Interatomic potentials of interactions in radiation physics

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Abstract. Current theoretical methods of calculating the pair, interatomic and averaged, potentials of ion interaction with the atoms of solids are discussed. Along with the traditional static approximations, nonstationary and quasi-stationary models are considered. In the other case, modification of the electron gas approximation taking account of the relative velocity of atoms v_1 is investigated. Furthermore, the effect of ion ionisation and dynamic screening of potentials by the electron gas is taken into account. Theoretical models are compared with each other and with the experimental data. The energy losses and the ion ranges in solids, angular distributions due to multiple scattering, bremsstrahlung losses of heavy ions in the process of a planar channelling, channelling radiation lines of the relativistic electrons and positrons, and other effects are considered.

1. Introduction

When we use atom-atom (ion-atom) potentials of interaction (IP), we can, in the first approximation and

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Received 4 April 1994, revised 25 January 1995 Uspekhi Fizicheskikh Nauk **165** (8) 919–953 (1995) Translated by O B Moskalev; edited by L Dwivedi independently of the problem considered, exclude the details of the electron structure of matter. Therefore the interpretation of the basic phenomena connected with the transport of particles in the medium is directly or indirectly based upon the concept of IP. It is common practice to distinguish between short-range and long-range interatomic forces. In this work we concentrate mainly on the shortrange forces because in the radiation physics of solids the particle impact parameters with respect to the target atoms are relatively small. However, in some cases long-range forces may also prove significant, as for example in the sliding interaction of a particle with the surface. The main theoretical considerations determining the calculations of the static IP of the isolated neutral particles are developed in detail (for example, see Refs [1-4]), but the problem remains when we calculate the ion-atom IP for an arbitrary degree of ionisation and for an arbitrary energy of the incident ions on the one hand and for the different combinations of the collision partners on the other hand. It is also evident that a frequent assumption concerning the additivity of the particle interactions with the separate target atoms has only a relative validity, estimation of its accuracy being not always straightforward. It is therefore desirable, based on the concept of IP, to take into account the dynamic and many-particle effects, and also the specific properties of a target. A good example of this is the phenomenon of channelling [5, 6], where a theoretical description has been made after the introduction of the concept of a continuous potential of the atomic chain (plane) [7].

Recently, along with the traditional application of IP in solid state and radiation physics, interest in these subjects has also been stimulated by the prediction and discovery of the radiation of the relativistic channelling particles [8–10, 305-309, 319], the diagnostic application of this radiation [10, 11, 306], and the growing demand of nuclear material science [12]. Besides, information concerning the repulsive IP is traditionally important for the problems of physical kinetics [13, 14] and laser excitation of the electrons [15, 16]. In the latter case, it is necessary to have the potential curves for the region of the energy minimum, i.e. in the transition region between the repulsive and long-range potentials.

Owing to the rapid development of these trends it might be interesting to review recent achievements in the application of theoretical methods for IP calculations, and their use for an explanation of different phenomena taking place during the transport of charged particles in matter. Most of the aspects mentioned above have not received sufficient attention (or have not been considered at all) and therefore this review might be a timely one.

The choice of material is determined, on the one hand, by the author's interests and, on the other hand, by the limited space of the article. Therefore, I have not considered (or only briefly touched on) the results associated with the dechannelling and the orientation effects at high energies, sputtering of solids by ion bombardment, the phase transformations due to irradiation, and other effects. Those interested in this subject are referred to a number of review articles and monographs [10, 12, 111, 145, 201, 306-309].

Section 2 includes a review of the most important theoretical methods employed for calculating the pair potentials in the molecular and ion-atom systems. Among them are the stationary quantum-mechanical models, the Thomas-Fermi and Thomas-Fermi-Dirac approximations, and an electron gas approximation. A great number of analytical models are also considered. Sec-2.7 tions 2.6 and deal with а nonstationary approximation and a quasi-static generalisation of the electron gas theory. In the latter case, the ion-atom IP depends upon the energy (velocity) resulting from the stripping of the electron shell and the varving effectiveness of the overlapping of the Fermi spheres of the electrons in the impulse space.

