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THE SUPERCONDUCTING TRANSITION TEMPERATURE OF DISORDERED A-15 COMPOUNDS

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The universal depression of the superconducting transition temperature T_c in disordered A-15 compounds is examined. Results of energy band calculations are used to calculate T_c as a function of residual resistivity ρ_o for a series of 10 different A-15 materials V_3X and Nb_3X, (X = Aℓ, Ga, Si, Ge and Sn).

In recent years, the properties of high-T_c superconductors with A-15 structure have been investigated both theoretically and experimentally with many interesting results.[1] Among them is the very large reduction of T_c due to defects[2,3] which seems to be a common feature of these A-15 compounds. The mechanism for the reduction of T_c has remained a source of some controversy. Various explanations are based on a sharp-density of states in a one-dimensional-type structure[4] which is easily decreased by disorder. Some other explanations have been based on gap anisotropy[5]. Another point of view has focused on the acoustic plasmon mechanism[6] and, finally, some arguments have been based on general smearing of the density of states with disorder.[7,8]

The purpose of the present work is, by using the ideas of a model first introduced by Testardi and Mattheiss[7], to calculate the density of states N(E), Fermi velocity $V_F(E)$, and Drude plasma frequency $\Omega_p(E)$ and other properties as a function of disorder Γ (or residual resistivity ρ_o) for 10 different A-15 compounds Nb_3X and V_3X, with X = Aℓ, Ga, Si, Ge, Sn. In applying this scheme, we have used the electronic band structure results of Klein, et. al.[9] for the N(E), $V_F(E)$, and $\Omega_p(E)$ for the perfectly ordered materials. We want to emphasize that a good quantitative understanding[10] of the superconducting properties of the A-15's has been derived from these band-structure results[9] without additional assumptions regarding quasi one-dimensionality or resorting to model density of states singularities.

In this short paper we only present the results for the dependence of T_c on the residual resistivity ρ_o for the 10 different A-15's. The details of the calculation and results for $N(E_F)$, $V_F(E_F)$, $\Omega_p(E_F)$ and other properties as a function of disorder will be presented elsewhere.[11]

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

$$\rho_o = 4\pi\hbar\Gamma/\Omega_p^2 = 4\pi\hbar^2/\Omega_p^2\tau \qquad (1)$$

where the plasma frequency Ω_p can be extracted from optical data. Hence the electron damping $\Gamma = \hbar/\tau$ will cause a broadening of structure in the density of states N(E) according to

$$N(E,\Gamma) = \int S(E,E',\Gamma)N(E',\Gamma=0)dE' \qquad (2)$$

where N(E, Γ=0) is density of states of the perfectly ordered material and S is an appropriate broadening function. We consider a Lorentzian form

$$S(E,E',\Gamma) = \pi^{-1}\Gamma/[(E-E')^2+\Gamma^2] \qquad (3)$$

and impose the essential constraint of the conservation of total states. Details on how to avoid complications from the broad Lorentzian wings and the exact normalization will be given elsewhere.[11]

Using Eqs. (2) and (3) and the band structure results[9] for N(E), $V_F(E)$, and $\Omega_p(E)$ of the perfectly ordered A-15's, we have calculated $N(E_F)$, $V_F(E_F)$ and $\Omega_p(E_F)$ as a function of electron damping Γ, which is a measure of the disorder. Γ is related to the resistivity ρ_o through Eq. (1). (In the appropriate units we have $\rho_o(\mu\Omega\text{-cm})=101.4925\ \Gamma\ (\text{mRy})/\Omega_p^2(\text{eV})$). The superconducting transition temperature T_c was obtained by assuming that $\lambda \sim N(E_F, \Gamma)$ and using McMillan's equation[12], with $\mu^* = 0.13$ and θ_D to be constant. We used that $\lambda=\lambda^{exp}N(E_F,\Gamma)/N(E_F,\Gamma=0)$, where λ^{exp} is the experimentally[10] measured λ by inverting McMillan's equation.

