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THE RELATION BETWEEN NORMAL STATE PROPERTIES AND $T_c$
FOR SOME Zr$_2$X COMPOUNDS

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We find that a certain feature of the normal state resistivity correlates with $T_c$ in a closely related group of superconductors.

THE INTERMETALLIC compounds, Zr$_2$Rh ($T_c = 11.5^\circ$K), Zr$_2$Ir ($T_c = 7^\circ$K), Zr$_2$Co ($T_c = 5^\circ$K) and Zr$_2$Ni ($T_c = 1.5^\circ$K), all crystallize in the tetragonal C16 structure. The first three compounds form an isoelectronic series, which is especially interesting because Zr$_2$Rh has one of the highest $T_c$'s of all the non-cubic inter-transition metal compounds. The investigation reported here was motivated by a desire to understand how a certain feature in the electrical resistivity correlates with $T_c$.

The resistance data are shown in Fig. 1. All the curves have a similar shape and we are interested particularly in the region of pronounced negative curvature. The negative curvature can be characterized by the inflection point which we shown in Table 1. For the isoelectronic compounds we note that as this region of negative curvature moves to high temperatures the $T_c$ decreases.

A least-squares fit has been made to the resistance data using the model of Cohen et al. in this model, developed to explain the resistivity and other normal state properties of A-15 compounds, one assumes an almost empty or full d-band overlying a low density of states s-band. The ratio of s-density of states to the total density of states at the Fermi level is called $\alpha$; $T_0$ is the effective Fermi temperature of

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Table 1. Inflection point of resistivity curves and best fit parameters to resistivity model of reference 2

<table>
<thead>
<tr>
<th>Compound</th>
<th>$T_{\text{inf}}$</th>
<th>$\theta_R$</th>
<th>$T_0$</th>
<th>$\alpha$</th>
<th>r.m.s Deviation of fit (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zr$_2$Rh</td>
<td>39</td>
<td>160</td>
<td>120</td>
<td>0.11</td>
<td>1.3</td>
</tr>
<tr>
<td>Zr$_2$Ir</td>
<td>50</td>
<td>205</td>
<td>90</td>
<td>0.11</td>
<td>1.2</td>
</tr>
<tr>
<td>Zr$_2$Co</td>
<td>69</td>
<td>305</td>
<td>95</td>
<td>0.11</td>
<td>1.4</td>
</tr>
<tr>
<td>Zr$_2$Ni</td>
<td>65</td>
<td>272</td>
<td>95</td>
<td>0.3</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Fig. 1. Temperature dependence of the electrical resistivity of Zr$_2$X compounds. All curves were scaled to make the room temperature values equal.

The $d$-band (electrons or holes for the almost empty or full cases, respectively); and $\theta_R$ denotes the Debye temperature. One simply assumes that the total density of states is dominated by the $d$-band and thus $s$ to $d$-state scattering dominates the electrical resistivity. These parameters, as determined by the least-squares fit, are given in Table 1. We notice that the fits, which are very good, show little variation in $T_0$ and $\alpha$ for the sequence Zr$_2$Co—Zr$_2$Rh—Zr$_2$Ir, but that $\theta_R$ varies significantly. The fit for Zr$_2$Ni, with $\alpha = 0.3$, indicates that the model is not as appropriate for this compound, since the $d$-density of states is not dominant.

Low temperature heat capacity measurements have been made on the same specimens by an a.c. calorimetry technique. The electronic heat capacity coefficient $\gamma$ and Debye temperature $\theta_D$ of Zr$_2$Ir and Zr$_2$Co have been determined by equating the entropy of normal and superconducting states below their respective $T_c$'s. The $T_c$ for Zr$_2$Ni was below the present temperature range of measurement and Zr$_2$Rh exhibited two distinct transitions (Fig. 2), most of the bulk $T_c$ being at the higher temperature 11.3 K. In these two cases $\gamma$ and $\theta_D$ values were deduced by simple extrapolation procedure of the $C/T$ vs $T^2$ plots from above $T_c$. The data are given in Table 2. It is interesting to note that $\theta_D$ varied only slightly from compound to compound whereas $\gamma$ changes considerably; but neither parameter seems to correlate with $T_c$. Similar anticorrelation has been pointed out in susceptibility measurements on these compounds earlier. The origin of the second heat capacity anomaly in Zr$_2$Rh is not clear at present.

What interests us here is that $\theta_R$ does not seem to depend sensitively on $\theta_D$. This suggests, therefore, that there are groups of special phonons especially connected with both the resistance and the superconductivity. It is, of course, possible that the Cohen model, which provides an accurate and convenient parametrization, may not be particularly appropriate.
Table 2. Experimental low temperature specific heat parameters and magnetic susceptibility from reference 1

<table>
<thead>
<tr>
<th>Compound</th>
<th>$T_c$ (°K)</th>
<th>$\theta_D$ (°K)</th>
<th>$\gamma$ (mJ/mol °K)$^2$</th>
<th>$\chi_{R,T} \times 10^4$ (emu/mol)$^1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zr$_2$Rh</td>
<td>11.3</td>
<td>188</td>
<td>46</td>
<td>3.7</td>
</tr>
<tr>
<td>Zr$_2$Ir</td>
<td>7.5</td>
<td>200</td>
<td>17</td>
<td>3.0</td>
</tr>
<tr>
<td>Zr$_2$Co</td>
<td>5.5</td>
<td>180</td>
<td>28</td>
<td>5.2</td>
</tr>
<tr>
<td>Zr$_2$Ni</td>
<td>1.6</td>
<td>221</td>
<td>18</td>
<td>3.2</td>
</tr>
</tbody>
</table>

Both experimental and theoretical work for $d$-band superconductors, however, indicate that peculiarities in phonon spectra are particularly important for $T_c$, a result consistent with our analysis.

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REFERENCES