

ON THE LONG RANGE PERIODIC POTENTIAL ACTING ON A FREE ELECTRON IN THE RIGID LATTICE OF POLARIZABLE ATOMS

BY P. WIELOPOLSKI AND J. STECKI

Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw*

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The classical electrostatic energy of a cubic crystal of polarizable ions and containing an additional charge at a given position is computed by the use of methods developed earlier and of multipole expansions. The polarization energy of a Frenkel defect is also calculated. In contradistinction to the case of a Schottky defect, the Mott-Littleton approximation gives poor results.

The effective potential acting on a free charge in the lattice of polarizable atoms, which should be taken into account in problems of scatterings or solvation of an electron, contains a long-range electrostatic part due to the polarizational interactions. In this paper we deal only with this part of the potential. At low energies of the electron it is the main interaction in the scattering problem [3, 4, 5]. If the velocity of the electron — v_{el} fulfills the inequality:

$$v_{at} \ll v_{el} \ll v_{orb} \quad (1.1)$$

where v_{at} is the linear velocity of the oscillations of the atoms and v_{orb} is the linear velocity of the atomic (bound) electrons, one can ignore the motion of atoms with respect to the motion of the free electron, and the motion of the free electron can be ignored in calculating the induced polarizations of the atomic electrons [6]. The potential acting on the electron whose velocity fulfills inequality (1.1), can be therefore approximated by the potential energy of a static electronic charge in a rigid lattice of polarizable atoms. Having fixed the position of the charge in space we can express the interaction energy in the crystal lattice of polarizable atoms in a form analogous to that of the polarizational energy of the crystal defects [1]. We have calculated the potential energy of an electronic charge in the simple cubic lattice of polarizable atoms. It is given in the following form:

$$V(r_e) = -\frac{1}{2} \sum_i \sum_j e S_{ei} A_{ij}^0 S_{je} e \quad (1.2)$$

* Address: Instytut Chemii Fizycznej PAN, Kasprzaka 44/52, 01-224 Warszawa, Poland.

where \mathbf{r}_e is the position vector of the electron, \underline{A}_{ij}^0 is the generalized polarizability tensor [1,2] and $e \mathbf{S}_{ei} \equiv e \frac{\mathbf{r}_{ei}}{|\mathbf{r}_{ei}|^3} = e \frac{\partial}{\partial \mathbf{r}_e} \frac{1}{|\mathbf{r}_{ei}|}$ is the electric field due to the electron at \mathbf{r}_e and acting on an atom at the lattice site i . Because of the translational symmetry of the lattice the energy given by Eq. (1.2) is a periodic function with the lattice period:

$$V(\mathbf{r}_e) = V(\mathbf{r}_e + \mathbf{R}_n)$$

where \mathbf{R}_n is an arbitrary lattice vector. An additional consequence of the lattice symmetry is the symmetry of the potential energy function inside the elementary cell. The lattice cell in which the electronic charge is placed, is taken as the origin of the coordinate system for that cell and we denote its position by the vector $\mathbf{r}_0 = \{0, 0, 0\}$. From the periodicity of the potential energy function and its symmetry inside the elementary cell it follows that it suffices to know its form in the cube $\frac{a}{2} \times \frac{a}{2} \times \frac{a}{2}$.

Inside this cube we can express the potential energy $V(\mathbf{r}_{e0})$ as a power series in \mathbf{r}_{e0} . Eq (1.2) takes the following form:

$$\begin{aligned} V(\mathbf{r}_{e0}) &= V_A(\mathbf{r}_{e0}) + V_B(\mathbf{r}_{e0}) + V_C(\mathbf{r}_{e0}) \\ V_A(\mathbf{r}_{e0}) &= -\frac{1}{2} e^2 \sum_{i \neq 0} \sum_{j \neq 0} \mathbf{S}_{ei} \underline{A}_{ij}^0 \mathbf{S}_{je} \\ V_B(\mathbf{r}_{e0}) &= -e^2 \sum_{j \neq 0} \mathbf{S}_{e0} \underline{A}_{0j}^0 \mathbf{S}_{je} \\ V_C(\mathbf{r}_{e0}) &= -\frac{1}{2} e^2 \mathbf{S}_{e0} \underline{A}_{00}^0 \mathbf{S}_{0e}. \end{aligned} \quad (1.3)$$

