The First-Minimum Position of the Wills-Harrison Effective Pair Potential in Liquid Ni

Vladimir Filippov\textsuperscript{1,2}

\textsuperscript{1)} Ural Federal University, Mira st. 19, 620002 Ekaterinburg, Russia
\textsuperscript{2)} Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences, Amundsen st. 101, 620016 Ekaterinburg, Russia

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Abstract

It is found that the position of the first minimum of the Wills-Harrison effective pair potential in the liquid Ni very slightly depends on the probability that not only the diagonal $d$-$d$ couplings between two atoms are possible. This result denotes that the account of the non-diagonal couplings is not such important for the liquid Ni as for both the liquid Fe and liquid Co.

Keywords: Transition metal, Wills-Harrison pair potential, $d$-state coupling

In [1] the Wills-Harrison (WH) model [2] was corrected by means the introduction the probability $p$ that 25 equiprobable $d$-$d$ couplings between two atoms are possible and the probability $(1 - p)$ that only 5 equiprobable diagonal couplings are possible.

Recently, we studied the influence of the magnitude $p$ on the position, $r_{\text{min}}$, of the first minimum of the WH effective pair potential, $\varphi_{\text{WH}}(r)$, in the liquid Fe and Co [3, 4]. Here, we fulfil the analogous study for the liquid Ni. Input data (values of parameters and the experimental mean atomic volume, $\Omega$) are listed in Table 1.

One can see from Fig. 1. that the calculated magnitude of the first-minimum position of $\varphi_{\text{WH}}(r)$ is practically constant up to $p = 0.9$. It denotes that the account of the non-diagonal couplings is almost not important in the case of the liquid Ni.

Table 1. Input data for the calculation

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<td>1.342</td>
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<td>8.6</td>
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<td>0.207</td>
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Figure 1. $r_{\text{min}}$ of $\varphi_{\text{wH}}(r)$ in liquid Ni at different $p$ ($T=1873$K).

References


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