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INTERATOMIC POTENTIALS DEDUCED FROM THE Kr-Al, Cs-Al, Xe-Ni, Xe-Cu AND Xe-Mo RANGE DATA

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Abstract: A semiempirical method to deduce an inverse power-low interatomic potential from the ion range data is proposed. Experimental data on 20—70 keV ion ranges in solids and usual matching procedure are used to derive the parameters of the power-low potentials for the Kr-Al, Cs-Al, Xe-Ni, Xe-Cu and Xe-Mo pairs. Comparing the obtained potentials and Bohr and Thomas-Fermi potentials, one can conclude that this method gives a representation of the interatomic potentials in this energetic region, as good as the Bohr or Thomas-Fermi potentials.

1. Introduction

Screening potentials could be represented by means of power-low function

$$f(r/a) = \frac{k_s}{s}(a/r)^{s-1}, \tag{1}$$

where

$$a = \frac{0.8853}{(Z_1^{2/3} + Z_2^{2/3})^{1/2}}, \text{ and}$$

where the parameters k_s and s are appropriately chosen constants. These constant parameters could be determined by analysing the particular experimental data or

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matching a dimensionless potential i. e., Bohr, Born-Mayer or Thomas-Fermi. Matching, naturally, is performed in the region where the theoretical potentials represent well the real ones. Due to simple calculations, this potential appears to be very convenient for the description of the collisional penetration of energetic ions in the amorphous materials.

Matching procedure consists in determining the parameters k_s and s from the conditions required that both equations have the same value for the function and its derivative in the point where the model potential represents well the real potential. For the Bohr and Born-Mayer potentials this point is the distance of maximum approach, r_0 while for the Thomas-Fermi potential this is a point in the asymptotic region. Equating the Bohr potential with the exponential screening function $f(t/a) = \exp(-r/a)$ and the chosen power-low potential function

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \exp(-r/a) = \frac{Z_1 Z_2 e^2}{r} \frac{k_s}{s} (a/r)^{s-1},$$

and setting the matching conditions of these two potential forms in the point r_0, we have for s and k_s

$$s = \frac{r_0}{a} + 1 \tag{2}$$

$$k_s = \left(\frac{r_0}{a} + 1\right) \left(\frac{r_0}{ea}\right)^{r_0/a}. \tag{3}$$

Generally, the constant k_s has to be close to unity. It appears from the expression (3) which is valid at low interatomic distances (r_0/a approaches zero), i. e. high particle energies, where the Bohr potential represents a good approximation of real potential. When in (3) $r_0/a \to 0$, $k_s = 1$. But since k_s is the energy independent this argument widens to the whole energetic region i. e., for finite interatomic distances.

2. *Evaluation of power-low potential parameters*

In this Section a semiempirical method for evaluation of k_s and s parameters will be presented. The basis of this semiempirical method for determining k_s and s in power-low potential of the form

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \frac{k_s}{s} \left(\frac{a}{r}\right)^{s-1}, \tag{4}$$

represent expressions for the moments of different order which for potential (4) has been introduced by Sanders[1]. Namely, the moment $p_1^1(\varepsilon)$ is in a simple way connected with experimentally measured most probable ranges. Potential (4) itself, for $2 \leq s < 4$ represents well the real interatomic potential when the collision energy is such that the inelastic collisions can be neglected.

In that case the moments $p_1^n(\varepsilon)$ are defined as

$$p_1^n = 4\pi \int_0^\infty p_1(r, \varepsilon)\, r^{n+2}\, \mathrm{d}r, \tag{5}$$

where $p_1(r, \varepsilon)$ is the coefficient in the Legendre polynom evolution of probability density $p(\vec{r}, \vec{n}, \varepsilon)$ that the projectile starting from the coordinate beginning, with energy ε in the direction $\vec{n}$, will come at rest (looses all the kinetic energy) in elementary volume $\mathrm{d}r^3$, around the point $\vec{r}$. Here ε means reduced energy, given by the expression

$$\varepsilon = E \frac{a M_2}{Z_1 Z_2 e^2 (M_1 + M_2)} = C_2 E. \tag{6}$$

Movements $p_1^n(\varepsilon)$ as functions of ε are given as

$$p_1^n(\varepsilon) = \lambda_1^n \varepsilon^{2n/s}, \tag{7}$$

where $\lambda = \text{const}$ dependent on potential parameters and masses of colliding particles. The moment $p_1^1(\varepsilon)$, which is connected with the reduced most probable range $\bar{\varrho}_p$ by the relation

$$p_1^1(\varepsilon) = \bar{\varrho}_p \tag{8}$$

is of special interest for us.

