The Softness of the Wills-Harrison Effective Pair Potential in Liquid Fe

Nikolay Dubinin\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
ned67@mail.ru

Copyright © 2013 Nikolay Dubinin. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

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 the increase of the softness of repulsive part in the Wills-Harrison effective pair potential for liquid Fe.

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, in [1] the WH effective pair potentials, \(\varphi_{\text{WH}}(r)\), were considered at different \(p\) for liquid Fe, Co and Ni.

Here, we consider how the magnitude \(p\) influences the softness of the repulsive part of \(\varphi_{\text{WH}}(r)\) for liquid Fe at absolute temperature \(T=1863\text{K}\).

The repulsive part of the pair potential \(\varphi(r)\) is considered here 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 of the model are taken from works [2] and [3]. The experimental value of the mean atomic volume equal to 89.29 a.u. is taken from the work [4].

The dependence \(\beta[\varphi_{\text{WH}}(r) - \varphi_{\text{WH}}(d)]\) on \(p\) is shown in Fig. 1. One can see that the increase of the probability \(p\) leads to the increase of the softness of repulsive part in the WH effective pair potential for liquid Fe.
Figure 1. $\beta(\varphi_{WH}(r) - \varphi_{WH}(d))$ in liquid Fe ($p = 0$ – solid line; $p = 0.5$ – dotted line; $p = 1$ – dashed-dotted line).

References


Received: April 30, 2013