Section 3 contains an analysis of the classical effects of the interaction between the ions and the light particles with the solids, with their description being based on the interatomic IP or the averaged potentials with respect to channelling (single and multiple scattering, stopping powers, and ranges). In Section 3.4 the problems of calculating the ion-atom (ion-ion) IP in solids are considered, with an account of the effect of dynamic screening by the electron gas. Section 3.5 gives a detailed description of the problem of connection between different approximations for the continuous potentials of the atomic chains (planes) taking into account (or ignoring) the external periodic fields. In Section 3.6 some surface effects are briefly described, and Section 3.7 deals with the special features of the interactions of particles with solids at high energies.

Section 4 contains comparisons of the theoretical models with some experimental data. Special emphasis is placed on the effects of the Z_1 -, Z_2 -oscillations of the cross sections of scattering and stopping, and the ranges of the

ions in semiconducting, metal, and gaseous targets (Section 4.1); the effects of correlation of the energy losses with the outgoing angle from the thin film and the features of multiple scattering of the partly 'stripped' ions (4.2); the question of dependence of the value $\psi_{1/2}\sqrt{E}$ (where $\psi_{1/2}$ is the angular half width of the inverse scattering during channelling, and E is the ion energy) upon the energy is discussed (4.3). In Sections 4.4 and 4.5 the measurements of the trajectories and potentials, as well as dependences of the bremsstrahlung losses of the heavy ions on the frequency of the oscillations in plane channelling conditions are analysed; in Section 4.6 theoretical and experimental data related to the characteristic radiation of the channelled electrons and positrons (in a plane regime) are compared and the problems related to a diagnostic application of this radiation are discussed. In the conclusions section some significant, and in the author's opinion still unresolved, problems and trends in the development of the theory of interaction potentials and the radiation effects are mentioned.

The list of references, although quite extensive, is far from being complete, notably with respect to developments over the last two years.

2. Theoretical discussion

Among the approximations most frequently used in radiation physics for the calculation of the pair and average potentials, atomic electron densities, form factors etc., a specific role is played by the stationary Thomas-Fermi and Thomas-Fermi-Dirac models and the related methods of the electron gas and of the electron density functional [22, 176, 40, 86]. More rigorous theoretical schemes based on the Schrodinger equation [16, 21, 324] have been used to a lesser extent because of their complexity and they are the last resort in application to radiation physics. Nevertheless, continuous progress in the field makes it necessary to refine the theory constantly in order to include more detailed interactions between the ions and atoms. Thus a broader perspective is offered for the development and new application of the nonstationary and quasistationary approximations in the theory of interatomic potentials. At the same time, many model analytical approximations retain their significance. Combination and analysis of the approximations mentioned in a single section makes it possible to use the information in it in a way that is autonomous with respect to other sections directly related to the interactions in solids.

2.1 Stationary quantum-mechanical models

An adiabatic approximation of the Schrodinger equation forms the basis of the quantum-mechanical calculations of the potential energy of the diatomic system. This enables us to separate the motion of the electrons from the motion of the nuclei. As a result of applying this approximation, we have [17]:

$$\left[\hat{H} - U(\boldsymbol{R})\right] \boldsymbol{\Phi}(\boldsymbol{R}, \boldsymbol{r}) = 0 , \qquad (2.1)$$

where r designates the electron coordinates, R is the coordinate of the relative motion of nuclei, the Hamiltonian \hat{H} includes the kinetic energy of the electrons and the potential energies of the mutual and cross interactions of nuclei and electrons. The function U(R), which is an eigenvalue of the operator \hat{H} , defines the energy of the system for a fixed distance R. When $R \to \infty$, we have $U(R) \to E_1 + E_2$, where $E_{1,2}$ are the energies of the isolated atoms. Interaction potential in a typical interpretation is defined as

