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Disorder and Superconductivity in *A*-15 Compounds

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The universal depression of the superconducting transition temperature T_c in disordered A-15 compounds is examined. Existing energy-band calculations are used to calculate the density of electron states, which is possibly enhanced by disorder in some cases such as Nb_3Ge. The dramatic drop in T_c in Nb_3Ge at a critical value of the resistivity is attributed to overdamping of acoustic plasmons which decreases the electron pairing interaction despite small changes in the density of states.

Disorder induced by crystal growth conditions, α-particle irradiation, and neutron damage yields a remarkable depression of the superconducting transition temperature T_c for the high-temperature superconducting A-15 compounds Nb_3Ge, V_3Si, and similar materials. Testardi, Poate, and Levinstein[1] have pointed out the universal nature of the depression of T_c by correlating it with the residual resistance ratio for various types of damage. A thorough investigation of neutron irradiation by Sweedler, Cox, and Moehlecke[2] demonstrated that the relative decrease of T_c in many A-15 compounds followed a similar pattern as a function of the neutron flux. The measured transition temperatures of disordered V_3Si samples are plotted versus the residual resistance $R(T = 25\,^{\circ}\mathrm{K})$ in Fig. 1. The drop in T_c from 18 to 4 °K is characteristic of the general trend for Nb_3Ge, Nb_3Al, and similar materials. Also the

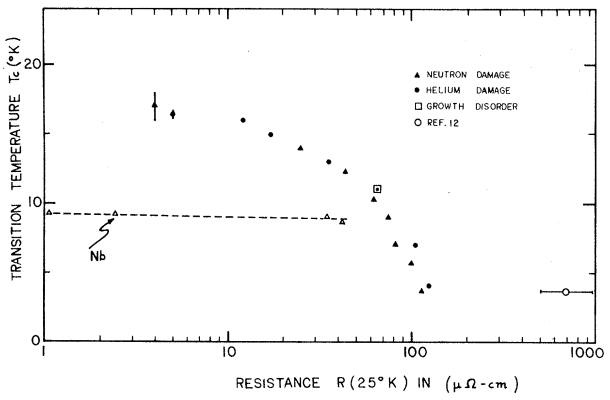

FIG. 1. Superconducting transition temperature of V_3Si subjected to various types of damage as a function of residual resistivity. The universal drop in T_c is common to other A-15 compounds, and is in sharp contrast to the behavior of Nb shown by the dotted curve.

persistence of low-temperature superconductivity ($T_c \simeq 4$ °K) at rather large resistance values is evident from Fig. 1.

By contrast, disorder appears to have very little influence on Nb samples which remain superconducting to $T_c \simeq 9$ °K over a wide range of residual resistance as shown in Fig. 1.[1] Further clues to the problem are provided by the disordered-enhanced superconducting temperature (from 1 to 5 °K) in Mo_3Ge which also exhibits the A-15 structure.[3]

On the basis of the phonon-exchange mechanism of the superconducting electron pairing it is difficult to reconcile changes in the phonon spectrum with the dramatic variations in T_c induced by disorder. However, changes in the electron density of states may have a profound influence on the transition temperature according to the BCS weak-coupling formula

$$T_c \simeq 0.7\theta_D \exp[-1/(\lambda_{ph} - \mu^*)], \quad (1)$$

where θ_D is the phonon Debye temperature, $\mu^* \simeq 0.1$ represents the Coulomb repulsion between electron pairs, and λ_{ph} is the attractive pairing parameter originating from exchange of phonons. Since $\lambda_{ph} \simeq N(0)V^2$, where $N(0)$ is the electron density of states at the Fermi surface and V^2 is an averaged electron-phonon matrix element, it is evident that changes in $N(0)$ will significantly alter the superconducting properties.

