

The calculation method of interaction between metal atoms under influence of the radiation

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Abstract. A method of calculation of interatomic interaction potentials in the presence of ionized states has been developed. They have been obtained for the atoms with different ionization degree on example of aluminum. The Heine-Abarenkov-Animalu model potential form factors was employed. The form factor parameters of ionized atoms was determined on the base of the quantum defect method using the atomic-spectroscopy data. The potential of interatomic interaction for different charged states with different degree of ionization were determined.

1. Introduction

It is known that intensive radiation generates ionized atoms within the track of a fast charged particle as well as near the solid surface. The potentials of interactions between these atoms and surrounding particles change considerably. The knowledge of corresponding potentials of interatomic interaction is necessary for studying the behavior of partially or entirely ionized matter.

Therefore, aluminum was taken as an example studying the interatomic potentials in metal containing ionized states. Calculations were based on the method of pseudopotentials using Heine-Abarenkov-Animalu model potentials with parameters which were determined from spectroscopic terms of free ions following the method of quantum defect.

2. Quantum defect method

The energetic levels E_{nl} of a single electron in the area of positive ions with the electron shells being similar to the spherically symmetric electron shells of inert gases, in particular Na^+ , Mg^{2+} , Al^{3+} , Si^{4+} , P^{5+} , S^{6+} , Cl^{7+} , are known to satisfy the relation [1]:

$$E_{nl} = -Z^2 / (n - \delta_{nl})^2 + \Delta_{nl}, \quad (1)$$

where Z is the ion-core charge, δ_{nl} and Δ_{nl} denotes quantum defects characterizing the $|Z\epsilon|$ -charge induced deviation of an atomic potential in such a configuration of inert gas shells from a Coulomb ones. Figure1 shows a linear dependence of the value of spectroscopic terms of the atomic series considered on a square of the ion-core charge.

It turns out that there also are similar dependences for additionally ionized cores (figure2). Here the following series Na^{2+} , Mg^{3+} , Al^{4+} , Si^{5+} , P^{6+} , S^{7+} , Cl^{8+} will be realized.

Using this empirical law we have determined the mode potential parameters of the additionally ionized cores with respect to the energies $\epsilon_{nl} = E_{nl} - \Delta_{nl}$, as it was done for transition metals in [1].

Radial wave equation with a model potential describing the electron motion is written as



$$\left[-\frac{1}{2} \frac{d}{dr^2} + \frac{l(l+1)}{2r^2} + v_l \right] \chi(r) = \frac{1}{2} \varepsilon \chi(r), \quad (2)$$

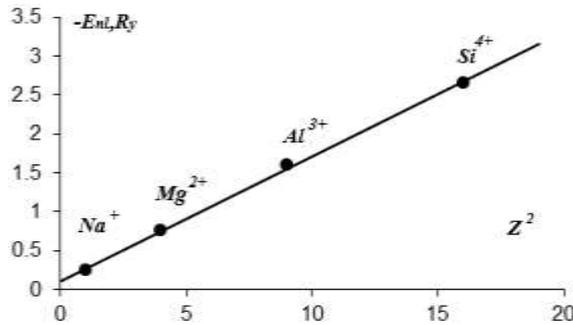


Figure 1. Spectroscopic term values E_{3p} as function of the chemical valence.

where $\chi(r)$ is the radial wave function and l is the angular momentum. With such a representation ε is given in rydbergs and vl in atomic units.

The model potential of the electron ion-core interaction has a form

- $V_l = -A_l(\varepsilon)$ for $r \leq R_m$
 - $V_l = -Z/r$ for $r > R_m$,
- (3)

here R_m is a model radius closed to the ion-core radius which provides for joining the inside and outside solutions of the wave equation.

After making a substitution of

$\rho = Zr$ and $\bar{\rho} = r\sqrt{2A_l - |\varepsilon|}$ into expression (2) it will be written as

- $\left[-\frac{1}{2} \frac{\partial^2}{\partial \bar{\rho}^2} + \frac{l(l+1)}{\bar{\rho}^2} + 1 \right] \chi = 0$ for $r \leq R_m$,

(4)

- $\left[-\frac{\partial^2}{\partial \rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2}{\rho} \right] \chi + \varepsilon' \chi = 0$ for $r > R_m$,

(5)

where $\varepsilon' = \varepsilon / z^2$.

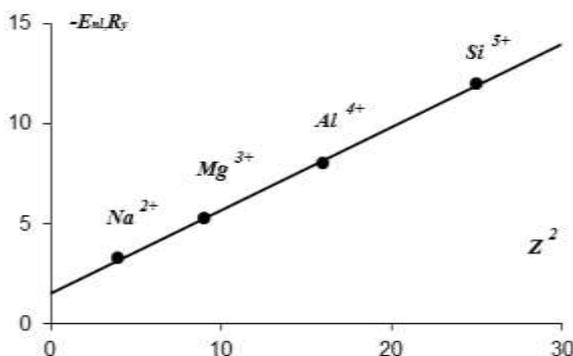


Figure 2. Spectroscopic term values E_{2p} as function of the ion-core charge.