The expansion in the power series in \mathbf{r}_{e0} is possible only in the case of the vectors \mathbf{S}_{ei} with $i \neq 0$. Making use of the definition for the electric field intensity, one obtains the energy $V_C(\mathbf{r}_{e0})$ in the following form:

$$V_C(\mathbf{r}_{e0}) = -\frac{1}{2} \frac{e^2}{a} \frac{\alpha'}{|\mathbf{r}'_{e0}|^4} \underline{A}'_{00}{}^0 \quad (1.4)$$

where

$$\alpha' = \frac{\alpha}{a^3}; \quad \mathbf{r}'_{e0} = \frac{\mathbf{r}_{e0}}{|a|}; \quad \underline{A}'_{00}{}^0 = \alpha^{-1} \underline{A}_{00}^0.$$

The function $\underline{A}'_{00}{}^0$ was calculated with the aid of the method given in [2]

$$\underline{A}'_{00}{}^0 = \alpha^{-1} \int_{\square} d\mathbf{k} \underline{a}(\mathbf{k}, \alpha) = \underline{U} \int_{\square} d\mathbf{k} \underline{a}'_{xx}(\mathbf{k}, \alpha) \quad (1.5)$$

where the last equality sign follows from the symmetry properties of $\underline{a}(\mathbf{k}, \alpha)$. The integral given by Eq. (1.5) was numerically calculated with the aid of the computer EMC ODRA 1204. The terms $V_A(\mathbf{r}_{e0})$ and $V_B(\mathbf{r}_{e0})$ of the equation (1.3) were expressed in the form of

the Fourier transforms [3]

$$\begin{aligned} V_A(\mathbf{r}_{e0}) &= -\frac{1}{2} e^2 \int_{\square} d\mathbf{k} S(\mathbf{k}, \mathbf{r}_{e0}) \underline{a}(\mathbf{k}, \alpha) S(-\mathbf{k}, \mathbf{r}_{e0}) \\ V_B(\mathbf{r}_{e0}) &= -e^2 S_{e0} \int_{\square} d\mathbf{k} \underline{a}(\mathbf{k}, \alpha) S(-\mathbf{k}, \mathbf{r}_{e0}) \end{aligned} \quad (1.6)$$

where $S(\mathbf{k}, \mathbf{r}_{e0})$ was developed in power series of \mathbf{r}_{e0}/a :

$$\begin{aligned} S(\mathbf{k}, \mathbf{r}_{e0}) &= \left[S(\mathbf{k}) - \underline{\tau}(\mathbf{k}) \mathbf{r}_{e0} + \frac{1}{2!} T^{(3)}(\mathbf{k}) \mathbf{r}_{e0} \mathbf{r}_{e0} + \frac{1}{3!} T^{(4)}(\mathbf{k}) \mathbf{r}_{e0} \mathbf{r}_{e0} \mathbf{r}_{e0} + \dots \right] \\ S(-\mathbf{k}, \mathbf{r}_{e0}) &= \left[S(-\mathbf{k}) - \underline{\tau}(\mathbf{k}) \mathbf{r}_{e0} + \frac{1}{2!} T^{(3)}(-\mathbf{k}) \mathbf{r}_{e0} \mathbf{r}_{e0} + \frac{1}{3!} T^{(4)}(-\mathbf{k}) \mathbf{r}_{e0} \mathbf{r}_{e0} \mathbf{r}_{e0} + \dots \right]. \end{aligned} \quad (1.7)$$

The Fourier transforms in Eq. (1.6) are defined in the following way:

$$\begin{aligned} S(\pm \mathbf{k}) &= \sum_{i \neq 0} \frac{r_{0i}}{|r_{0i}|^3} e^{\pm 2\pi i \mathbf{k} r_{0i}} \\ \underline{\tau}(\mathbf{k}) = \underline{\tau}(-\mathbf{k}) &= - \sum_{i \neq 0} \left[\frac{\partial}{\partial \mathbf{r}_e} \frac{\partial}{\partial \mathbf{r}_e} \frac{1}{|r_{ei}|} \right]_{r_e=r_0} e^{2\pi i \mathbf{k} r_{0i}} \\ T^{(4)}(\pm \mathbf{k}) &= \sum_{i \neq 0} \left[\frac{4}{r^4} \frac{1}{|r_{ei}|} \right]_{r_e=r_0} e^{\pm 2\pi i \mathbf{k} r_{0i}}. \end{aligned} \quad (1.8)$$