Measurements of the specific heat C_v and magnetic susceptibility of V_3Si indeed suggest a reduction in the density of states with increased neutron damage, but a quantitative analysis gives discrepancies with the measured transition temperatures of this and other A-15 compounds.[5]

The purpose of the present work is twofold. First we compute the density of states including disorder using band-structure results of augmented-plane-wave (APW) and pseudopotential methods. These calculations will show the general trends in T_c to be expected with disorder, and, in particular, will exhibit possible T_c enhancement with disorder. We then calculate the influence of the electron relaxation time τ on an alternative pairing mechanism based on exchange of acoustic plasmons; the usual criterion for overdamped excitations will be shown to correspond to the universal drop in T_c for disordered Nb_3Ge and some other A-15 superconductors.

A primary and general consequence of disorder is to limit the electron relaxation time τ and thereby increase the resistivity R by the Einstein relation

$$R = (4\pi/\omega_{pl}^2)\tau^{-1}, \quad (2)$$

where the plasma frequency $\omega_{pl}^2 = 4\pi ne^2/m^*$ may be extracted from optical data. Hence the electron damping $\Gamma = \tau^{-1}$ will cause a broadening of structure in the density of states $N(E)$ according to

$$N(E,\Gamma) = \int S(E,E',\Gamma)N^{(0)}(E')dE', \quad (3)$$

where S is an appropriate broadening function. We consider a Lorentzian form

$$S(E,E',\Gamma) = \pi^{-1}\Gamma/[(E-E')^2 + \Gamma^2], \quad (4)$$

and impose the essential constraint of the conservation of total states. The latter point is crucial since a finite range of energies is considered, which is not necessarily much greater than Γ in the extremely disordered cases. Thus we compute $N(E,\Gamma)$ from Eqs. (3) and (4) numerically by allowing a shift of the Fermi energy E_F' to preserve the total density.

We present here the analysis of Nb_3Ge using the self-consistent APW band-structure calculations of Klein *et al.*[6] and independently using the pseudopotential bands of Ho, Cohen, and Pickett.[7] A final element of our calculation is the value of the plasma frequency $\omega_{pl} \cong 2.3$ eV obtained from optical data.[8] Our results for the density of states including damping are shown in Fig. 2: They demonstrate the expected smearing of structure in $N(E)$ for $\Gamma \sim 0.05$ eV, but show relatively small changes in $N(E_F)$ with disorder! The significance of these changes in the density of states is greatly amplified in the superconducting transition temperature T_c shown in Fig. 3. The T_c was evaluated from the McMillan equation which incorporates strong-coupling corrections to Eq. (1), and the values of the electron-phonon coupling parameter $\lambda = V^2N(E_F)$ were scaled to yield $T_c = 23$ °K for the ordered Nb_3Ge: This requires $V^2 = 0.13$ eV for the pseudopotential results and $V^2 = 0.25$ eV for the APW bands. Since the Fermi level lies near a peak in $N(E)$ in the calculations of Ref. 7, the lower portion of the shaded region in Fig. 3 represents a *lower* bound on T_c, whereas the results of Ref. 6 indicate an *upper* bound on the T_c variation reflecting a Fermi energy near a valley in $N(E)$.

Clearly the results of the independent band-structure calculations shown in Fig. 3 yield a much smaller variation in T_c than observed experimentally for Nb_3Ge. The discrepancy be-