The relation between the reduced range $\bar{\varrho}_p$ and the experimental range $\bar{R}_p$ is given by the relation

$$\bar{\varrho}_p = \bar{R}_p \left(1 + \frac{\mu s^2}{4(2s-1)}\right) N\pi a^2 \frac{4M_1 M_2}{(M_1 + M_2)^2} = C_1 \bar{R}_p, \tag{9}$$

where $\mu = \dfrac{M_1}{M_2} \leq 1$, and N the atom concentration.

Thus, for $\bar{\varrho}_p$ we have

$$\bar{\varrho}_p = \lambda_s \varepsilon^{2/s}, \tag{10}$$

where λ_s is a constant of the form

$$\lambda_s = \left[\frac{1}{\gamma}\left(\frac{\gamma_s k_s}{2}\right)^{2/s}\left\{\frac{M_1 + M_2}{2M_1}(1-\gamma)^{2/s+1/2} + \frac{M_1 - M_2}{2M_1}(1-\gamma)^{2/s-1/2} - \right.\right.$$

$$- 1 + \gamma^{1/s}\left(\frac{M_1 + M_2}{2M_1}(2/s + 1/2)\, B_\gamma(1 - 1/s;\ \ 2/s + 1/2) + \right.$$

$$\left.\left.\left. + \frac{M_1 - M_2}{2M_1}(2/s - 1/2)\, B_\gamma(1 - 1/s;\ \ 2/s - 1/2) - 1\right)\right]\right\}^{-1}.$$

Here, γ is the maximum collisional energy transfer, B_γ is the incomplete beta-function, and $\gamma_s = \frac{1}{2} B\left(\frac{1}{2};\ \frac{s+1}{2}\right)$.

The equations (10), (6) and (9) give for assumed potential (4) and for ion energy E, $\bar{R}_p$ as

$$\bar{R}_p(E) = K(k_s, s)\, E^{2/s}, \tag{11}$$

where

$$K(k_s, s) = \frac{\lambda_s C_2^{2/s}}{C_1} \tag{12}$$

is an energy independent constant. Obviously from (11) it is possible to determine s using two experimental points $\bar{R}_1(E_1)$ and $\bar{R}_2(E_2)$ as

$$s = 2\frac{\log\frac{E_1}{E_2}}{\log\frac{\bar{R}_1}{\bar{R}_2}}. \tag{13}$$

Table

The interatomic potential parameters s and k_s.

Atomic pair	Reference	s	$r_0(a_0)$	k_s
Kr-Al	Davies[4]	2.4624	0.3194	0.9946
Cs-Al	Davies[5]	2.4572	0.2885	0.9905
Xe-Ni	Jokić[6]	2.9724	0.3602	0.1579
Xe-Cu	„	2.5727	0.2858	1.0878
Xe-Mo	„	2.3193	0.2274	0.8936

Having determined s, the constant $K(k_s, s)$ can also be determined from each experimental point $\bar{R}_e(E_e)$ as

$$K_e = \frac{\bar{R}_e}{E_e^{2/s}}. \tag{14}$$

By equalizing this „ experimental„ value for K with the expression (12) the unknown parameter k_s is obtained. The parameter s of the potential (4) could be determined from the equation

$$K(k_s, s) = K_e. \tag{15}$$

Naturally, this procedure has to be used for numerous experimental points and then averaged.