The numerical calculations of the lattice sums defined by Eqs (1.8) were done with the aid of De Wette's method [8] for the same values of the \mathbf{k} -vector for which the function $\underline{a}(\mathbf{k}, \alpha)$ was calculated. We have found the symmetry rules for the tensor $T^{(n)}(\mathbf{k})$, which allowed us to reduce the number of the calculated points. Because the integration in the Eq. (1.6) is performed over the whole volume of the first Brillouin zone, only the integrals which satisfy the condition of the threefold parity are not equal to zero:

$$f(\pm k_x, \pm k_y, \pm k_z) = f(|k_x|, |k_y|, |k_z|).$$

Making use of the condition of the threefold parity and the symmetry rules for tensors $T^{(n)}(\mathbf{k})$, $\underline{a}(\mathbf{k}, \alpha)$ we have calculated numerically the integrals which are coefficients of the expansion in the power series. The potential energy of the electron was expressed in the form of a linear combination of the Legendre polynomials [8]. The numerical calculations were performed for four values of the reduced polarizability $\alpha' = 0.04, 0.06, 0.08, 0.1$.

The calculated form of the free electron potential energy in the simple cubic lattice of polarizable atoms is:

$$\alpha' = 0.1$$

$$\begin{aligned}
V(r'_{00}) - \frac{e^2}{a} \left\{ -\frac{0.0589136701}{r'_{00}{}^4} - \frac{0.1782734018}{r'_{00}} - 0.4530753551 - r'_{00} \times \right. \\
\times [0.0480215347(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) + 0.80355397(2\pi)^{1/2}Y_{4,0}] \\
- r'_{00}{}^2 0.891367009 + r'_{00}{}^3 [0.0346455417(2\pi)^{1/2}(Y_{6,4} + Y_{6,-4}) + \\
- 0.926201741(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) - 0.0185188211(2\pi)^{1/2}Y_{6,0} - \\
- 0.15498319552(2\pi)^{1/2}Y_{4,0}] + r'_{00}{}^4 [0.1276097188(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) + \\
\left. + 0.2135319013(2\pi)^{1/2}Y_{4,0} - 0.2096086163(4\pi)^{1/2}Y_{0,0}] + \dots \right\}.
\end{aligned}$$

$$\alpha' = 0.08$$

$$\begin{aligned}
V(r'_{00}) - \frac{e^2}{a} \left\{ -\frac{0.0443052843}{r'_{00}{}^4} - \frac{0.1076321084}{r'_{00}} - 0.3982848836 - r'_{00} \times \right. \\
\times [0.0267921488(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) + 0.0448318397(2\pi)^{1/2}Y_{4,0}] + \\
- r'_{00}{}^2 0.6727006775 + r'_{00}{}^3 [0.0192209381(2\pi)^{1/2}(Y_{6,4} + Y_{6,-4}) + \\
- 0.0546039808(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) - 0.0102740235(2\pi)^{1/2}Y_{6,0} - \\
- 0.091369936(2\pi)^{1/2}Y_{4,0}] + r'_{00}{}^4 [0.1238789818(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) + \\
\left. + 0.2072891844(2\pi)^{1/2}Y_{4,0} - 0.1636127603(4\pi)^{1/2}Y_{0,0}] + \dots \right\}.
\end{aligned}$$

$$\alpha' = 0.06$$

$$\begin{aligned}
V(r'_{00}) - \frac{e^2}{a} \left\{ -\frac{0.031753314}{r'_{00}{}^4} - \frac{0.0584437143}{r'_{00}} - 0.3303325163 - r'_{00} \times \right. \\
\times [0.013370485(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) + 0.0223731006(2\pi)^{1/2}Y_{4,0}] + \\
- r'_{00}{}^2 0.4870309525 + r'_{00}{}^3 [0.0095386093(2\pi)^{1/2}(Y_{6,4} + Y_{6,-4}) + \\
- 0.0291355738(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) - 0.0050992015(2\pi)^{1/2}Y_{6,0} - \\
- 0.0487531382(2\pi)^{1/2}Y_{4,0}] + r'_{00}{}^4 [0.1087722966(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) + \\
\left. + 0.1829119853(2\pi)^{1/2}Y_{4,0} - 0.1211445921(4\pi)^{1/2}Y_{0,0}] + \dots \right\}.
\end{aligned}$$

