the lattice constant, making the broadening $\hbar/\tau\sim 0.3$–0.4 eV. In Fig. 1, we show the detailed structure of $N(E)$ near E_F for Nb_3Ge, using a Fourier-series interpolation scheme described previously.[5] It can be seen that E_F lies in a peak of width $W\approx 0.07$ eV. It is evident that this structure will be completely smeared out well below room temperature, where $\hbar/\tau=0.4$ eV. The resultant drop in the effective value of $N(E_F)$ when $\hbar/\tau(T)\sim W/2$ (i.e., when the peak becomes smeared out), of the order of (20–30)%, would have a drastic effect on T_c. The situation in Nb_3Al is similar, although somewhat less drastic.

In the following we estimate the temperature at which the smearing of $N(E)$ becomes important using three models for the resistivity.

In the high-temperature ($T>\Theta_D$) limit, the electron-phonon scattering time τ can be written in the form[7]

$$\tau^{-1}=2\pi\lambda_{tr}k_B T/\hbar, \tag{1}$$

where λ_{tr} is closely related to the superconductivity coupling parameter λ ($\lambda_{tr}\simeq\lambda$). Smearing of the density of states will become important when the energy uncertainty $\hbar/\tau$ is of the order of half the peak width. With a peak width $W\sim 0.1$ eV, the condition $\hbar/\tau\sim W/2$ would then give the temperature

$$T\sim(90/\lambda)\text{°K} \tag{2}$$

at which the peak becomes completely smeared out (without allowing for temperature smearing). For strong-electron-phonon-coupling materials, the value of λ is $\gtrsim 1.5$; in these cases, the expression (1) for τ is no longer applicable, since we are not in the high-temperature limit. We can use the Bloch formula[8] for the $T\ll\Theta_D$ expression:

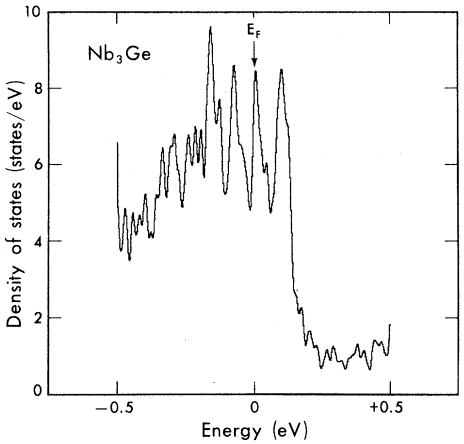

FIG. 1. Detailed electronic density of states near the Fermi energy, E_F, for Nb_3Ge, obtained from self-consistent pseudopotential band-structure calculations.

$$\frac{\tau_{T_1}}{\tau_{T_2}}=\frac{\rho_L(T_2)}{\rho_L(T_1)}=497.6\left(\frac{T_2}{\Theta_D}\right)^4\frac{T_2}{T_1}$$

$$\text{for } T_2\ll\Theta_D\ll T_1. \tag{3}$$

By use of (1) and (3), we get for the strong-coupling case

$$T\sim 0.7\Theta_D{}^{4/5}\lambda^{-1/5}\text{°K} \tag{4}$$

For $\Theta_D\sim 300$°K and $\lambda\sim 1.8$, this gives a temperature of 60°K at which the peak is destroyed by scattering.

Experimentally,[9] it has been found that the low-temperature resistivities of the high-T_c $A15$ materials can be described quite well by the empirical expression

$$\rho=A+BT^2. \tag{5}$$

Experimental resistivity data[9] give values of $B\sim 4.2\times10^{-3}$ and 4.5×10^{-3} $\mu\Omega$ cm/K^2 for Nb_3Ge and Nb_3Al, respectively. The electron-phonon resistivity can be expressed as

$$\rho_L=4\pi/\Omega_P{}^2\tau, \tag{6}$$

where

$$\Omega_P{}^2=\frac{4\pi e^2}{3}\sum_{k,n}v_{kn}{}^2\delta(\epsilon_{kn}-\epsilon_F)$$

$$=\frac{4\pi e^2}{3}N(\epsilon_F)\langle v^2(\epsilon_F)\rangle. \tag{7}$$

For Nb_3Ge and Nb_3Al, the values of Ω_p can be estimated from previous band-structure calculations.[4] The result for both materials is $\hbar\Omega_P$

~ 3.7 eV. Using these values,

$$T \sim \left(\frac{1}{B}\,\frac{4\pi}{\Omega_P^2}\,\frac{W}{2\hbar}\right)^{1/2}; \tag{8}$$

the results are 80 and 75°K for Nb_3Ge and Nb_3Al, respectively. At these temperatures the peak is *virtually destroyed.* However, at much lower temperatures the effective coupling constant $\lambda(T)$ can already be much reduced from $\lambda(0)$. One can envision a situation in which an increase in $\lambda(0)$ would actually lead to a decrease in $\lambda(T)$ due to the increased scattering.

Although we have no evidence that this regime has been reached in any known $A15$ materials, phonon broadening may be adversely affecting T_c (relative to the calculated value using $T=0$ band structures) for the high-T_c members. To estimate the magnitude of the effect in Nb_3Ge, we approximate the peak in $N(E)$ at E_F (Fig. 1) by a symmetric triangular peak centered at E_F, with full width $W=0.07$ eV and height 3, over a background density of states of 5, in units of states/(eV spin unit-cell). Obtaining the broadening from Eqs. (5)–(7), for $T_c \simeq 25$°K we have $2/W\tau = (25/80)^2 = 0.1$, resulting in ~ 8% decrease in $N(E_F)$. Using[5] $\lambda = 1.8$, $\mu^* = 0.1$, and estimating $d\ln T_c/d\lambda = 0.56$ from the Allen-Dynes equation,[3] we get a reduction $\Delta T_c = 2$°K. [We assume that $\lambda \propto N(E_F)$ and use the phonon moments of Nb_3Sn.]

