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TRANSITION TEMPERATURE IN SOME A-15 COMPOUNDS

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MODE SOFTENING AND HIGH SUPERCONDUCTING
TRANSITION TEMPERATURE IN SOME A-15 COMPOUNDS*

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ABSTRACT

The electronic density of states at the Fermi level, $N(E_F)$, and the geometric mean phonon frequencies, ω_g , were determined from heat-capacity data for a number of A-15 superconductors. Although ω_g is an appropriate average phonon parameter for evaluating McMillan's expression for λ , we found that the T_C values cannot be reliably estimated using ω_g . There are, however, strong correlations between λ , $N(E_F)$, and the temperature dependence of ω_g , $d\ln\omega_g/dT$. The high- T_C , high- $N(E_F)$ materials V_3Si and V_3Ga show the largest phonon-mode softening on cooling. We propose that, for the higher- $N(E_F)$ materials, particular phonon-modes strongly couple to the electronic system and enhance T_C to a greater extent than average phonon properties would indicate.

The high- T_C A-15 superconductors have anomalous electronic and phonon properties.⁽¹⁾ In earlier papers,^(2,3) we analyzed heat-capacity data on A-15 compounds, to determine certain average electronic and phonon properties relevant to superconductivity. In this paper, we present data on an additional compound, $Nb_3Sn_{0.7}Sb_{0.3}$. With the new data we show that there are correlations between the electron-phonon mass enhancement λ , and the electronic density of states at the Fermi level $N(E_F)$. There is also a correlation between the temperature dependence of the geometric mean phonon-mode frequency and $N(E_F)$. We explain these correlations by suggesting that a relatively small number of phonon-modes strongly couple to the electronic system and selectively soften because of electronic screening effects, which in turn depend strongly on $N(E_F)$.

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The sample of $\text{Nb}_3\text{Sn}_{0.7}\text{Sb}_{0.3}$ was prepared⁽³⁾ in the same manner as Nb_3Sn . Its T_c value was 14.9 K and metallographic analysis showed that it was 85-90% single phase. The heat capacity was measured over the temperature range of 2-400 K. The electronic density of states at the Fermi level can be determined from the low-temperature heat-capacity data. The higher-temperature entropy can be analyzed to determine the geometric mean frequency, $\omega_g = \left[\frac{3N}{11s} \omega_g \right] \frac{1}{3N}$ and its temperature dependence.⁽³⁾ In Fig. 1 we display the ω_g values, for all samples, as effective Debye temperatures $\theta \equiv e^{1/3} \hbar \omega_g / k_B$. Note that the high- T_c vanadium compounds show large temperature dependencies of θ , indicating that there is considerable phonon-mode softening with decreasing temperature.

To test whether the differences in ω_g (at $T = T_c$) can account for the different T_c values, we obtained λ -values from McMillan's expression for T_c and related ω_g to λ by the usual expression $\lambda = N \langle I^2 \rangle / M \omega_g^2$, where $\langle I^2 \rangle$ is the average electron-phonon coupling parameter and M is the gram atomic weight. (See Table I). McMillan showed that $N(E_F) \langle I^2 \rangle$ was approximately constant, based on an analysis of some bcc transition metals. This is clearly not the case for these A-15 compounds, as can be seen in Table I, and the differences in T_c must be caused by differences in $N \langle I^2 \rangle$. In Fig. 2(a), we plot λ versus $N(E_F)$ for all compounds. Note that for the V_3X compounds, λ is approximately linearly related to $N(E_F)$ when $N(E_F)$ is greater than 2 states/eV-atom, whereas it is not clear whether this is true for the Nb_3X compounds. In Fig. 2(b), the normalized slope of ω_g , $\frac{A}{3R} \equiv -\frac{1}{\omega_g} \frac{\partial \omega_g}{\partial T}$, is plotted versus $N(E_F)$, where R is the gas constant. Within experimental error, there is a linear relationship between A and $N(E_F)$ for all compounds.

The relationship between λ , $N(E_F)$, and $\frac{1}{\omega_g} \frac{\partial \omega_g}{\partial T}$ and the lack of correlation between $M\omega_g^2$ and λ can be explained if we postulate that a relatively small number of modes are strongly coupled to the electronic system. Then, these modes can dominate the magnitude of λ , while the softening will affect $M\omega_g^2$ much less dramatically. Therefore, $N\langle I^2 \rangle \equiv \lambda M\omega_g^2$ is not expected to be constant. For the Nb_3X compounds, since $N(E_F)$ is lower than for the V_3X compounds, the contribution to λ from particular modes will not dominate λ . Therefore, we would expect that $N\langle I^2 \rangle$, as obtained from $\lambda M\omega_g^2$, would be more constant for these materials. From Table I it is clear that for the Nb_3X compounds, the $N\langle I^2 \rangle$ values are quite constant, except for Nb_3Sb , which, because of its low $N(E_F)$, can hardly be classified a transition-metal superconductor. (5)

The correlation of $\frac{1}{\omega_g} \frac{\partial \omega_g}{\partial T}$ with $N(E_F)$ is another manifestation of strong selective electronic screening. The high $N(E_F)$ can cause the frequencies of certain phonon modes to decrease significantly. These frequencies can be temperature dependent for two reasons. Firstly, electronic screening could cause the effective second-order term in the phonon potential energy to be reduced relative to the third and fourth-order terms. This reduction enhances the anharmonicity as measured by A . Secondly, electronic screening, by near-Fermi-energy electronic states, will be quite temperature dependent because of sharp structure in $N(E)$ near E_F . If the same percentage of the modes shows this anomalous screening, for all of the compounds, then the correlation between A and $N(E_F)$ is explained.

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FIGURE CAPTIONS

- Fig. 1. The temperature dependence of the effective Debye temperature associated with the geometric mean phonon-mode frequencies for the indicated compounds.
- Fig. 2. The electron-phonon mass enhancement [Fig. 2(a)] and the phonon frequency shift parameter [Fig. 2(b)] as functions of $N(E_F)$.

Table I. Calorimetrically determined properties of A-15 compounds.

Compounds	T_c (°K)	$N(E_F)^*$	λ	$M\omega_B^2 \left(\frac{eV}{A^2} \right)$	$N\langle I^2 \rangle \left(\frac{eV}{A^2} \right)$
Nb_3Al	18.5	1.6	1.07	7.82	8.4
Nb_3Sn	17.9	2.4	1.17	7.18	8.4
$Nb_3Sn_{0.7}Sb_{0.3}$	14.9	1.5	1.0	8.17	8.2
Nb_3Sb	0.2	0.4	0.3	10.85	3.3
V_3Si	16.5	3.8	0.86	8.61	7.4
V_3Ga	14.3	4.8	0.91	6.43	5.9
$V_3Ga_{0.5}Sn_{0.5}$	5.6	2.7	0.62	7.30	4.5
V_3Sn	3.8	2.0	0.56	8.14	4.6

* in units of states/eV-atom

Fig. 1. The temperature dependence of the effective Debye temperature associated with the geometric mean phonon-mode frequencies for the indicated compounds.

Fig. 2. The electron-phonon mass enhancement [Fig. 2(a)] and the phonon frequency shift parameter [Fig. 2(b)] as functions of $N(E_F)$.