$$\alpha' = 0.04$$

$$\begin{aligned}
V(r'_{00}) - \frac{e^2}{a} \left\{ - \frac{0.0205139334}{r'_{00}{}^4} - \frac{0.0256966713}{r'_{00}} - 0.245700166 - r'_{00} \times \right. \\
\times [0.005331763(\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) - 0.008921746(2\pi)^{1/2}Y_{4,0}] - \\
- r'_{00}{}^2 0.3212083913 + r'_{00}{}^3 [0.0037848264(2\pi)^{1/2}(Y_{6,4} + Y_{6,-4}) - \\
- 0.012568994(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) - 0.0020230751(2\pi)^{1/2}Y_{6,0} - \\
- 0.021031951(2\pi)^{1/2}Y_{4,0}] + r'_{00}{}^4 0.0835731577(2\pi)^{1/2}(Y_{4,4} + Y_{4,-4}) + \\
\left. + 0.1398446405(2\pi)^{1/2}Y_{4,0} - 0.0804552857(4\pi)^{1/2}Y_{0,0} \right] + \dots \left. \right\}.
\end{aligned}$$

Making use of the continuum approximation for the functions $\underline{a}(\mathbf{k}, \alpha)$ [2], one can easily show that the influence of the terms $V_A(\mathbf{r}_{e0})$ and $V_B(\mathbf{r}_{e0})$, Eq. (1.3) upon the total polarizational energy of the electron is not a large one. Besides, the continuum approximation allows us to take into account the effect of the replacement of the exact local field by the Lorentz field. We now express Eq. (1.2) in the following form:

$$\begin{aligned}
V(\mathbf{r}_{e0}) &= -\frac{1}{2} e^2 \sum_i S_{ei} d\mathbf{k} e^{-2\pi i \mathbf{k}(\mathbf{r}^0_0 - \mathbf{r}^0_i)} \underline{a}(\mathbf{k}, \alpha) \sum_j S_{je} e^{-2\pi i \mathbf{k}(\mathbf{r}^0_j - \mathbf{r}^0_0)} = \\
&= -\frac{1}{2} e^2 \sum_i S_{ei} d\mathbf{k} e^{-2\pi i \mathbf{k}(\mathbf{r}^0_0 - \mathbf{r}^0_i)} \underline{a}(\mathbf{k}, \alpha) e^{-2\pi i \mathbf{k}(\mathbf{r}_e - \mathbf{r}^0_0)} \sum_j S_{je} e^{-2\pi i \mathbf{k}(\mathbf{r}^0_j - \mathbf{r}_e)}. \quad (1.9)
\end{aligned}$$

The function

$$S(-\mathbf{k}, \mathbf{r}_e) = \sum_j S_{je} e^{-2\pi i \mathbf{k}(\mathbf{r}^0_j - \mathbf{r}_e)} \quad (1.9a)$$

is a periodic function with the lattice period, therefore we can express it in terms of the following Fourier series:

$$S(-\mathbf{k}, \mathbf{r}_e) = \sum_{\mathbf{v}} S(-\mathbf{k}, \mathbf{K}_{\mathbf{v}}) e^{2\pi i \mathbf{K}_{\mathbf{v}} \mathbf{r}_e} \quad (1.10)$$

where $\mathbf{K}_{\mathbf{v}}$ are vectors of the reciprocal lattice an

$$S(-\mathbf{k}, \mathbf{K}_{\mathbf{v}}) = \frac{1}{v_0} \int_{v_0} d\mathbf{r}_e \sum_j S(\mathbf{r}_j^0 - \mathbf{r}_e) e^{-2\pi i \mathbf{k}(\mathbf{r}^0_j - \mathbf{r}_e)} e^{-2\pi i \mathbf{K}_{\mathbf{v}} \mathbf{r}_e} \quad (1.11)$$

where $v_0 = a^3$ is the volume of the elementary cell. Making use of the property of $\mathbf{K}_{\mathbf{v}}$, namely that: $e^{2\pi i \mathbf{K}_{\mathbf{v}} \mathbf{r}_j^0} = 1$, for every lattice vector \mathbf{r}_j^0 , we obtain:

$$S(-\mathbf{k}, \mathbf{K}_{\mathbf{v}}) = \frac{1}{v_0} \int_{v_0} d\mathbf{r}_e \sum_j S(\mathbf{r}_j^0 - \mathbf{r}_e) e^{2\pi i (\mathbf{K}_{\mathbf{v}} - \mathbf{k}) (\mathbf{r}^0_j - \mathbf{r}_e)}.$$

