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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, $\omega_p$, were determined from heat-capacity data for a number of A-15 superconductors. Although $\omega_p$ 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 $\omega_p$. There are, however, strong correlations between $\lambda$, $N(E_F)$ and the temperature dependence of $\omega_p$, $d\ln \omega_p/dT$. The high-$T_c$, high-$N(E_F)$ materials $V_3$Si and $V_3$Ga 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. In earlier papers, 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$_3$Sn$_{0.7}$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$_3$Sn$_{0.7}$Sb$_{0.3}$ was prepared in the same manner as Nb$_3$Sn. Its $T_c$ value was 14.9 K and metallurgical 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,

$$\omega_p = \left[ \frac{3N}{\sum \omega_p^3} \right]^{1/3}$$

and its temperature dependence. In Figure 1 we display the $\omega_p$ values for all samples, as effective Debye temperatures $\theta \equiv e^{1/3}h\omega_p/k_B$. 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 $\omega_p$ (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 $\omega_p$ to $\lambda$ by the usual expression $\lambda = N\langle t^2 \rangle/M\omega_p^2$, where $\langle t^2 \rangle$ is the average electron-phonon coupling parameter and $M$ is the gram atomic weight. 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 $N\langle t^2 \rangle$. In Figure 2(a), we plot $\lambda$ vs. $N(E_F)$ for all compounds. Note that for the $V_3$X compounds, $\lambda$ is approximately linearly related to $N(E_F)$ when $N(E_F)$

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is greater than 2 states/eV-atom, whereas it is not clear whether this is true for the Nb$_3$X 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 \(Mg^2\) 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

![Graph showing temperature dependence of effective Debye temperature associated with geometric mean phonon-mode frequencies for indicated compounds.](image)

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

![Graph showing electron-phonon mass enhancement and phonon frequency shift parameter as functions of \(N(E_F)\).](image)

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

\(Mg^2\) much less dramatically. Therefore, \(N(I^2) \equiv \lambda Mg^2\) is not expected to be constant. For the Nb$_3$X compounds, since \(N(E_F)\) is lower than for the V$_3$X compounds, the contribution to \(\lambda\) from particular modes will not dominate \(\lambda\). Therefore, we would expect that \(N(I^2)\), as obtained from \(\lambda Mg^2\), would be more constant for these materials. From Table I it is clear that for the Nb$_3$X compounds, the \(N(I^2)\) values are quite constant, except for Nb$_3$Sb, which,

<table>
<thead>
<tr>
<th>Compounds</th>
<th>(T_c)(K)</th>
<th>(N(E_F)) (^a)</th>
<th>(\lambda)</th>
<th>(Mg^2) (\frac{\text{eV}}{\AA^2})</th>
<th>(N(I^2)) (\frac{\text{eV}}{\AA^2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nb$_3$Al</td>
<td>18.5</td>
<td>1.6</td>
<td>1.07</td>
<td>7.82</td>
<td>8.4</td>
</tr>
<tr>
<td>Nb$_3$Sn</td>
<td>17.9</td>
<td>2.4</td>
<td>1.17</td>
<td>7.18</td>
<td>8.4</td>
</tr>
<tr>
<td>Nb$<em>3$Sn$</em>{0.7}$Sb$_{0.3}$</td>
<td>14.9</td>
<td>1.5</td>
<td>1.0</td>
<td>8.17</td>
<td>8.2</td>
</tr>
<tr>
<td>Nb$_3$Sb</td>
<td>0.2</td>
<td>0.4</td>
<td>0.3</td>
<td>10.85</td>
<td>3.3</td>
</tr>
<tr>
<td>V$_3$Si</td>
<td>16.5</td>
<td>3.8</td>
<td>0.86</td>
<td>8.61</td>
<td>7.4</td>
</tr>
<tr>
<td>V$_3$Ga</td>
<td>14.3</td>
<td>4.8</td>
<td>0.91</td>
<td>6.43</td>
<td>5.9</td>
</tr>
<tr>
<td>V$<em>3$Ga$</em>{0.5}$Sn$_{0.5}$</td>
<td>5.6</td>
<td>2.7</td>
<td>0.62</td>
<td>7.30</td>
<td>4.5</td>
</tr>
<tr>
<td>V$_3$Sn</td>
<td>3.8</td>
<td>2.7</td>
<td>0.56</td>
<td>8.14</td>
<td>4.6</td>
</tr>
</tbody>
</table>

\(^a\) In units of states/eV-atom.
because of its low $N(E_F)$, can hardly be classified a transition-metal superconductor.\textsuperscript{5}

The correlation of $(1/\omega_p)(d\omega_p/dT)$ 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.

REFERENCES