$$V(\mathbf{R}) = U(\mathbf{R}) - U(\infty) . \qquad (2.2)$$

Solution of Eqn (2.1) for the needs of radiation physics is still a remote possibility. Therefore more simple computational schemes are of interest, in particular the method of separating the contributions of the interactions of the atomic cores and of the valence electrons [16]:

$$\hat{H} = \hat{H}_{1} + \hat{H}_{2} + \hat{H}_{v} + \hat{H}_{12} ,$$

$$V(\mathbf{R}) = V_{c}(\mathbf{R}) + V_{v}(\mathbf{R}) ,$$

$$\Phi(\mathbf{R}, \mathbf{r}) = \Phi_{1}(\mathbf{R}, \mathbf{r}) \Phi_{2}(\mathbf{R}, \mathbf{r}) \Phi_{v}(\mathbf{R}, \mathbf{r}) ,$$
(2.3)

where $\hat{H}_{1,2}$ are the Hamiltonians of the cores, \hat{H}_v is the Hamiltonian of the valence electrons, \hat{H}_{12} is the interaction of the cores, $\Phi_{1,2}(\mathbf{R}, \mathbf{r})$ and $\Phi_v(\mathbf{R}, \mathbf{r})$ are the wave functions of the core and valence electrons. Assuming that $U(\infty) = E_1 + E_2 + E_v$, substituting (2.3) into (2.1) and separating the variables, we get (for simplicity designations of the variables \mathbf{R} and \mathbf{r} are omitted):

$$(\hat{H}_{1} + \hat{H}_{2}) \Phi_{1} \Phi_{2} - V_{c} \Phi_{1} \Phi_{2} = (E_{1} + E_{2}) \Phi_{1} \Phi_{2} ,$$

$$H_{v} \Phi_{v} - V_{v} \Phi_{v} = E_{v} \Phi_{v} .$$
(2.4)

Functions Φ_1 , Φ_2 , and Φ_v should, in addition, satisfy the orthogonality relations

$$\langle \boldsymbol{\Phi}_i | \boldsymbol{\Phi}_{\mathbf{v}} \rangle = 0, \quad i = 1, 2.$$
(2.5)

If the overlapping of the ion cores is small, potential $V_c(R)$ is calculated in the first order of the perturbation theory (assuming that wave functions $\Phi_{1,2}$ of the ion cores are known):

$$V_{\rm c}(R) = \langle \boldsymbol{\Phi}_1 \boldsymbol{\Phi}_2 | \hat{H}_{12} | \boldsymbol{\Phi}_1 \boldsymbol{\Phi}_2 \rangle . \qquad (2.6)$$

Thus, the problem of finding the IP reduces to the computation of integral (2.6) and to the solution of the simpler (the second one) of the two equations (2.4), where $\hat{H}_{\rm v}$ contains only operators of the kinetic energy of the valence electrons and of their interactions between themselves and with the cores. However, even in this case the problem remains sufficiently complex and therefore, in practice, the method of the model potentials [18-21] is widely used. This method involves representation of the Hamiltonian in the form of a sum $\hat{H}_{v} = \hat{T} + v_{m}$, where \hat{T} is an operator of the kinetic energy of the electrons, and $v_{\rm m}$ is a model potential. Various forms of such potentials can be found in Ref. [16]. The accuracy of the computations of the IP by this method guarantees agreement with the experimental data related to the scattering of the molecular beams and to the spectroscopy in the range of 5-10% (at the minimum of the potential curves). The method of the electron density functional provides similar accuracy [86].

