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

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The electronic density of states at the Fermi level,  $N(E_F)$ , and the geometric mean phonon frequencies,  $\omega_g$ , were determined from heat-capacity data for a number of A-15 superconductors. Although  $\omega_g$  is an appropriate average phonon parameter for evaluating McMillan's expression for  $\lambda$ , we found that the  $T_c$  values cannot be reliably estimated using  $\omega_g$ . There are, however, strong correlations between  $\lambda$ ,  $N(E_F)$  and the temperature dependence of  $\omega_g$ ,  $d \ln \omega_g/dT$ . 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.<sup>1</sup> In earlier papers,<sup>2,3</sup> 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,  $\lambda$ , 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  $N(E_F)$ .

The sample of  $Nb_3Sn_{0.7}Sb_{0.3}$  was prepared<sup>3</sup> 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 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,

$$\omega_g = \left[ \frac{3N}{s} \prod \omega_g \right]^{1/3N}$$

and its temperature dependence.<sup>3</sup> In Figure 1 we display the  $\omega_g$  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  $\theta$ , indicating that there is considerable phonon-mode softening with decreasing temperature.

To test whether the differences in  $\omega_g$  (at  $T = T_c$ ) can account for the different  $T_c$  values, we obtained  $\lambda$ -values from McMillan's expression for  $T_c$  and related  $\omega_g$  to  $\lambda$  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 Figure 2(a), we plot  $\lambda$  vs.  $N(E_F)$  for all compounds. Note that for the  $V_3X$  compounds,  $\lambda$  is approximately linearly related to  $N(E_F)$  when  $N(E_F)$

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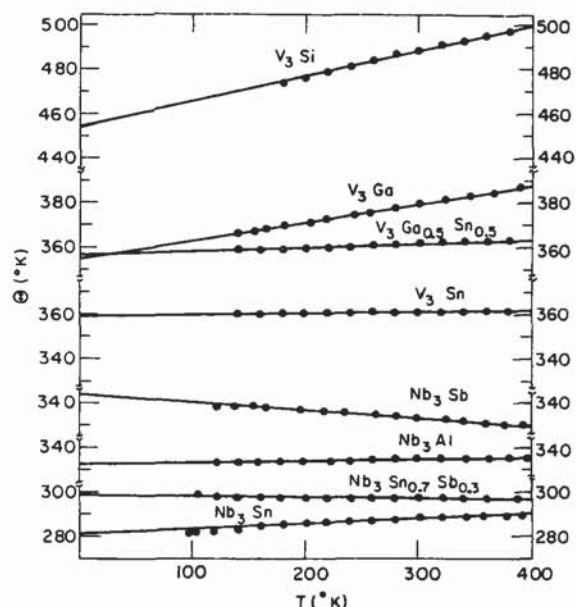


FIGURE 1 The temperature dependence of the effective Debye temperature associated with the geometric mean phonon-mode frequencies for the indicated compounds.

is greater than 2 states/eV-atom, whereas it is not clear whether this is true for the  $Nb_3X$  compounds. In Figure 2(b), the normalized slope of  $\omega_g$ ,  $(A/3R) \equiv -(1/\omega_g)(\partial\omega_g/\partial T)$ , is plotted vs.  $N(E_F)$ , where  $R$  is gas constant. Within experimental error, there is a linear relationship between  $A$  and  $N(E_F)$  for all compounds.

The relationship between  $\lambda$ ,  $(NE_F)$ , and  $(1/\omega_g)(\partial\omega_g/\partial T)$  and the lack of correlation between  $M\omega_g^2$  and  $\lambda$  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  $\lambda$ , while the softening will affect

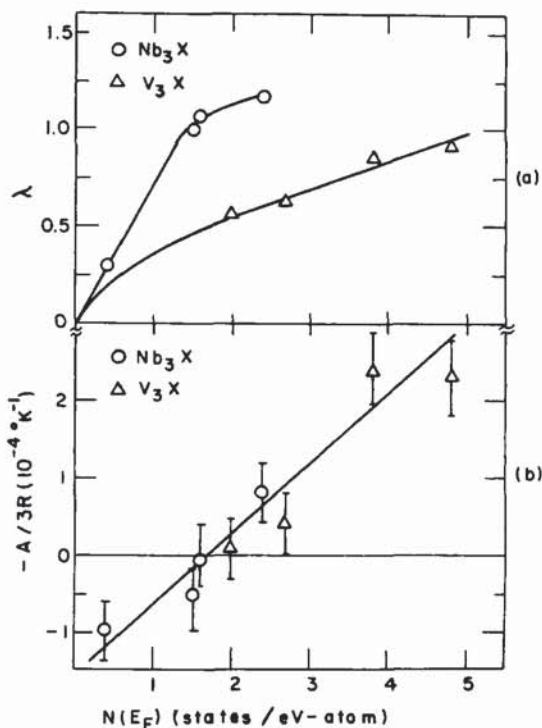


FIGURE 2 The electron-phonon mass enhancement [Figure 2(a)] and the phonon frequency shift parameter [Figure 2(b)] as functions of  $N(E_F)$ .

$M\omega_g^2$  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  $\lambda$  from particular modes will not dominate  $\lambda$ . 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,

TABLE I  
Calorimetrically determined properties of A-15 compounds

Compounds	$T_c$ (°K)	$N(E_F)^a$	$\lambda$	$M_g^2 \frac{eV}{\text{\AA}^2}$	$N\langle I^2 \rangle \frac{eV}{\text{\AA}^2}$
$Nb_3Al$	18.5	1.6	1.07	7.82	8.4
$Nb_3Sn$	17.9	2.4	1.17	7.18	8.4
$Nb_2Sn_{0.7}Sb_{0.3}$	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	2.7	0.56	8.14	4.6

<sup>a</sup> In units of states/eV-atom.



because of its low  $N(E_F)$ , can hardly be classified a transition-metal superconductor.<sup>5</sup>

The correlation of  $(1/\omega_g)(\partial\omega_g/\partial T)$  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. First, 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  $A$ . Second, 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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