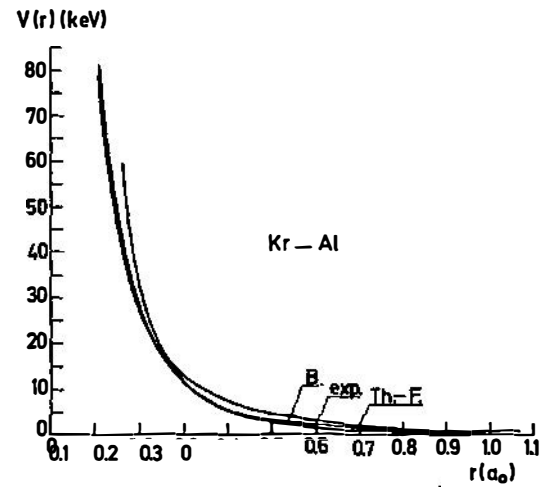

Fig. 1. Interatomic potential for Kr-Al as a function of distance of colliding atoms.

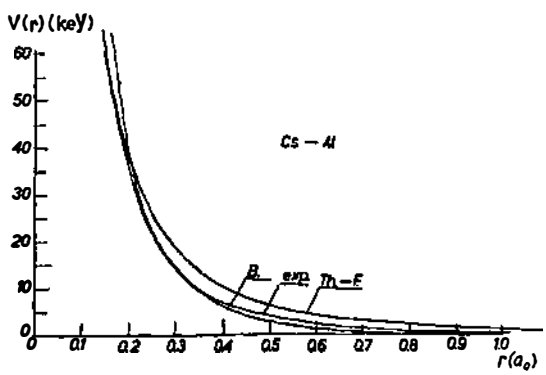

Fig. 2. Interatomic potential for Cs-Al as a function of distance of colliding atoms.

Similar semiempirical method for the determination of parameters k_s and s of the potential (4) was recently proposed by G. Carter and W. Grant[2]. This method comprises the differential cross section analysis and the use of experimental data on ranges. Although, in principle correct, this method does not give correct k_s values. Thus, for Kr-Al and Cs-Al one could calculate parameter k_s equal to 0.5530 and 0.0218 respectively, in no case near to unity.

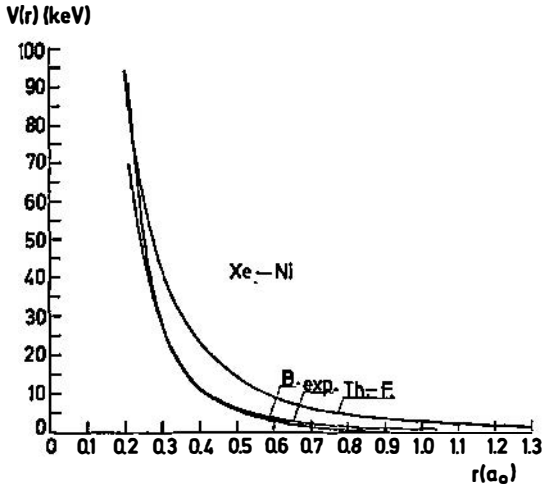

Fig. 3. Interatomic potentials between colliding atoms Xe and Ni.

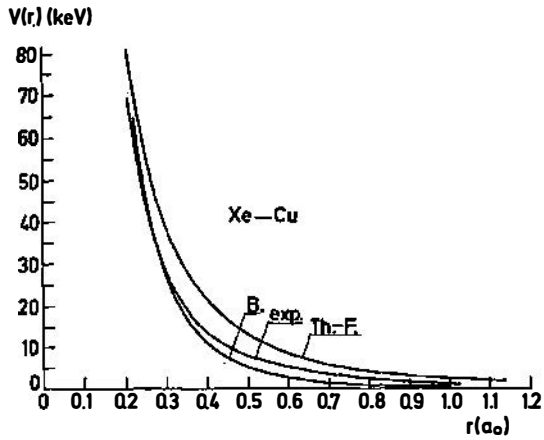

Fig. 4. Interatomic potentials for Xe-Cu.

The other semiempirical method proposed earlier by D. Corkhill and G. Carter[3] consists in matching R_p and differential cross section. However, the matching of R_p with differential cross section based on hard core conception cannot give the potential of the type $V(r) = C/r^4$.