Our results for T_c/T_{co} vs ρ_o are shown in Figs. 1 and 2 for the Nb_3X and V_3X respectively, where X = Aℓ, Ga, Si, Ge, and Sn. For the Nb-base A-15's (Fig. 1) we have found that Nb_3Ga, $Nb_3A\ell$ and Nb_3Sn decrease by 80% when ρ_o reaches 150-200 μΩ-cm in qualitatively agreement with experiment[2]. Our detailed calculations for Nb_3Ge yield a smaller variation in T_c than observed experimentally. Hence for Nb_3Ge, the drop in T_c seen experimentally is not coming from the drop of $N(E_F)$. Ruvalds and Soukoulis[6] attributed the drop in T_c in Nb_3Ge to overdamping of acoustic plasmons. For

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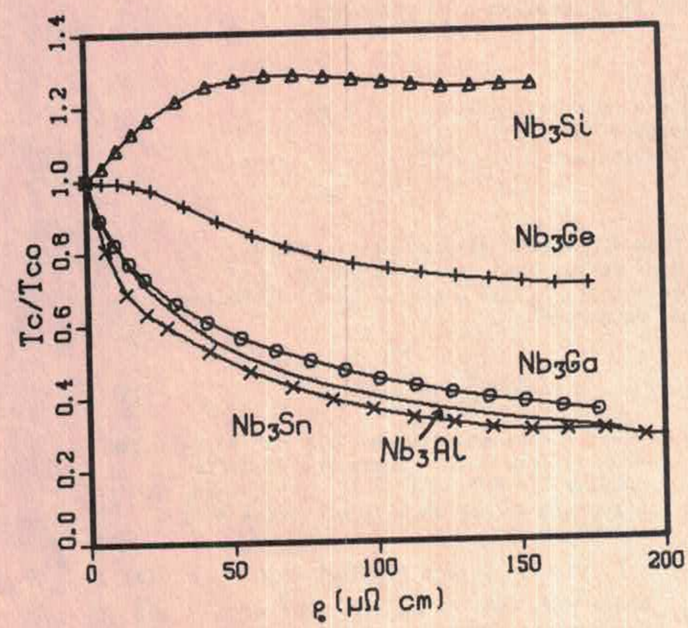

Fig. 1: T_c/T_{co} vs ρ_o for the Nb-base A-15's.

Nb_3Si we predict that T_c will increase by 30% as disorder increases which may explain the disagreement between experimental expectations and the low λ and T_c values calculated at full stochiometry.[9,10] As far as the V-base A-15's (Fig. 2), we have found that the T_c drop in

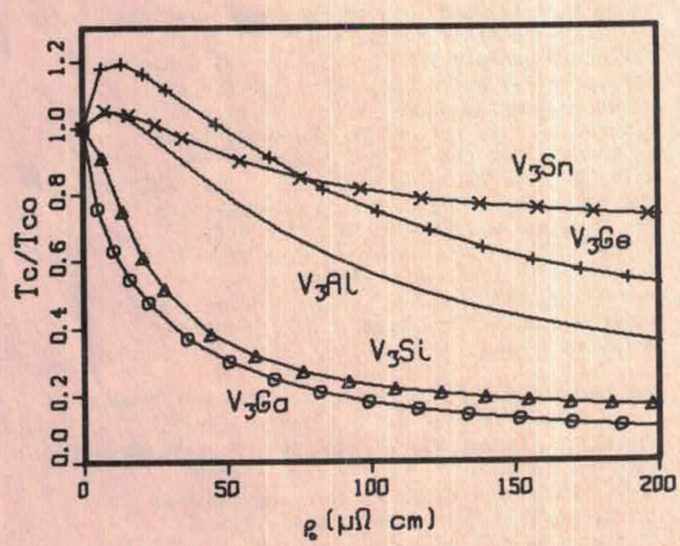

Fig. 2: T_c/T_{co} vs ρ_o for the V-base A-15's.

V_3Si and V_3Ga is in qualitative agreement with experiment.[3] The existing measured values of T_c for V_3Ge[3] are also in qualitative agreement with our results, but there is no experimental values in the region with $\rho_o \leq 50$ μΩ-cm to check if the calculated initial increase in T_c with ρ_o is real. For V_3Sn and $V_3A\ell$, the decrease of T_c is 20% and 60% respectively. Insufficient or no data on V_3Sn and $V_3A\ell$ prohibits us from comparing our results with experiments.

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