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

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Abstract

It is found that the position of the first minimum of the Wills-Harrison effective pair potential in liquid Fe begins to shift significantly to the right-hand side when the \( d-d \)-non-diagonal coupling begins to predominate in the metal under consideration.

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 all 25 \( d-d \) couplings between two different atoms are equiprobable and probability \( (1 - p) \) that only 5 equiprobable diagonal couplings are possible.

Here, we consider how the magnitude \( p \) influences the position, \( r_{\text{min}} \), and the magnitude of the first minimum of the WH effective pair potential, \( \phi_{\text{WH}}(r) \), in liquid Fe.

We use the local Bretonnet-Silbert (BS) model pseudopotential [3] for description the \( s \)-electron contribution to \( \phi_{\text{WH}}(r) \). Input data (WH and BS parameters and the experimental mean atomic volume, \( \Omega \)) are listed in Table 1.

Figure 2 shows that magnitude of the first minimum quite monotonously increases with increasing \( p \) for pair potential under consideration. At the same time, as follows from Figure 1, the first-minimum position begins to increase harshly from \( p = 0.6 \) approximately. Since the portion of the non-diagonal \( d-d \) couplings in a metal is equal to \( 0.8p \), it denotes that significant shift of the
\( \varphi_{W_H}(r) \) first minimum to the right is occurred when the non-diagonal coupling begins to predominate in liquid Fe.

**Figure 1.** \( r_{\min} \) of \( \varphi_{W_H}(r) \) in liquid Fe at different \( p \) (\( T=1863 \)K).

**Figure 2.** \( \varphi_{W_H}(r_{\min}) \) in liquid Fe at different \( p \) (\( T=1863 \)K).
Table 1. Input data for calculation

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References


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