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TRANSITION TEMPERATURE OF ISOTROPIC SUPERCONDUCTORS

S. J. Poon

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California Institute of Technology
W. M. Keck Laboratory of Engineering Materials

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by

S. J. Poon

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Professor Pol Duwez, principal investigator.

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Using the self-consistent solutions of the Eliashberg theory⁽¹⁾, we discuss in this paper the limitations on the superconducting critical temperature T_c of isotropic superconductors. It was observed⁽²⁾ that the maximum T_c of alloys in the transition metal (TM) series is given by the relation $T_c \lesssim k \frac{T_m}{M}$ (k is a constant, T_m is the melting temperature from the solidus, and M is the average ionic mass). We show that this empirical relation can be explained by Leaven's⁽³⁾ least upper bound on T_c . However, it is necessary to remark that Leaven's result is consistent with Allen's approximate T_c equation, once the area A of the electron-phonon spectral function $\alpha^2 F(\omega)$ is fixed. The differences in the bound values are within two percents. Leaven's result can be expressed in the form $T_c \lesssim \frac{C(\mu^*)}{2} \frac{\eta}{M} \frac{\langle \omega \rangle}{\langle \omega^2 \rangle}$, where η and the frequency moments are defined in the usual way, $C(\mu^*)$ is a μ^* dependent constant. For the class of alloys considered in reference 2, $\frac{\eta \langle \omega \rangle}{\langle \omega^2 \rangle} \sim \frac{\eta}{\theta_D}$ scales well with T_m . The errors in this approximation are at most within a few percents. Thus Poon and Johnson's maximum T_c relation is obvious. Leaven's result is good for analyzing the T_c trend in a particular class of alloys, when the trend of A is known. To study the possibility of obtaining high T_c materials, it might be more informative to consider the fundamental atomic parameter η , since it depends explicitly on the self-consistent ionic potentials. We also prefer using Allen's approximate T_c equation.

We first discuss the case of d-band isotropic superconductors. The asymptotic critical temperature can be expressed⁽³⁾ in the form $T_c \rightarrow 0.15 (\eta/M)^{\frac{1}{2}} (\mu^* = 0.1)$ as $\lambda \rightarrow \infty$. If we take $\eta \sim 12 \text{ eV/\AA}^2$, the maximum value expected based on cohesive energy arguments⁽²⁾, and a small value of $M = 50 \text{ amu}$ for TM elements; then

$T_c \rightarrow 60^\circ\text{K}$ as $\lambda \rightarrow \infty$. Experimentally, λ is limited to order of unity because $\langle \omega^2 \rangle \rightarrow 0$ signifies a lattice instability. However, using an expression of the form⁽⁴⁾ $\langle \omega^2 \rangle = \langle \Omega^2 \rangle - 2 \langle \Omega \text{Re} \Pi \rangle$ only gives the condition for $\langle \omega^2 \rangle \rightarrow 0$ or $\lambda \rightarrow \infty$. Metallurgically, once a phase transformation occurs, $\langle \omega^2 \rangle$ again sets on some finite values. It might be more useful to consider the relation $\langle \omega^2 \rangle \approx \frac{\omega_M^2}{\langle \epsilon(q, \omega) \rangle}$ for the jellium model, where ω_M is the ion plasma frequency, and $\epsilon(q, \omega)$ is the linear dielectric function of the medium. It is found that⁽⁵⁾ by taking the empirical static dielectric function of Bennemann and Garland⁽⁶⁾, the values of $\langle \omega^2 \rangle$ for TM elements and Nb_3Sn scale well with the numerical results of reference 3. One can show that $\langle \epsilon(q, 0) \rangle$ is applicable to d-band isotropic superconductors in general.⁽⁵⁾ The most important parameter in $\langle \epsilon(q, 0) \rangle$ is the density of states $N(\epsilon_f)$. For a given η (say $\sim 10 \text{ eV}/\text{\AA}^2$) a high value of λ is determined from a small $\langle \omega^2 \rangle$ (or large $N(\epsilon_f)$).

It was shown in reference 4 that $\langle \omega^2 \rangle \rightarrow 0$ as the product $\omega_c N(\epsilon_f) \rightarrow \sim 4$ states/atom, where ω_c is a cutoff frequency. This result seems to be quite general for tight-binding metals.⁽⁵⁾ For metals, the value of ω_c cannot be significantly less than the intra-atomic Coulomb interaction, which is the order of a few eV.⁽⁷⁾ Moreover, this lattice instability condition does not take into account the Gibbs free energies of the different competing phases, which might set a even more stringent condition on $N(\epsilon_f)$. It is reasonable to assume $N(\epsilon_f) \lesssim 3$ states/eV atom. Comparing the value of $\langle \omega^2 \rangle$ obtained this way together with $\eta \sim 10 \text{ eV}/\text{\AA}^2$ to the case of bad superconductors (e.g. Mo, W), we get $\lambda \lesssim 2-3$.

For the 3d series and some intermetallics,

we might face another type of instability, namely ferromagnetism. In this case, the classical Slater-Stoner condition $N(\epsilon_f)\delta E \lesssim 1$ sets an upper limit on $N(\epsilon_f)$, where δE is the effective exchange energy. Usually, $\delta E \sim 0.5$ eV for the 3d series and is smaller for the 4d and 5d series.⁽⁷⁾ The limit on $\langle \omega^2 \rangle$ is again obvious and λ does not seem to exceed the value obtained from lattice instability condition.

Actually, the difficulty for increasing T_c when $\lambda \gtrsim 1$ is obvious from the approximate T_c equation. In fact, the derivative $\frac{dT_c}{d\lambda}$ reaches a maximum around $\lambda \sim 1$ and then tails off for larger λ ($\mu^* \sim 0.1$, constant η). By taking $\eta \sim 10$ eV/Å², $\mu^* \sim 0.1$ and $\lambda \lesssim 3$, a maximum T_c of $\sim 30^\circ$ K is obtained assuming an Einstein spectrum. However, we must also consider the possibility of enhancing μ^* and thus lowering T_c because it is an increasing function of $N(\epsilon_f)$. Tunneling experiments on TM elements and compounds are needed to study the effects of the pair (λ, μ^*) on T_c . The T_c value for d-band superconductors obtained here might have been a marginal value. The metallurgical feasibility of particular phases has been ignored.

For the simple metals, the light elements (e.g. metallic phases of H, Be and C) are potentially high T_c superconductors. The T_c benefits from the small mass even though η ($\lesssim 2.5$ eV/Å²) is small. The small η is universal of the one-OPW approximation of the Fermi surface. To obtain larger η might require a multiple-OPW approximation⁽⁸⁾, which signifies a tendency towards covalent-metallic instability. Although, this does not increase λ appreciably since the Debye temperatures are high, yet the fact that $\lambda \lesssim 0.5$ ($\frac{dT_c}{d\lambda}$ still increasing as mentioned earlier) is promising in further enhancing T_c . A T_c as high as $\sim 11^\circ$ K has been obtained in metastable Be films.⁽⁹⁾ For intermetallics

from the fourth period and higher in the periodic table, it was observed⁽²⁾ that the maximum T_c ($\lesssim 10^{\circ}\text{K}$) is independent of the melting temperature. It is reasonable to expect higher values of T_c from the lower periods with small atomic mass.

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