2.2 Thomas – Fermi and Thomas – Fermi – Dirac approximations

When we use the Thomas-Fermi (TF) or Thomas-Fermi-Dirac (TFD) theories, the energy of the two-centre system can be written in the form [22] (here and hereafter we use atomic units: $e = \hbar = m_e = 1$)

$$U(R) = \frac{Z_1 Z_2}{R} - \int \left(\frac{Z_1}{r_1} + \frac{Z_2}{r_2}\right) \rho(\mathbf{r}) d^3 \mathbf{r} + \frac{1}{2} \int \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r} d^3 \mathbf{r}' + \frac{3}{10} (3\pi^2)^{2/3} \int \rho(\mathbf{r})^{5/3} d^3 \mathbf{r} - \frac{3}{4} \left(\frac{3}{\pi}\right)^{1/3} \int \rho(\mathbf{r})^{4/3} d^3 \mathbf{r} , \qquad (2.7)$$

where $\rho(\mathbf{r})$ is the electron density at the point \mathbf{r} of the coordinate space, $Z_{1,2}$ are the charges of the nuclei, $r_{1,2}$ are the distances from the point \mathbf{r} to the nuclei, and R is the internuclear distance. Formula (2.7) corresponds to the TFD theory and without the last (exchange) term it corresponds to the TF theory. The proof of the fact that the extremum of the functional U(R) with respect to $\rho(\mathbf{r})$ gives the minimum energy of the system for the TFD approximation in Ref. [24]. In these two cases, when we minimise U(R) with respect to $\rho(\mathbf{r})$, we obtain the known relations between the density and the electric potential $V_e(\mathbf{r})$ of the system [22]:

$$\rho_{\rm TF} = \frac{2^{3/2}}{3\pi^2} \left(V_{\rm e} - V_0 \right)^{3/2} \,, \tag{2.8}$$

$$\rho_{\rm TFD} = \frac{2^{3/2}}{3\pi^2} \left[\left(V_{\rm e} - V_0 + \tau_0^2 \right)^{1/2} + \tau_0 \right]^3 \,, \tag{2.9}$$

where V_0 is the chemical potential, and $\tau_0 = 1/\sqrt{2\pi}$. The potential $V_c(R)$ satisfies the Poisson equation for the charge densities given by Eqns (2.8) and (2.9):

$$\Delta V_{\rm e} = 4\pi\rho - 4\pi \left[Z_1 \delta(\boldsymbol{r} - \boldsymbol{r}_1) + Z_2 \delta(\boldsymbol{r} - \boldsymbol{r}_2) \right] \,. \tag{2.10}$$

Substituting Eqns (2.8) and (2.9) into Eqn (2.10), we obtain the standard equations of the TF and TFD theories for the molecules. If we substitute in Eqn (2.7) the approximate values of the density ρ , it is evident that the value U(R)that we obtain is an upper limit of the energy. In the case of a neutral diatomic molecule, in the TF approximation, Firsov [23] obtained a maximising functional $U_1(R)$. Using the latter for an improved estimation of energy of the system with an approximate density, we can take a halfsum value $[U(R) + U_1(R)]/2$. So far as we know, no correct form of the maximising functional has been found in the TFD theory, and no correct form of the ion-atom systems has been found in the TF theory.

The authors of Ref. [325] considered a modification of the TF equation by changing $\rho^{5/3}$ in Eqn (2.7) to $\alpha(N)\rho^{4/3}/r$, where N is the number of electrons. Firsov [25] showed that within the accuracy bounds of the TFD model one can expand the density [Eqn (2.9)] with respect to the small parameter τ_0^2 and restrict it to the first two terms. Then, taking into account Eqns (2.9) and (2.10), a modified equation of the TFD will be presented as

$$\Delta V_{\rm e} = 0.81 V_{\rm e} + 1.2 V_{\rm e}^{3/2} -4\pi [Z_1 \delta(\mathbf{r} - \mathbf{r}_1) + Z_2 \delta(\mathbf{r} - \mathbf{r}_2)] . \qquad (2.11)$$

Although Eqn (2.11) in the case of the neutral systems is more convenient for computations than the standard TFD equation (because it does not lead to a finite radius of the molecule), this advantage disappears when we turn to the ion-atom system.

