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

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Abstract

The partial Wills-Harrison effective pair potentials in liquid equiatomic Fe-Ni alloy are considered. It is shown that the account of the non-diagonal $d$-$d$ couplings between electrons leads to the same changes in characteristics of the pair-potential first minimum as in the case of the pure transition metals.

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

The Wills-Harrison (WH) [1] partial effective pair potentials, $\phi_{\text{WH}}(r)$, between atoms Fe and Ni in equiatomic Fe-Ni alloy at $T=1873K$ 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].

We use the local Bretonnet-Silbert (BS) model pseudopotential [4] for description the $s$-electron contributions to partial pair interactions. As follows from [3, 5], $\phi_{\text{WH}}(r) = \phi_{\text{BS}}(r)$ at $p = 1$. Values of the WH and BS parameters are taken from [1, 6]. The experimental values of the mean atomic volumes, $\Omega$, of pure Fe and Ni are taken from [7]. For alloy $\Omega$ calculated as an average. All input data are listed in Table 1. The partial coordination numbers are taken equal to 12.

Results obtained are similar (Fig. 1) that obtained earlier for Fe-Co equiatomic alloy [5]: changing $p$ from 0 up to 0.5 slightly influences the depth and position of the first minimum of $\phi_{\text{WH}}(r)$, whereas these characteristics become
strong different at \( p = 1 \).

**Table 1.** Input data for calculation

<table>
<thead>
<tr>
<th></th>
<th>( r_{di} ) (a.u.)</th>
<th>( z_{di} )</th>
<th>( z_i )</th>
<th>( R_{ci} ) (a.u.)</th>
<th>( a_i ) (a.u.)</th>
<th>( \Omega )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>1.512</td>
<td>1.4</td>
<td>6.6</td>
<td>1.54</td>
<td>0.363</td>
<td>89.29</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>

**Figure 1.** \( \varphi_{WH}(r) \) between atoms Fe and Ni in liquid equiatomic Fe-Ni alloy (\( p = 0 \) – solid line; \( p = 0.5 \) – dotted line; \( p = 1 \) – dashed-dotted line).

**References**


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