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# Non-Diagonal Couplings between *d* Electrons: Generalization to Binary Alloys of Transition Metals

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**Abstract**

Suggested earlier correction to the Wills-Harrison model is extended to a binary mixture of transition metals. It is found that the full account of the non-diagonal couplings between *d* electrons leads to the vanishing the *d*-electron contributions to the partial pair interactions.

**Keywords:** Binary alloy, transition metal, Wills-Harrison model, *d*-state coupling

The Wills-Harrison partial effective pair potentials are expressed as follows [1, 2]:

$$\varphi_{ij\mathrm{WH}}(r) = \varphi_{sij}(r) + \varphi_{dij}(r)\,, \qquad (1)$$

where $\varphi_{sij}(r)$ and $\varphi_{dij}(r)$ are the contributions due to *s*- and *d*-electron states, respectively. The last term in the right-hand side of (1) consists of two parts:

$$\varphi_{dij}(r) = \varphi_{bij}(r) + \varphi_{cij}(r)\,, \qquad (2)$$

where $\varphi_{bij}(r)$ is the partial *d*-band-width term, $\varphi_{cij}(r)$ - partial *d*-band-center-shift term:

$$\varphi_{bij}(r) = -\bar{z}_d \left(\frac{10-\bar{z}_d}{10}\right)\left(\frac{12}{\nu_{ij}}\right)^{1/2} \frac{(r_{di} r_{dj})^{3/2}}{r^5} K_b \;\;, \qquad (3)$$

$$\varphi_{cij}(r) = \bar{z}_d \frac{(r_{di} r_{dj})^3}{r^8} K_c \quad , \tag{4}$$

where $\bar{z}_d = c_1 z_{d1} + c_2 z_{d2}$ is the average alloy valence, $\nu_{ij}$ - partial coordination number, $r_{di}$ - *d*-state radius of the free atom of the *i*-th kind, $z_{di}$ - effective number of valence *d* electrons per ion in the pure metal of the *i*-th kind, $c_i$ - concentration of the *i*-th-kind component, $K_b$ and $K_c$ - combinatoric coefficients which in a general case depend on the diagonal and non-diagonal couplings between *d* electrons [3].

In [4, 5] was shown that $K_b$ and $K_c$ are equal to zero in the case of the full account of the non-diagonal *d-d* couplings.

Thus, it is obviously that $\varphi_{ij\mathrm{WH}}(r) = \varphi_{sij}(r)$ at $K_b = K_c = 0$, and, therefore, that $\varphi_{ij\mathrm{WH}}(r)$ is determined in this case by the form of the pseudopotential model used for description of the contribution $\varphi_{sij}(r)$**.**

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