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

Nikolay Dubinin$^{1,2}$

$^1$Ural Federal University, Mira st. 19, 620002 Ekaterinburg, Russia
$^2$Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences, Amundsen st. 101, 620016 Ekaterinburg, Russia
ned67@mail.ru

Abstract

The partial Wills-Harrison effective pair potentials in liquid equiatomic Fe-Co 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 Fe-Co alloy, transition metal, Wills-Harrison model, $d$-state coupling

The Wills-Harrison [1] partial effective pair potentials, $\phi_{WH}(r)$, between atoms Fe and Co in equiatomic Fe-Co alloy at $T=1863$K 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.

Following [3] we use the local Bretonnet-Silbert (BS) model pseudopotential [4] extended to binary alloys in [5] for description the $s$-electron contribution, $\phi_{sij}(r)$, to $\phi_{WH}(r)$.

As follows from the previous paper, $\phi_{WH}(r) = \phi_{sij}(r)$ at $p=1$. It denotes here that $\phi_{WH}(r) = \phi_{BS}(r)$ at $p=1$.

It is clear from Fig.1 that changing $p$ from 0 up to 0.5 slightly influences the depth and position of the first minimum of $\phi_{WH}(r)$. At the same time, these characteristics become strong different at $p=1$. Such a tendency is the same as it
was observed in the case of pure transition metals [2].

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

References


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