So far, few attempts have been made at numerical integration of the general TF and TFD equations for the molecules. For the homonuclear pairs the classic works [26-28] which offer the solutions to the TF equation are known. The systems of Ne–Ne, He–Ar and Mg–O were considered in Ref. [29], and in Ref. [30] the TFD equation was solved. Calculation of the IP of a homoatomic pair by applying the maximal and minimal principles of the TF model within the framework of the variational method was made in Ref. [31].

From Eqn (2.7) it is evident that, if $Z_1 = Z_2$ and the densities ρ are obtained from the solution to the TF equation, the energy of the system can be represented in a universal form

$$U(Z, R) = Z^{7/3} \left[\frac{1}{RZ^{1/3}} + f_1(RZ^{1/3}) + Z^{-2/3} f_2(RZ^{1/3}) \right],$$
(2.12)

where the last term represents the contribution of the exchange energy calculated for $\rho = \rho_{\rm TF}$ as a small perturbation, and $f_1(x)$ and $f_2(x)$ are the known functions.

In Ref. [32] it is shown that the addition to the functional (2.7) of the Kirzhnits nonhomogeneity correction [33],

$$\Delta U_{\rm K} = \frac{1}{72} \int \frac{\left(\nabla \rho\right)^2}{\rho} \, \mathrm{d}^3 \boldsymbol{r} \,, \qquad (2.13)$$

leads to a rise in the exchange energy in Eqn (2.12) by 2/9 of its previous value (in this case, $\Delta U_{\rm K}$ is also treated as a small adjustment). In fact, assuming that $V_0 = 0$ in Eqn (2.8) (for the neutral system of identical atoms), and taking into account Eqns (2.8), (2.10), and Green's formula, we can transform Eqn (2.13) as follows:

$$\Delta U_{\rm K} = \frac{\sqrt{2}}{24\pi^2} \int (\nabla V_{\rm e}^{1/2}) \nabla V_{\rm e} \, \mathrm{d}^3 \boldsymbol{r} = -\frac{2}{9\pi^3} \int V_{\rm e}^2 \, \mathrm{d}^3 \boldsymbol{r}$$
$$= -\frac{2}{9} \frac{3}{4} \left(\frac{3}{\pi}\right)^{1/3} \int \rho^{4/3} \, \mathrm{d}^3 \boldsymbol{r} \,, \qquad (2.14)$$

which is QED. Thus, taking into account the nonhomogeneity of the electron gas reduces the energy of a diatomic system, while in the case of a single atom the situation is reversed. This conclusion is also evident from a direct analysis of Eqn (2.13) if we take into account the fact that within the space between the nuclei the electron density gradient becomes smaller.

In Ref. [32] a correction to the energy is obtained, which is similar to the known correction of Scott [34] for an atom, and which takes account of the contribution of the strongly bounded electrons:

$$\Delta U_q(R, Z) = Z^2 f_3(RZ) . \qquad (2.15)$$

The function $f_3(x)$ varies within the limits from 1 to 2 and is tabulated in Ref. [32]. Table 1 contains the comparative figures of the IP for the N-N system calculated on the basis of Ref. [32], results obtained by the Hartree-Fock (HF) method [35], and those obtained by the variational computation [31] for the half-sum of the upper and lower energy estimates based on the TF theory. In the latter case, a scaled version of the TF model and an interpolation of the results of Ref. [31] for the values of R are used to obtain the necessary values of R.

Table 1. N - N potential of interaction.

R/a.u.	Z^2/R	V(R)/a.u.			
		Ref. [31]	Ref. [32]	Ref. [35]	
0.2	245	140	129.2	132.6	
0.5	98	28	21.4	24.8	
1.0	49	6.8	-0.8	4.1	
1.5	32.7	2.25	-4.8	0.2	
2.0	24.5	1.0	-6.0	-0.4	
3.0	16.35	0.29	-6.65	-0.05	

The figures in Table 1 show that taking into account the corrections given by Eqns (2.14) and (2.15), calculated in a nonselfconsistent way [32], will lead to considerably underestimated values of the IP for R > 1. On the contrary, the potential [31] that corresponds to the TF theory decreases too slowly if R increases. These conclusions are likely to be valid for the case of the IP of a pair of identical positive ions, where a universal function of N and N/Z (N is the number of electrons) is obtained in Ref. [36]. On the whole, it can be mentioned that so far the TFD theory in its classical interpretation has not led to any essential results in IP calculation .