Because the sum over indices j runs through all lattice sites, there is an equality:

$$\frac{1}{v_0} \int d\mathbf{r}_e \sum_j S(\mathbf{r}_j^0 - \mathbf{r}_e) e^{2\pi i(\mathbf{K}_v - \mathbf{k})(\mathbf{r}_j^0 - \mathbf{r}_e)} = \frac{1}{v_0} \int dR S(\mathbf{R}) e^{2\pi i(\mathbf{K}_v - \mathbf{k})R} \quad (1.12)$$

where V is the macroscopic volume of the crystal and $S(\mathbf{R}) = \frac{R}{R^3}$. Because we are treating the system as an infinite lattice, we obtain [3]:

$$S(-\mathbf{k}, \mathbf{K}_v) = \frac{1}{a^3} \iiint_{-\infty}^{\infty} d\mathbf{R} \frac{R}{R^3} e^{2\pi i(\mathbf{K}_v - \mathbf{k})R} = \frac{1}{a^3} S'^{\text{con}}(\mathbf{K}_v - \mathbf{k}). \quad (1.13)$$

Representing $S'^{\text{con}}(\mathbf{K}_v - \mathbf{k})$ in non-dimensional form $S^{\text{con}}(\mathbf{K}_v - \mathbf{k})$, we obtain:

$$S(-\mathbf{k}, \mathbf{K}_v) = \frac{1}{a^2} S^{\text{con}}(\mathbf{K}_v - \mathbf{k})$$

therefore

$$S(-\mathbf{k}, \mathbf{r}_e) = \frac{1}{a^2} \sum_v S^{\text{con}}(\mathbf{K}_v - \mathbf{k}) e^{2\pi i \mathbf{K}_v \mathbf{r}_e}. \quad (1.14)$$

Introducing the function $S(-\mathbf{k}, \mathbf{r}_e)$ defined by Eq. (1.14) into the expression for the potential energy of the electron, we obtain:

$$V(\mathbf{r}_{e0}) = -\frac{1}{2} e^2 \frac{1}{a^2} \sum_i S_{ei} \sum_v \int_{\square} d\mathbf{k} e^{-2\pi i(\mathbf{K}_v - \mathbf{k})\mathbf{r}'_{ei}} \underline{a}(\mathbf{k}, \alpha) S^{\text{con}}(\mathbf{K}_v - \mathbf{k}). \quad (1.15)$$

In this representation, vector \mathbf{r}'_{ei} is non-dimensional. Making use of the periodicity of the function $\underline{a}(\mathbf{k}, \alpha)$, $\underline{a}(\mathbf{k}, \alpha) = \underline{a}(\pm \mathbf{K}_v + \mathbf{k}, \alpha)$, we express Eq. (1.15) in the following form:

$$\begin{aligned} V(\mathbf{r}_{e0}) &= -\frac{1}{2} e^2 \frac{1}{a^2} \sum_i S_{ei} \sum_v \int_{\square} d\mathbf{k} e^{-2\pi i(\mathbf{K}_v - \mathbf{k})\mathbf{r}'_{ei}} \underline{a}(-\mathbf{K}_v + \mathbf{k}, \alpha) S^{\text{con}}(\mathbf{K}_v - \mathbf{k}) = \\ &= -\frac{1}{2} e^2 \frac{1}{a^2} \sum_i S_{ei} \int_{V_{\text{reo}}} d\mathbf{k} e^{-2\pi i \mathbf{k} \mathbf{r}'_{ei}} \underline{a}(\mathbf{k}, \alpha) S^{\text{con}}(\mathbf{k}) \end{aligned}$$

where V_{reo} denotes the volume of the reciprocal lattice and

$$\mathbf{k} = \mathbf{K} - \mathbf{k}.$$

Introducing the continuum approximation for the function $\underline{a}(\mathbf{k}, \alpha)$ [2], we obtain the potential energy of the electron in the crystal lattice calculated with the assumption that the local field is a Lorentz local field:

TABLE I

Values of the coefficients of the term

$$|r'_{eo}|^{-4}; W'(\alpha') \equiv \left(\frac{e^2}{a}\right)^{-1} W(\alpha')$$

α'	Exact solution $W'_{\text{ex}}(\alpha')$	Approximate solution $W'_{\text{app}}(\alpha')$	$\frac{W'_{\text{ex}}(\alpha')}{W'_{\text{app}}(\alpha')}$
0.04	0.02051	0.01498	1.37
0.06	0.03175	0.01996	1.59
0.08	0.04430	0.02395	1.85
0.1	0.05891	0.02721	2.16