3. *Results and comparison with the Bohr and Thomas-Fermi potentials*

The parameters of interatomic potentials obtained by the outlined procedure are presented in Table. Experimental range data are used from references[4-6].

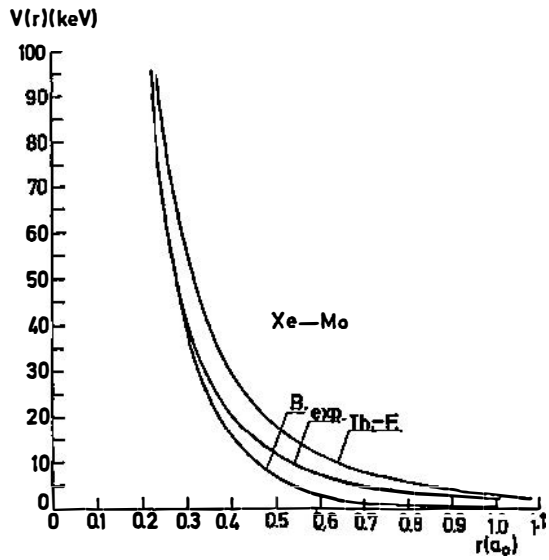

Fig. 5. Interatomic potentials for Xe-Mo.

All the s values are between 2.5 and 3, whilst parameter k_s is near to unity.

The potentials deduced by the procedure outlined and the Bohr and Thomas--Fermi potentials for the corresponding ion-atom pairs are shown in Figs.1 to 5.

4. *Discussion*

Figs. 1 to 5 show that interatomic potentials in the ion energy region investigated lie between the Bohr and Thomas-Fermi potentials when $r > r_0$. Thence the power-low potential (4) with parameters k_s and s given in the Table represent a real interatomic potential as good as the Bohr or Thomas-Fermi potentials.

Lindhard proposed a model similar to (4) with fixed parameters $k_s = 1$ and $s = 2$. This model is very simple because for $\overline{\varrho} = f(\varepsilon)$ gives straight line (see (10). But our analysis shows that for colliding atomic pairs investigated k_s values are near, but not equal to unity whilst the parameter s varies between 2.3 and 2.9.

A particular model for the interatomic potential (Bohr's, Bern-Meyer's, Thomas--Fermi's, Lindhard's and power-low (4)) represents well the real interatomic forces only at certain finite interatomic distances. Hence, it can be used in the penetration studies with more or less exactness depending on the energy of bombarding particles. The applicability of these models is usually limited to narrow distance regions. Therefore, to achieve a better knowledge of the real potentials between colliding atomic particles, further theoretical and experimental investigations are required.

References

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INTERATOMSKI POTENCIJALI IZVEDENI IZ DOMETA Kr u Al, Cs u Al, Xe u Ni, Xe u Cu i Xe u Mo

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Sadržaj

U radu su dati interatomski potencijali za određeni broj atomskih parova. Dobijeni potencijali izvedeni su iz eksperimentalnih podataka o prodiranju energetskih jona u čvrsto telo.

U stepenoj funkciji (1) koja predstavlja interatomski potencijal, parametri k_s i s određeni su analizom eksperimentalnih podataka o dubini prodiranja, tj. iz odnosa (9) i procedurom povezivanja sa nekim od bezdimenzionalnih potencijala, na pr. Bohr-ovim, Born-Meyer-ovim ili Thomas-Fermi-evim. Na pr., povezivanje sa Bohr-ovim potencijalom (4) uz uslov tangiranja u tački najvećeg približenja $r_0 = (s - 1)\, a$, za k_s je dobijeno

$$k_s = s \left(\frac{s - 1}{e} \right)^{s-1}.$$

Parametri s i k_s datoga potencijala za posmatrane atomske parove dati su u tablici. Sve vrednosti za s leže između 2.3 i 2.9, dok se za parametar k_s dobijaju vrednosti bliske jedinici.

»Eksperimentalno« određivanje realnog interatomskog potencijala je moguće. Međutim, stvarni potencijal je moguće predstaviti samo u određenim oblastima međuatomskih rastojanja, pa i ovako dobijeni potencijali pokazuju zavisnost od dubine prodiranja samo u određenim oblastima energije.