The Softness of the Wills-Harrison

Effective Pair Potential in Liquid Ni

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Abstract

It is found that an account of the non-diagonal couplings between \(d\) electrons sited on different atoms in a transition metal leads to increase of the softness of repulsive part in the Wills-Harrison effective pair potential of liquid Ni.

Keywords: Transition metal, Wills-Harrison model, \(d\)-state coupling

In [1] the Wills-Harrison (WH) model [2] was corrected by means the introduction the probability \(p\) that all 25 \(d-d\) couplings between two different atoms are equiprobable and probability \((1-p)\) that only 5 equiprobable diagonal couplings are possible. Then, the softness of the repulsive part of the WH effective pair potential, \(\varphi_{\text{WH}}(r)\), were considered at different \(p\) for liquid Fe [3] and liquid Co [4].

Here, we study how the magnitude \(p\) influences the softness of the repulsive part of \(\varphi_{\text{WH}}(r)\) for liquid Ni at absolute temperature \(T=1873\)K.

The repulsive part of the pair potential \(\varphi(r)\) is considered in the reduced form that is \(\beta[\varphi(r) - \varphi(d)]\), where \(\beta = 1/(k_B T)\), \(k_B\) - Boltzmann constant, \(d\) - position of the first minimum of \(\varphi(r)\). The input parameters are taken from works [2] and [5] and listed in Table 1. The experimental value of the mean atomic volume equal to 85.24 a.u. is taken from the work [6]. The coordination number is taken equal to 12.
The dependence $\beta[\varphi_{\text{WH}}(r) - \varphi_{\text{WH}}(d)]$ on $p$ is shown in Fig. 1. It is found that for liquid Ni an account of the non-diagonal couplings between $d$ electrons leads to increase the softness of the repulsive part of the WH effective pair potential almost in the same degree as for liquid Co [4] and in less degree than for liquid Fe [3].

Table 1. Input data for the calculation

<table>
<thead>
<tr>
<th>$R_C$ (a.u.)</th>
<th>$\alpha$ (a.u.)</th>
<th>$z_s$</th>
<th>$z_d$</th>
<th>$r_d$ (a.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.03</td>
<td>0.207</td>
<td>1.4</td>
<td>8.6</td>
<td>1.342</td>
</tr>
</tbody>
</table>

Figure 1. $\beta[\varphi_{\text{WH}}(r) - \varphi_{\text{WH}}(d)]$ in liquid Ni ($p = 0$ – solid line; $p = 0.5$ – dotted line; $p = 1$ – dashed-dotted line).
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References


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