Account of Non-Diagonal $d$-$d$-Electron Couplings in Co-Ni Liquid Alloy

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Abstract

The partial Wills-Harrison effective pair potentials in liquid equiatomic Co-Ni alloy are considered. It is shown that the account of the non-diagonal $d$-$d$ couplings between electrons leads to similar changes in characteristics of the pair-potential first minimum as for Fe-Co and Fe-Ni equiatomic alloys.

Keywords: Liquid transition-metal alloy, Wills-Harrison model, $d$-state coupling

The Wills-Harrison (WH) [1] partial effective pair potentials, $\varphi_{\text{WH}}(r)$, between atoms Co and Ni in equiatomic Co-Ni alloy at $T=1873$K are calculated at different values of the suggested in [2] probability $p$ that not only diagonal $d$-$d$ couplings are possible at condition that all $d$-$d$ couplings (diagonal and non-diagonal) are equiprobable in this case. This approach was extended to binary alloys in [3] and applied to equiatomic Fe-Co and Fe-Ni liquid alloys in [4] and [5], respectively. All input data are listed in Table 1. The partial coordination numbers are taken equal to 12.

Table 1. Input data for calculation

<table>
<thead>
<tr>
<th></th>
<th>$r_{di}$ (a.u.)</th>
<th>$z_{di}$</th>
<th>$z_{zi}$</th>
<th>$R_{Ci}$ (a.u.)</th>
<th>$a_i$ (a.u.)</th>
<th>$\Omega$ (a.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co</td>
<td>1.437</td>
<td>1.4</td>
<td>7.6</td>
<td>1.64</td>
<td>0.393</td>
<td>85.85</td>
</tr>
<tr>
<td>Ni</td>
<td>1.342</td>
<td>1.4</td>
<td>8.6</td>
<td>1.03</td>
<td>0.207</td>
<td>85.24</td>
</tr>
</tbody>
</table>

Results obtained (Fig. 1) are similar to that obtained earlier for Fe-Co [4] and Fe-Ni [5] equiatomic alloys.
Figure 1. \( \varphi_{\text{WHT}}(r) \) between atoms Co and Ni in liquid equiatomic Co-Ni alloy (\( p = 0 \) – solid line; \( p = 0.5 \) – dotted line; \( p = 1 \) – dashed-dotted line).

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References


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