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EFFECTIVE INTERIONIC INTERACTION IN TRANSITION METALS

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Taking into consideration the third order corrections of perturbation theory for electron-ionic pseudopotential, the calculation of the effective interionic interaction potentials in $3d$–transition metals was carried out. For more full consideration of the model potential nonlocality in determination of its form-factors the procedure of the angular coordinates averaging was used. The analysis of the calculated potentials shows that the consideration of the third order corrections for model potential results in the increasing of the first minimum depth and decreasing of the equilibrium distance between ions.

One of the most important characteristics of metals that determines their equilibrium properties are effective potentials of interionic interaction. Usually the interionic interaction is represented in the form of a sum of pair-wise Coulomb potential and indirect interaction of ions through conducting electrons. An investigation of the interionic interaction for simple metals was performed in many works in which there were considered both the pair-wise interaction [1-3] (the second order of perturbation theory for pseudopotential) and the terms of perturbation theory of higher orders [4-6]. Concerning transition metals that problem is studied insufficiently.

Previously we carried out calculation of the effective potential of interionic interaction for $3d$–transition metals in the second order perturbation theory for pseudopotential [7]. For determination of the formfactors of the nonlocal model potential (MP) the semilocal approximation of Fermi sphere was used [2]. However, it is known that for quantitative calculations of the properties of metals the following aspects are actual. First, the more precise consideration of the electron-ion MP nonlocality. That can be achieved by using the procedure of formfactor averaging over angular coordinates [8] instead of the Fermi sphere approximation. Second, it is important to consider the perturbation theory terms of higher orders for MP that corresponds to many-particles correlations in the electronic subsystem.

Taking into account the above mentioned suggestions we express the effective two-particle potential of interionic interaction as a power series in MP

$$V_{eff.}(r) = V_{i-i}(r) + \sum_n V_2^{(n)}(r), \qquad (1)$$

where the first term describes the direct interaction of ions (the most frequently used here is the pure Coulomb potential z^2/r), and $V_2^{(n)}(r)$ is the contribution of the n-order of perturbation theory in the pair-wise indirect

interionic interaction. In particular, in the second order the correction to the effective potential of interionic interaction for transition metals is presented in the form [7]

$$V_2^{(2)}(r) = \frac{2}{N}\sum_{\vec{q}\neq 0} V_2^{(n)}(r)F(q)e^{-i\vec{q}\vec{r}} - \tag{2}$$

$$\frac{1}{N}\sum_{\vec{k}}\sum_{m}\beta_r^m\cos(\vec{k}\vec{r})\left\{\langle\vec{k}|w_{add}^{(0)}|\vec{k}\rangle + \langle\vec{k}|w_{hybr}^{(0)}|\vec{k}\rangle\right\},$$

here β_r^m is the overlap integral of d-orbitals, m is quantum magnetic number. The characteristic function of band structure $F(q)$, matrix elements of additional $\langle\vec{k}|w_{add}^{(0)}|\vec{k}\rangle$ and hybridization $\langle\vec{k}|w_{hybr}^{(0)}|\vec{k}\rangle$ for transition metals are determined in [8]. Let us remark that the second term in (2) describes the indirect interaction between external d-shell neighbouring ions as a result of their overlapping.

If we move in (2) from summation to integration then for the component $V_2^{(2)}(r)$ we obtain

$$V_2^{(2)}(r) = \frac{\Omega_0}{2\pi^2}\int_0^\infty F(q)q^2\frac{\sin qr}{qr}\mathrm{d}q + \tag{3}$$

$$\int_0^{k_F}\sum_m \beta_r^m\frac{\sin(kr)}{r}\left[\left\{\langle\vec{k}|w_{add}^{(0)}|\vec{k}\rangle + \langle\vec{k}|w_{hybr}^{(0)}|\vec{k}\rangle\right\}\mathrm{d}k\right].$$

Similarly we can write the correction of the third order to $V_{eff.}(r)$

$$V_2^{(3)}(r) = \frac{3\Omega_0}{4\pi^4}\int_0^\infty F^{(3)}(q)q^2\frac{\sin qr}{qr}\mathrm{d}q \tag{4}$$

where

$$F^{(3)}(q) = \int_0^\infty \mathrm{d}q_1 q_1^2\int_{-1}^1 \mathrm{d}\cos(\vec{q}\vec{q}_1)\Phi(q,q_1)\Lambda^{(3)}(q,q_1,|\vec{q}+\vec{q}_1|),$$

$$\Phi(q,\,q_1) = \int_0^{k_F}\langle\vec{k}|\vec{w}|\vec{k}+\vec{q}'\rangle\langle\vec{k}+\vec{q}'|w|\vec{k}+\vec{q}\rangle\langle\vec{k}+\vec{q}|w|\vec{k}\rangle\ln\left|\frac{q-2k}{q+2k}\right|\ln\left|\frac{q_1-2k}{q_1+2k}\right|\mathrm{d}k,$$

here $\Lambda^{(3)}(\vec{q}_1,\vec{q}_2,\vec{q}_3)$ is electron threepole for which we used the expression obtained in [9]; form–factors of the screened MP $\langle\vec{k}+\vec{q}|w|\vec{k}\rangle$ are determined in [8].

