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Probabilities of Diagonal and Non-Diagonal Couplings between *d* Electrons in Transition Metal

I. The *d*-Band Energy

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Abstract

It is shown that the full account of the non-diagonal couplings between *d* electrons sited on different atoms in a transition metal implemented within the framework of the Wills-Harrison model leads to vanishing the *d*-band contribution to the internal energy.

Keywords: Transition metal, Wills-Harrison model, *d*-state coupling

In the Wills-Harrison (WH) model [1] for the transition-metal internal energy, the *d*-band energy, E_b, is represented as follows (hereafter, per atom):

$$E_b = -\frac{1}{2} z_d \left(\frac{10 - z_d}{10} \right) W \quad , \tag{1}$$

where z_d is the effective *d*-electron valence, W - *d*-band width:

$$W = \left(\frac{12}{N} \sum_{m=1}^{N} \sum_{\substack{l=1 \\ l \neq m}}^{N} V_d^2(\vec{r}_{ml}) \right)^{1/2} \quad , \tag{2}$$

where N is the number of atoms, $V_b(r)$ - effective potential of the *d*-*d* interaction (hereafter, in atomic units):

$$V_b(r) = \frac{r_d^3}{r^5} K_b \quad . \tag{3}$$

Here, r_d is the *d*-state radius, K_b - combinatoric coefficient, which in the WH approximation depends on diagonal only couplings between *d* electrons sited on different atoms:

$$K_b^{\mathrm{WH}} = \left(\sum_{m=-2}^{2} \frac{y_m^2}{5} \right)^{\frac{1}{2}} , \tag{4}$$

where *m* is the magnet quantum number,

$$y_m = y_{|m|} = -\frac{(-1)^{|m|} 180}{\pi (2+|m|)!(2-|m|)!} . \tag{5}$$

From (4), (5)

$$K_b^{\mathrm{WH}} = 28.06/\pi . \tag{6}$$

In [2] was introduced the probability *p* that all 25 *d*-*d* couplings between two different atoms in a metal are equiprobable. Then, the probability of the WH limit case that only 5 equiprobable diagonal couplings are possible is $(1-p)$. From this assumption, the probability of a non-diagonal coupling is $0.8p$, probability of a diagonal coupling is $(1-0.8p)$ and

$$K_b = \left[\frac{1}{5} \left(\left(1 - \frac{4p}{5} \right) y_0^2 + \left(2 - \frac{6p}{5} \right) (y_2^2 + y_1^2) + \frac{4p}{5} y_0 (y_1 + y_2) + \frac{8p}{5} y_1 y_2 \right) \right]^{\frac{1}{2}} . \tag{7}$$

Now, allow us to apply (5) to (7). As a result,

$$K_b = K_b^{\mathrm{WH}} \sqrt{1-p} . \tag{8}$$

This surprising result denotes that at full account of the non-diagonal couplings between *d* electrons sited on different atoms $(p=1)$, the *d*-band energy in a transition metal is being become equal to zero.

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