MODE SOFTENING AND HIGH SUPERCONDUCTING 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, \( \omega_g \), 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 \( \omega_g \) and \( \frac{d\ln\omega_g}{dT} \). 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. 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 \( \lambda \), 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 \( N(E_F) \).

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The sample of Nb$_3$Sn$_{0.7}$Sb$_{0.3}$ was prepared$^3$ in the same manner as Nb$_3$Sn. 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, $\omega_g = \left( \frac{3N}{T} \omega_g \right) \frac{1}{3N}$, and its temperature dependence.$^3$ In Fig. 1 we display the $\omega_g$ values, for all samples, as effective Debye temperatures $\theta \equiv e^{1/3} / k_B$. 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 Fig. 2(a), we plot $\lambda$ versus $N(E_F)$ for all compounds. Note that for the V$_3$X compounds, $\lambda$ is approximately linearly related to $N(E_F)$ when $N(E_F)$ is greater than 2 states/eV-atom, whereas it is not clear whether this is true for the Nb$_3$X compounds. In Fig. 2(b), the normalized slope of $\omega_g$, $\frac{A}{3R} \equiv -\frac{1}{\omega_g} \frac{\partial \omega_g}{\partial T}$, 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 $\lambda$, $N(E_F)$, and $\frac{1}{\omega_g} \frac{\partial \omega}{\partial T}$ and the lack of correlation between $M_\omega^2$ 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 $M_\omega^2$ much less dramatically. Therefore, $N\langle T^2 \rangle \equiv \lambda M_\omega^2$ 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 $N\langle T^2 \rangle$, as obtained from $\lambda M_\omega^2$, would be more constant for these materials. From Table I it is clear that for the Nb$_3$X compounds, the $N\langle T^2 \rangle$ values are quite constant, except for Nb$_3$Sb, which, because of its low $N(E_F)$, can hardly be classified a transition-metal superconductor.

The correlation of $\frac{1}{\omega_g} \frac{\partial \omega}{\partial T}$ 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.

REFERENCES


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.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>$T_c$ (°K)</th>
<th>$N(E_F)^*$</th>
<th>$\lambda$</th>
<th>$N_\omega^2 \left( \frac{\text{eV}}{\text{Å}^2} \right)$</th>
<th>$N&lt;\gamma^2&gt; \left( \frac{\text{eV}}{\text{Å}^2} \right)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nb$_3$Al</td>
<td>18.5</td>
<td>1.6</td>
<td>1.07</td>
<td>7.62</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>3.17</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>2.0</td>
<td>0.56</td>
<td>8.14</td>
<td>4.6</td>
</tr>
</tbody>
</table>

* 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 $N(E_F)$. 