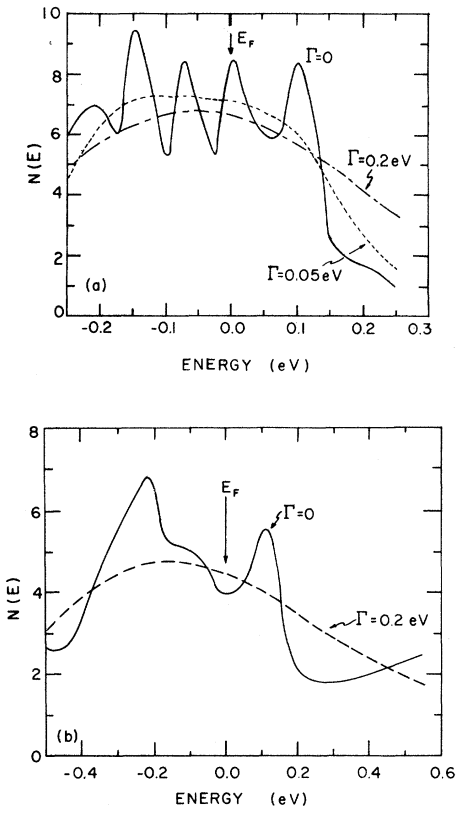

FIG. 2. Electron density of states for Nb_3Ge from (a) pseudopotential calculations (Ref. 7) and (b) from APW band structures (Ref. 6). The solid curves are in the limit of infinite electron lifetime $\Gamma = \tau^{-1} = 0$. Structure is significantly broadened for $\Gamma = 0.05$ eV, although $N(E_F)$ is only slightly modified in both calculations even in the extreme disordered case of $\Gamma = 0.2$ eV.

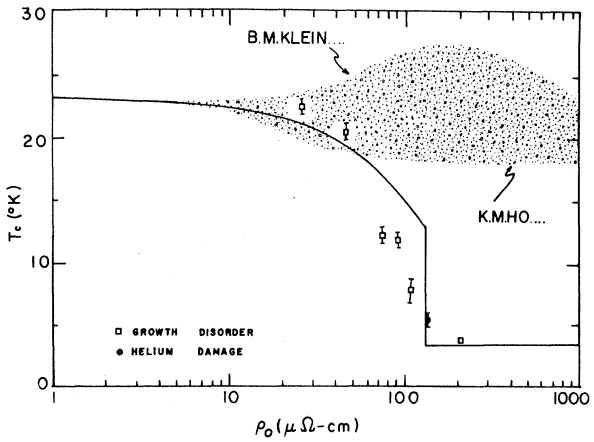

FIG. 3. Superconducting transition temperature for Nb_3Ge as a function of resistivity is indicated by experimental points from Ref. 1. The shaded region indicated the expected decrease in T_c from variations in the density of states obtained from pseudopotential calculations (Ho, Cohen, and Pickett), and the predicted increase from the APW band structure (Klein *et al.*). The solid curve results from the damping of the acoustic plasmons which becomes critical at the value $\rho_0 \simeq 120\ \mu\Omega$ cm.

tween T_c variations and the disordered $N(E)$ is considerably less for V_3Si as shown by the independent work of Testardi and Mattheiss using a similar analysis of APW band calculations.[9] However, the cases of Nb_3Al and other A-15's resemble the Nb_3Ge situation.[5]

To explain the anomalous depression of superconductivity in disordered Nb_3Ge, we consider the additional pairing mechanism achieved by exchange of acoustic plasmons.[10] The acoustic branch represents d-electron oscillations screened by lighter-mass electrons. *A priori*, it is clear that disorder will strongly affect the electron damping and thus eliminate the plasmon mechanism at some critical resistivity, even though the phonons may persist as well-defined excitations.

Denoting the electron pairing parameters induced by phonons and plasmons, respectively, as λ_{ph} and λ_{pl}, the transition temperature may be expressed as[10]

$$T_c \cong 0.7\theta_{ph}\left(\frac{\theta_{pl}}{\theta_{ph}}\right)\frac{\lambda_{pl}}{\lambda_T}\exp\left(-\frac{1+\lambda_T}{\lambda_T-\mu^*}\right), \qquad (5)$$

where $\lambda_T = \lambda_{ph} + \lambda_{pl}$, $\theta_{ph} \simeq 300$ °K is the phonon Debye energy, and θ_{pl} represents the corresponding maximal acoustic plasmon energy. The Coulomb repulsion term is $\mu^* \cong 0.1$. Noting that the transition temperature persists at $T_c \simeq 5$ °K at large disorder for both V_3Si and Nb_3Ge, we take $\lambda_{ph} = 0.45$ to achieve this saturation in the regime of overdamped plasmons.