TABLE II

Potential energy of the electron in the simple cubic lattice of polarizable atoms. Energy is presented in non-dimensional form defined by the equation:

$$v''(r'_{00}, \alpha') = \left(\frac{e^4}{a}\right)^{-1} v(r'_{00}, \alpha')$$

r	$\alpha' - 0.04$	$\alpha' - 0.06$	$\alpha' - 0.08$	$\alpha' - 0.1$
Direction 1 $\theta = 90^\circ; \varphi = 0^\circ$				
0.2	-13.2120776762	-20.4978514737	-28.6744950456	-38.2369512506
0.3	-2.9016217275	-4.5043748899	-6.3196246121	-8.4592538401
0.4	-1.160311485	-1.5562057269	-2.5507261822	-3.4278095012
0.5	-0.7077906508	-1.0987533695	-1.5484053687	-2.0912002073
Direction 2 $\theta = 90^\circ; \varphi = 45^\circ$				
0.2	-13.20738504468	-20.485451369	-28.6491103309	-38.1820638905
0.3	-2.8921543811	-4.4860747586	-6.2800146658	-8.38547559
0.4	-1.163476107	-1.7896844665	-2.4973388134	-3.30501396
0.5	-0.7104745774	-1.0788302478	-1.4844371085	-1.9531890206
$\frac{\sqrt{2}}{2}$	-0.5531029987	-0.8129317212	-1.0834566836	-1.3800247926
Direction 3 $\theta = 54.7^\circ; \varphi = 45^\circ$				
0.2	-13.2059973499	-20.4617628596	-28.6415454034	-38.1772495119
0.3	-2.8907618104	-4.4814761139	-6.269837524	-8.3663360471
0.4	-1.1634196345	-1.7888315986	-2.4867152706	-3.3007780204
0.5	-0.7141272358	-1.0791401285	-1.4771244187	-1.9324316209
$\frac{\sqrt{3}}{2}$	-0.6849592915	-0.9753014173	-1.2541976044	-1.5327987697