Solution of equation (4) are the spherical Bessel functions and equation (5) is the Coulomb wave one which was solved according to the procedure described in [2].

By setting the logarithmic derivatives from solutions of equation (4) equal to those in equation (5) at $r=R_m$ one obtains an expression for determining the parameters A_l :

$$\frac{xj_{l-1}(x)}{j_l} - l = \frac{{}^0D^l(ZR_m) + \gamma(N, l) {}^1D^l(ZR_m)}{{}^0U^l(ZR_m) + \gamma(N, l) {}^1U^l(ZR_m)}, \quad (6)$$

where $x = R_m \sqrt{2A_l - |\varepsilon_{nl}|}$, $j_l(x)$ denotes the spherical Bessel functions, ${}^0U^l, {}^1U^l$ are regular and irregular parts of the Coulomb wave function respectively, $N = n - \delta_{nl}$ expresses an effective quantum number, $D^l = \rho(dU^l/d\rho)$,

$$\gamma(N, l) = \frac{\Gamma(N-l)N^{2l+1} \lg \pi(N-l-1)}{\Gamma(N+l+1)}, \quad (7)$$

where Γ is a gamma-function [3].

The values of spectroscopic terms $\varepsilon = \varepsilon_{nl}$ were calculated from tables [4]. All values as function of energy $\varepsilon = \varepsilon_{nl}$ at fixed l .

A_l may be calculated precisely only for the energies which are consistent with the lines observed in the electron emission spectra of a core potential. There in the function $A_l(\varepsilon_{nl})$ is chosen so that the model potential will give eigen values consistent with ε_{nl} . Therefore, first, we estimate A_l for as many energy values as experimental lines exist, after wards linear interpolation and extrapolation to the Fermi energies is made.

Here the question arises, what value is a real energy of the conduction electrons. In contrast to isolated ion (equation 2) Schrodinger equation for the conduction electron in metal has a form

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + (V + \Sigma)_{ion} + (V + \Sigma)_{rest} \right] \Psi = \varepsilon \Psi, \quad (8)$$

where $(V + \Sigma)_{ion}$ is the potential of this ion and $(V + \Psi)_{rest}$ is the potential caused by other ions and conduction electrons.

Expression (8) may be written as

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + (V + \Sigma)_{ion} + (V + \Sigma)_{rest} \right] \Psi = \varepsilon \Psi, \quad (9)$$

Equation (9) is similar to equation (2) for an isolated ion with electron energy

$$E_F = eF - (V + S)_{rest}, \quad (10)$$

where

$$\varepsilon_F = -|I_i| - |I_c| + \mu_x + \mu_c + \frac{2}{5} \left(\frac{\hbar^2 k_F^2}{2m^*} \right) - E_x - E_c + \frac{0,6Ze^2}{R_a}, \quad (11)$$

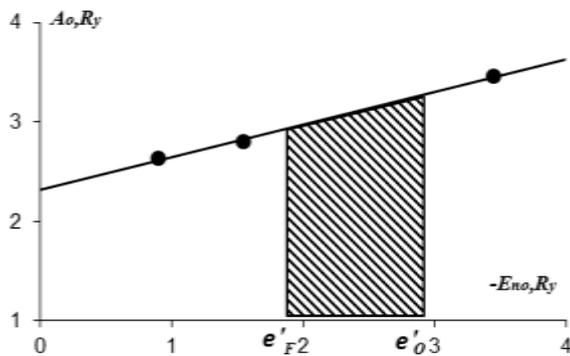


Figure 3. Energetic dependence of the parameters A_l for $l=0$ and $z=3$. Dashed region corresponds to the energies of the occupied conduction electron states.

I_i is the ionization energy of outside electron in a free atom, I_c is the electron cohesive energy, k_F is the Fermi radius, m^* is the effective electron mass, E_x is the exchange energy, E_c is the correlation energy of a free electronic gas per an electron, μ_x and μ_c are respectively, exchange and correlation potentials, and R_a is an atomic radius.

The potential $(V+\Sigma)_{rest}$ induced by the rest residual ions and conduction electrons may be written as [5]:

$$\Sigma_{rest} = \mu_x + \mu_c, \quad (12)$$

$$V_{rest} = \frac{Ze^2}{R_a} \left[3 - \frac{3}{4} \left(\frac{R_m}{R_a} \right)^2 \right]. \quad (13)$$

Figure 3 shows an energetic dependence of parameter A_0 for an electron in the field of a three-charged ion. The energy levels ε_n in Al^{3+} -ion, the Fermi energy ε'_F and that of the bottom of conduction band $\varepsilon'_0 = \varepsilon'_F - \hbar^2 k_F^2 / 2m$ are shown in terms of the ion energy [6].