Figure 1 show the results of calculation of the pair–wise effective potential of interionic interaction for 3d-transition metals ($1-Fe$, $2-Co$, $3-Ni$). Figures 2–4 show, for comparison, the potential $V_{eff.}(r)$ calculated with the consideration of second (1) and third (2) order perturbation theory corrections. As it is seen from the figures, the consideration of the third order term essentially influence on the form of the effective potential of interionic

interaction. For all three metals the consideration of $V_2^{(3)}(r)$ results in the increasing of the first minimum depth and decreasing of the equilibrium distance between ions. Obviously, $V_2^{(3)}(r)$ will have the essential role for $4d-$ and $5d-$ transition metals since MP is more strong for them. That is why while summing up the perturbation series in MP we can not restrict ourselves by lower orders of perturbation theory.

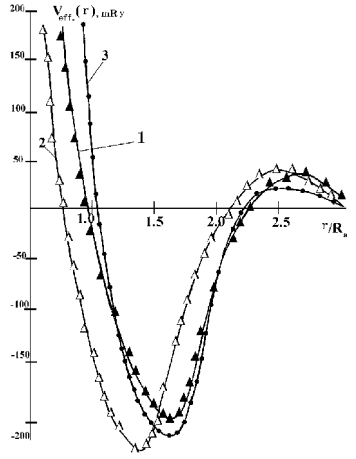

Figure1. Effective interionic interaction in transition metals ($1-Fe$, $2-Co$, $3-Ni$).

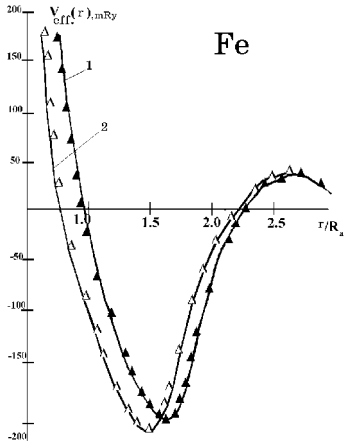

Figure 2. Effective interionic interaction for Fe (1 - second order correction, 2 - third order correction).

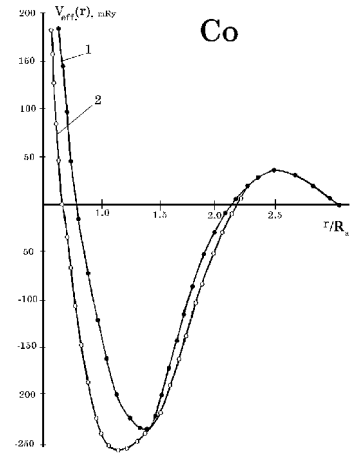

Figure3. Effective interionic interaction for Co (1 - second order correction, 2 - third order correction).

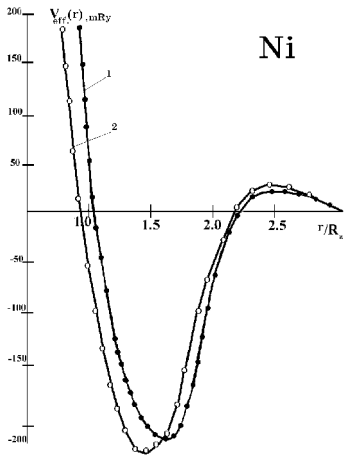

Figure 4. Effective interionic interaction for Ni (1 - second order correction, 2 - third order correction).

References

[1] Yukhnovskii I.R., Gurskii Z.A. Quantum-statistical theory of disordered systems. Kiev, Naukova Dumka, 1991 (in Russian).

[2] Harrison W.A. Pseudopotentials in the theory of metals. N.Y., W.A Benjamin, 1966.
[3] Dutchak Y.I., Yakibchuk P.M., Baryljak G.I. Effective potentials of interionic interaction and interionic force constant of simple metals in nonlocal pseudopotential theory. // Fiz. Met. Met., 1977, vol. 44, No 5, p. 938-944.
[4] Vavrukh M.V., Krokhmalskii T.Ye. Many particles electron correlations and effective ionic interactions in metals. Kiev, 1980. Preprint Acad. Sci. Ukr. SSR. Inst. Theor. Phys. ITP-80-38R (in Russian).
[5] Kovalenko N.P., Kuzmina L.M. // Ukr. Phys. Zhurn., 1980, vol. 25, No 5, p. 809-812 (in Russian).
[6] Bykov O.Y., Shvets V.T. Effective pair-wise interionic interaction in alkali metals. // Ukr. Fiz. Zhurn., 1991, vol. 36, No 3, p. 469-471 (in Ukrainian).
[7] Zhovtanetckii M.I., Gurskii Z.A., Dutchak Y.I., Yakibchuk P.M. Method of model pseudopotential in transition metals theory II. Equilibrium atomic properties. // Metalophysics, 1983, vol. 5, No 3, p. 16-22 (in Russian)
[8] Fourman V.V., Yakibchuk P.M. Pseudopotential within the phase functions method. Structure of model pseudopotential of transition and rare-earth metals. // Jour. Phys. Studies, 1, No 1, 1996, p. 134-137 (in Ukrainian).
[9] Browman E.G., Kagan Y.M. Phonons in nontransition metals. // Usp. Fiz. Nauk, 1974, vol. 112, No 3, p. 369-426 (in Russian).

ЕФЕКТИВНА МІЖІОННА ВЗАЄМОДІЯ В ПЕРЕХІДНИХ МЕТАЛАХ

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Враховуючи поправки третього порядку теорії збурень за електрон-іонним псевдопотенціалом обчислені ефективні потенціали міжіонної взаємодії $3d$ перехідних металів. Для більш повного врахування нелокальності модельного потенціалу при розрахунку його формфакторів використано процедуру усереднення за кутовими координатами. Аналіз обчислених потенціалів показує, що врахування поправок третього порядку теорієї збурень за псевдопотенціалом приводить до зростання глибини першого мінімуму та зменшення рівноважного атомного радіусу.