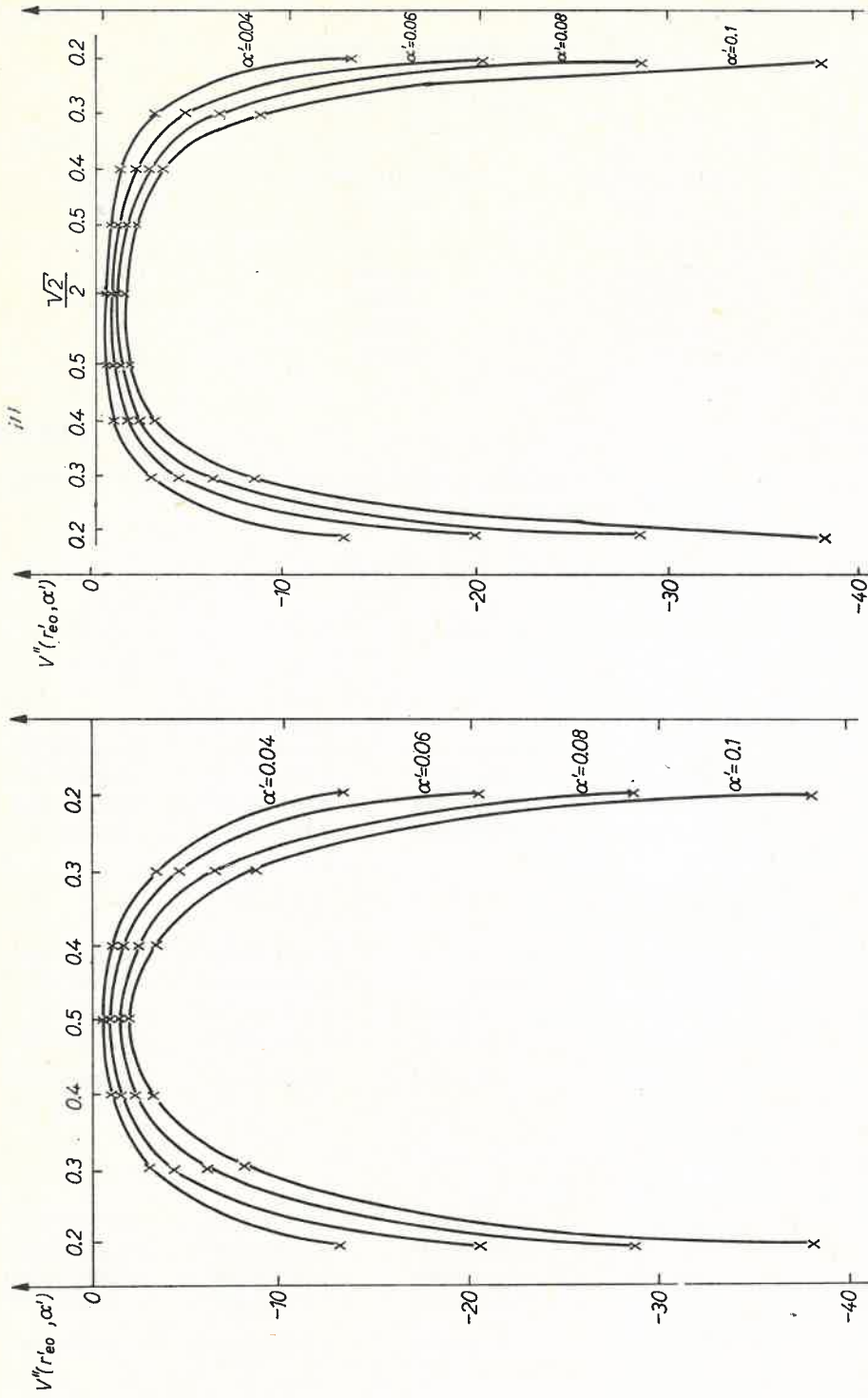


Fig. 1. Potential energy of the electron in the simple cubic lattice of polarizable atoms. Direction [1, 0, 0]

Fig. 2. Potential energy of the electron in the simple cubic lattice of polarizable atoms. Direction [1, 1, 0]

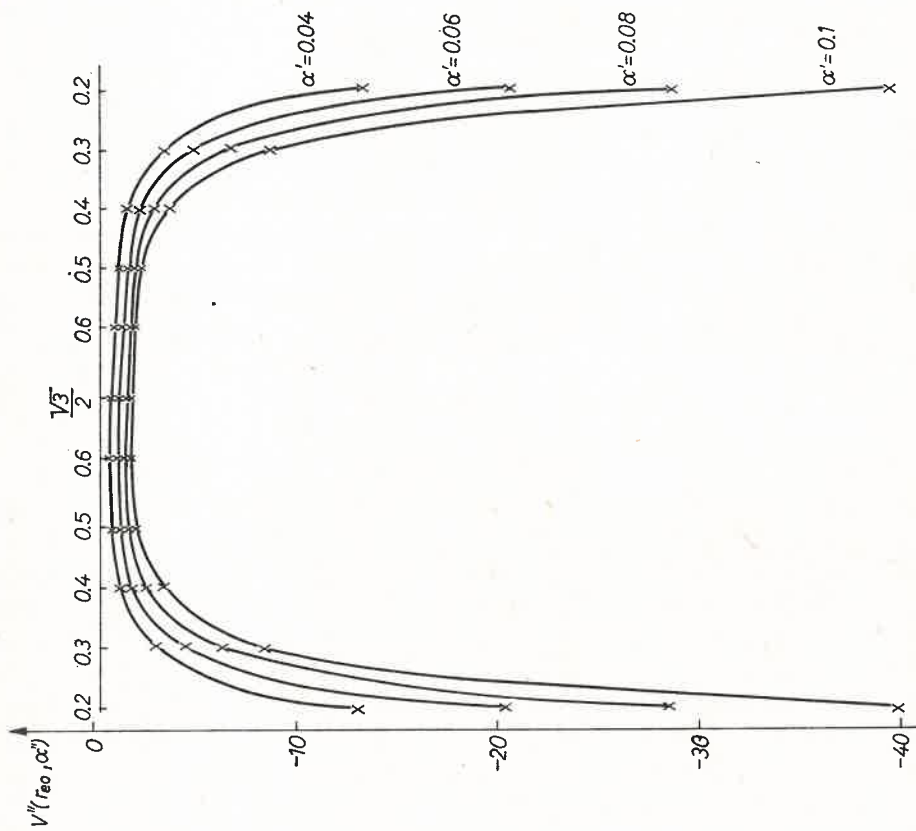


Fig. 3. Potential energy of the electron in the simple cubic lattice of polarizable atoms. Direction [1, 1, 1]