A rigorous treatment of the effects we discuss can be obtained by solving the Eliashberg equations in the "dirty" limit, but retaining the energy variation[10] in the band structure. For a general density of states this is a formidable task. A simpler but related method of finding a better estimate of the reduction in T_c is by using the functional derivative $\delta T_c/\delta N(E)$ for Nb_3Sn calculated by Lie and Carbotte.[11] Phonon broadening is implicitly included in this function, and we need only use the difference $\Delta N(E)$ between the correct $N(E)$ (the model used above) and the constant $N(E)=8$ to evaluate the reduction

$$\Delta T_c = \int [\delta T_c/\delta N(E)]\Delta N(E)\,dE. \tag{9}$$

To use the published curve[11] of $\delta T_c/\delta N(E)$, we have cut off the function at $E = 25T_c$ and renormalized to the correct value of $\delta T_c/\delta N(E_F)$. Equation (9) gives $\Delta T_c = 4.2$°K, probably a more accurate estimate than the 2°K value found above.

Enhancement of the gap $[\Delta(0)]$ to transition-temperature ratio $2\Delta(0)/k_B T_c$ over the weak-coupling value of 3.52 is a consequence of retardation and damping of the electron-phonon interaction, as was first demonstrated by Swihart, Scalapino, and Wada.[12] Including the effect of damping on the electronic density of states further enhances this ratio, since T_c is lowered while $\Delta(0)$ is unchanged. Because of the difficulty of preparing good tunnel junctions with $A15$ materials, experimental determinations of this ratio are scarce; however, a value of $2\Delta(0)/k_B T_c = 4.2$ has been reported[13] for Nb_3Ge. This provides some verification of our theory, expecially considering that impurities at the interface reduce the measured gap.

The effect we are discussing, depends, of course, on fine structure in the density of states. A number of band-structure calculations[14] have found large peaks in the region near E_F in $A15$ compounds, although widths as narrow as those we find have not been emphasized previously. We emphasize that the peaks which we find are not related to the "one-dimensional–band-structure" peaks used in model fits to data. The presence of narrow peaks in $N(E)$ near E_F is not as accidental as it might at first seem. In the $A15$ structure, there are six transition-metal atoms per unit cell. Thirty d bands are constrained to lie in an energy interval of 9–10 eV. Strong band-band interactions and the fact that no band crossings are allowed off symmetry planes result in sharp peaks in $N(E)$ from each band. We can get an estimate of the peak widths in the $A15$ materials by comparison with Nb. Nb has five d bands and a similar d-band width. The peak widths in Nb are less than 1 eV; therefore peaks in $A15$ structures should have widths $W < 0.15$ eV. Similar considerations also hold for Chevrel-phase compounds which have six Mo atoms per cell and have even smaller d-band widths.[15]

In conclusion, we have shown that strong scattering of electrons by phonons in $A15$ materials causes a smearing of the electronic spectrum which can have adverse effects on T_c. For $A15$ materials with $T_c \simeq 25$°K, the reduction of T_c is estimated to be 2–4°K; if impurities are present, the additional scattering may cause further reduction from the stoichiometric $T=0$ band-structure value. We suggest that in some systems there may be regimes in which increasing the electron-phonon coupling causes a decrease in T_c. The Chevrel-phase compounds, with even narrower d bands and higher resistivities than the $A15$ materials, are possible candidates to encounter an effective limit on T_c via this mechanism. Of course, for *very* large λ, all band structure is smoothed and we again will find the Allen-Dynes limiting behavior $T_c \sim \omega' \lambda^{1/2}$, albeit

with a reduced effective frequency ω'.

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Effects of Voids on the Thermal Magnetoresistivity of Metals

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The influence of cylindrical voids on the thermal magnetoresistance of a model metal is calculated. In the absence of lattice thermal conduction a linear thermal magnetoresistivity results from the presence of the voids in a manner similar to the electrical magnetoresistivity. However, when the lattice conductivity is present, marked deviations from linearity occur.

The question of the anomalous magnetoresistances of the simple metals is considered to be one of the great unsolved problems of metals physics. After nearly 50 years of research, the source of these anomalies is still unknown. The semiclassical magnetoresistance theory of Lifshitz, Azbel', and Kagnaov[1] predicts that closed-orbit, uncompensated metals should have electrical and thermal magnetoresistivities which saturate in strong fields. However, in many of the simple metals[2-4] (the alkalis[2] and metals such as indium[3] and aluminum[4]) a linear transverse electrical magnetoresistivity is observed. In potassium, the archetypical simple metal, the transverse thermal magnetoresistance contains terms linear and quadratic in the field[5] (similarly, the other magnetotransport coefficients show unexplained behavior). In fact, to our knowledge, no experiments in the simple metals have been reported in which a saturating magnetoresistivity has been observed. The question of whether the source of the anomalies is intrinsic or extrinsic has not been resolved. Noting that the linear magnetoresistance of the simple metals varies unpredictably with sample handling and fabrication techniques, several authors[6,7] suggested that sample inhomogeneities (voids, inclusions, grain boundaries, dislocations, etc.) may be responsible for the anomalous behavior. Fletcher has also argued in a different manner for an extrinsic cause.[8] A recent Letter by Beers *et al.*[9] describes a measurement of the electrical magnetoresistance of a pure indium specimen into which cylindrical voids were introduced. Beers *et al.* find a large enhancement in the linear electrical magnetoresistance due to the presence of