The ion-core radius R_c is an important value for calculating interatomic potential. Its procedure estimation is following.

According to [7,8] the wave electron function outside the core has a form

$$\Psi = -\frac{2}{n} \sqrt{\frac{(n-l-1)!}{[(n+l)!]^3}} \exp(-\rho^*/2) \rho^* L_{n+l}^{2l+1} \rho^*, \quad (14)$$

where L is the added Lagerr polynomial, $\rho^* = 2Zr/na_0$, a_0 is a Bohr radius.

Then the wave function will be

$$\Psi_{ni} = -\frac{2}{n} \sqrt{\frac{(n-2)!}{[(n+l)!]^3}} \exp(-\rho^*/2) \rho^* \sum_{k=0}^{n-2} \frac{(-1)^{k+l} [(n+1)!]^2 \rho^{*k}}{(n-2-k)! (k+3)! k!}. \quad (15)$$

Inside the core it is

$$\Psi_{ni} = A r j_l(\tilde{\rho}). \quad (16)$$

Here A is a normalization factor, $\tilde{\rho} = yr$, $y = \sqrt{2A_i - |\varepsilon_{ni}|}$.

Expression (15) included the numbers up to $(n-2)$ order, ρ^{*n-2} and ρ^{*n-3} are the major ones. If keep only these two members, one may think that n adopts any fractional values. At $r = R_c$ the logarithmic derivatives from expressions (15) and (16) may be set equal :

$$\left[-\frac{1}{2} + \frac{1}{\rho^*} + \frac{n-2}{\rho^* - (n+1)(n-2)} \right] \frac{2Z}{na_0} = \left(\frac{\tilde{\rho}}{1 - \tilde{\rho} \operatorname{ctg} \tilde{\rho}} - \frac{2}{\tilde{\rho}} \right) y. \quad (17)$$

By solving graphically equation (17) we hand found the ion-core radius of additionally ionized atom.

As it should be guess R_c value seemed to be not very sensitive to the degree of ionization.

As for an effective mass and charge of electron conduction, we counted $m^*/m = 1$, as it was done in [1], while the parameter inserted in expression to define the effective charge $e^* = e(1 + \alpha)$, which results from orthogonality correction, was calculated from a formulae

$$\alpha = (R_c / R_a)^3 / 2. \quad (18)$$

Table 1. Parameters of model potential

| Z | A ₀ | A ₁ | A ₂ | R _m | R _c | α |
|---|----------------|----------------|----------------|----------------|----------------|-------|
| 3 | 1,38 | 1,64 | 1,92 | 2 | 1,08 | 0,024 |
| 4 | 1,35 | 1,756 | 1,46 | 2 | 1,05 | 0,022 |

Table 1 illustrates the parameters of a model potential for usually charged aluminum, taken from reference [1], and those obtained by us for additionally ionized core for comparison. All the measured values are in atomic units.

3. Results and discussion

Figure 4 represents the potential of interatomic interaction for different charged states in aluminum which were estimated using the above data. Calculation was done for a situation when the ionized atom concentration is small and consequently the conduction electron concentration does not differ from an usual one.

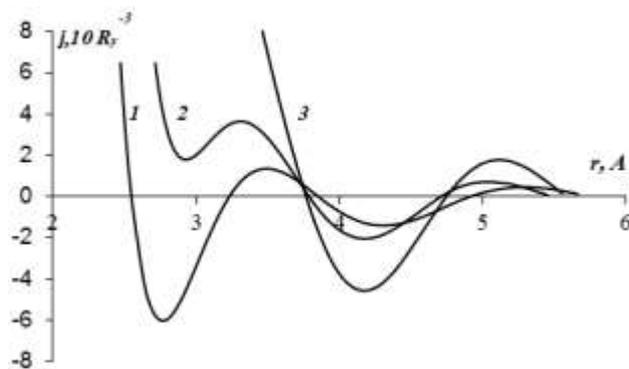


Figure 4. Interatomic potential: 1 – Al^{3+} and Al^{3+} ; 2 – Al^{4+} and Al^{3+} ; 3 – Al^{4+} and Al^{4+} .

This figure shows that ionization leads to the strong decrease in the depth of the first minimum of the potential function corresponding to the distance area between the nearest neighbors for three- or four-charged ions. Moreover, for the pair of particles with four charges the first minimum disappears absolutely. Atoms fall to the repulsion branch of interaction potential. As a result, the crystal lattice changes to the state of nonequilibrium.

On the basis of the similar potentials of interatomic interactions, applying the method of molecular dynamics, we modeled the dispersion of aluminum surface within the track of charged particles. It was shown that ionization greatly affects the dispersion process of surfaces of metals. However, the molecular-dynamic dispersion modeling in many cases is qualitative. For the more thorough investigation of destruction processes of surfaces we should solve the equation of thermal elasticity, where in its turn we should know the equation of substance condition.

References

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