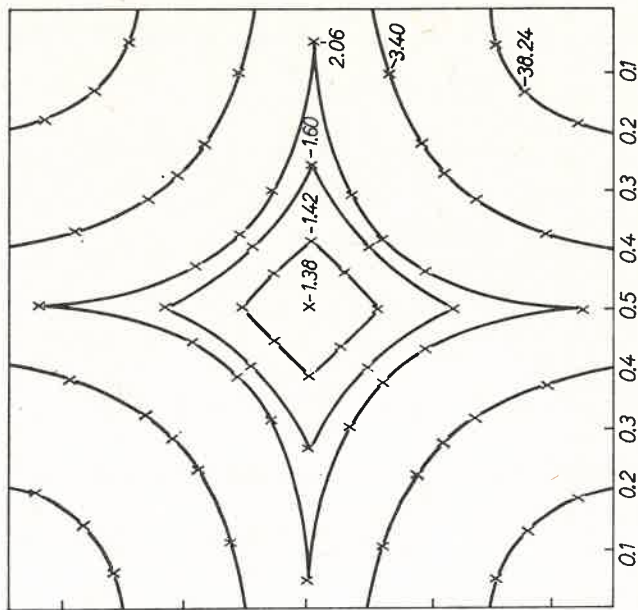


Fig. 4. Map of the electron potential energy in the s.c. lattice of polarizable atoms. Plane XY of the elementary cell, $Z = 0$

$$\begin{aligned}
 V(\mathbf{r}_{e0}) &= -\frac{1}{2} e^2 \frac{1}{a^2} \sum_i \mathcal{S}_{ei} \int_{V^{-1}} d\kappa e^{-2\pi i \kappa \mathbf{r}'_{ei}} \underline{\alpha}^{\text{con}}(\kappa, \alpha) S^{\text{con}}(\kappa) = \\
 &= -\frac{1}{2} e^2 \frac{1}{a^2} \sum_i \mathcal{S}_{ei} \int_{V^{-1}} d\kappa e^{-2\pi i \kappa \mathbf{r}'_{ei}} \frac{\alpha}{1+2B} \cdot \frac{2i\kappa}{\kappa^2} = \\
 &= -\frac{1}{2} e^2 \frac{1}{a^2} \frac{\alpha}{(1+2B)} \sum_i \mathcal{S}_{ei} \frac{\mathbf{r}'_{ei}}{|\mathbf{r}'_{ei}|^3}
 \end{aligned} \tag{1.16}$$

where

$$B = \frac{4\pi}{3} \alpha'; \quad \alpha' = \frac{\alpha}{a^3}.$$

Representing the vector \mathcal{S}_{ei} (Eq. (1.2)) in non-dimensional form, we obtain:

$$\begin{aligned}
 V(\mathbf{r}_{e0}) &= -\frac{1}{2} \frac{e^2}{a} \frac{\alpha'}{(1+2B)} \sum_i \frac{1}{|\mathbf{r}'_{ei}|^4} = \\
 &= -\frac{1}{2} \frac{e^2}{a} \frac{\alpha'}{(1+2B)} \frac{1}{|\mathbf{r}'_{e0}|^4} - \frac{1}{2} \frac{e^2}{a} \frac{\alpha'}{(1+2B)} \sum_{i \neq 0} \frac{1}{|\mathbf{r}'_{ei}|^4}.
 \end{aligned} \tag{1.17}$$

From Eq. (1.17) it follows that the term proportional to $|\mathbf{r}'_{e0}|^{-4}$ is the most important one in the calculation of the electron energy. Comparing the coefficients connected with the term $|\mathbf{r}'_{e0}|^{-4}$ in the exact and approximated solutions (Table I) one can see that the Lorentz local field gives large errors in the calculation of the electron potential energy.

In Table II and in Figs 1, 2, 3, 4 we present the numerical calculations of the electron potential energy according to the exact solution. The results are shown for three directions [1, 1, 1], [1, 1, 0], [1, 0, 0], of the vector \mathbf{r}_{e0} .

Conclusions

The presented of the calculation of the long range part of the electron energy, due to the ionic or atomic polarizabilities can be easily adopted to the calculations of the polarizational energy of Frenkel-type defects. From the comparison of the results obtained in Table I it follows that the approximate solution, which represents in fact the zero-order Mott-Littleton method [10] for the Frenkel type defect causes large errors in the calculations of the polarizational energy. The results obtained by the Mott-Littleton method were very close to the exact solution in the case of a Schottky defect [3]; it follows, that the exact solution for the local field intensity is of great importance in the case of defects which destroy the cubic symmetry of the lattice. The exact function of the electron potential energy allows us to calculate its energy in the whole volume of the lattice cell and to find the energy barrier between the lattice cells.

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