The plasmon damping Γ is related to the resistivity R by Eq. (2). The relevant dimensionless parameter is $x = \Gamma/\theta_{pl}$, so that the acoustic plasmons cease to exist for $x > 1$. Analysis[10] of the band-structure results for Nb_3Ge yields $\theta_{pl} \cong 0.15$ eV, so that we expect the plasmon mechanism to become inoperative at $R_c \cong 4\pi\theta_{pl}/\omega_{pl}^2 \cong 200\ \mu\Omega$ cm. This value is in good agreement with experiment, as shown in Fig. 3.

To make a realistic comparison over a wider range of resistivity, we consider a linear acoustic plasmon dispersion, $\Omega = sq$, where s is a "sound" velocity, and a matrix element g_2 for the coupling of electrons to the acoustic plasmon mode. Treating the damping Γ as independent of

momentum and energy, we find the pairing parameter

$$\lambda_{pl} = \frac{N(0) g_2^2 \theta_{pl}}{\Gamma (s k_F)^2} \times \left[\frac{x}{4} \ln\left(1 + \frac{4}{x^2}\right) + \tan^{-1}\left(\frac{2}{x}\right) - \frac{x}{2} \right], \quad (6)$$

where k_F is the Fermi momentum. Microscopic calculations of g_2 are faced with difficulties and uncertainties similar to the evaluation of the electron-phonon coupling, and thus we adjust λ_{pl} ($x = 0$) to fit T_c at the lowest resistivity value. The resulting behavior of the calculated T_c from Eqs. (5) and (6) is shown by the solid curve in Fig. 3, in comparison to the data on Nb_3Ge. At the highest point, $T_c = 23\,^{\circ}K$, we find $\lambda_{pl} \cong 0.22$, in comparison to the phonon contribution $\lambda_{ph} = 0.45$. We have included the additional Landau damping of the acoustic plasmons by decay into the screening electron continuum: This yields a corresponding width $X_L = \Gamma_{Landau}/\theta_{pl} = 0.4$.

In conclusion, the damping of acoustic plasmons explains the anomalous behavior of T_c in Nb_3Ge even though the electron density of states remains unchanged with disorder. In view of detailed uncertainties in the band-structure calculations which limit our knowledge of the acoustic plasmon parameters, the agreement with existing experiments is quite reasonable.

Optical data on the disordered A-15 materials would provide independent tests of the electron damping as a function of resistivity. Preliminary data[8] on one disordered sample of V_3Si gives a positive real part of the dielectric function which may be associated with overdamped plasmon modes. Our analysis of this data suggests a high value of resistivity ($R \sim 400$–$700\ \mu\Omega$ cm). Nevertheless the sample is superconducting with $T_c \simeq 4\,^{\circ}K$. It is interesting to note that the highly disordered V_3Si samples exhibit resistivities[1] an order of magnitude greater than the room temperature value of $R(300\,^{\circ}K) \cong 80\ \mu\Omega$ cm for pure V_3Si. Thus the peculiar temperature-dependent resistivity is far from a saturation value, in agreement with the estimated long mean free paths of electrons in V_3Si.[8]

Finally, we comment on the prospects of achieving higher superconducting temperatures by shifting the Fermi energy to a favorable maximum in $N(E_F)$. Alloying may reduce the electron lifetime and thereby reduce the acoustic plasmon mechanism. However, it may be of interest to change the electronic structure by ion implantation of hydrogen in compounds such as Nb_3Al, with the goal of increasing $N(E_F)$, while minimizing disorder. Furthermore our results may be relevant to Nb_3Si, whose band structure favors the acoustic plasmon formation, so that a high T_c would require rather well-ordered crystals with minimal defects and other electron scattering centers.

As an independent check on the analysis we have calculated the influence of compositional order on T_c for a realistic three-dimensional band model by extending the method of Labbé and Van Reuth.[11] These results support the present conclusions and will be published elsewhere.[5]

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