2.3 Electron gas approximation

An essential improvement of the results in IP calculations has been achieved by replacement of the electron density in Eqn (2.7) by the sum of the densities of the electrons of isolated atoms which have, however, been taken from the calculation by the Hartree–Fock (HF) method [37–40, 51, 282]. Somewhat earlier, exactly the same calculations were carried out with the TFD densities [41, 42]. In Refs [38–40, 51] a contribution due to the correlation energy of the electron gas was added to the energy functional. A corresponding value per unit volume is approximated by the expression [38]:

$$g_{\rm cor}(\rho)$$

$$= \begin{cases} \left[-0.048 - 0.01r_{s} + \ln r_{s}(0.0311 + 0.009r_{s})\right]\rho \\ r_{s} < 0.7 \\ (0.07064 + 0.00633 \ln \rho)\rho, \\ 0.7 \le r_{s} \le 10, \\ (-0.438r_{s}^{-1} + 1.325r_{s}^{-3/2}s - 1.47r_{s}^{-2}s - 0.4r_{s}^{-5/2})\rho, \\ r_{s} > 10 . \end{cases}$$

$$(2.16)$$

In addition to the assumption concerning additivity, the electron atomic densities are assumed to be spherically symmetric, which enables us to carry out the integration with respect to all angular variables in Eqn (2.7). For convenience, the resulting IP can be decomposed into several terms:

$$V(R) = V_{\rm C}(R) + V_{\rm kin}(R) + V_{\rm exch}(R) + V_{\rm cor}(R)$$
, (2.17)

where separate terms correspond to the contributions of the Coulomb, kinetic, exchange, and correlation energies. It is appropriate to write the formula for $V_C(R)$ in the form that takes into account arbitrary degrees of ionisation of the interacting particles [22, 43] ($q_i = 1 - N_i/Z_i$, i = 1, 2):

$$V_{\rm K}(R) = \frac{q_1 q_2 Z_1 Z_2}{R} + \frac{1}{2} Z_1 (1 + q_1) G_2(R) + \frac{1}{2} Z_2 (1 + q_2) G_1(R) - \frac{1}{2} \int [G_1(r_1) \rho_2(r_2) + G_2(r_2) \rho_1(r_1)] d^3 \mathbf{r}, (2.18)$$

where the function $G_i(r_i)$ is linked with the electrical potential of the electrons $V_{ei}(r_i)$ by the following relation:

$$G_i(r) = \frac{N_i}{r} + V_{ei}(r) .$$
 (2.19)

In the case of a spherical symmetry of $\rho_i(r)$, the potentials $V_{\rm ei}(r)$ reduce to single integrals:

$$V_{\rm ci}(r) = -\int \frac{\rho_i(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}^3 r' = -\frac{4\pi}{r} \int_0^r r'^2 \rho_i(r') \, \mathrm{d}r' - 4\pi \int_r^\infty r' \rho(r') \, \mathrm{d}r' \,.$$
(2.20)

Formulas (2.18)-(2.20) are especially convenient when integration in Eqn (2.20) can be carried out analytically. When we substitute numerical densities for $V_C(R)$, it is appropriate to employ a formula that combines all the contributions in one double integral [38]:

$$V_{\rm C}(R) = (4\pi)^2 \int_0^\infty r_1^2 \,\mathrm{d}r_1 \int_0^\infty r_2^2 \,\mathrm{d}r_2 \rho_1(r_1) \,\rho_2(r_2) \,I(R, r_1, r_2) , \qquad (2.21)$$

where the function $I(R, r_1, r_2)$ is calculated separately for the homoatomic, heteroatomic, and ion pairs. In particular, in the heteroatomic case we have [38]:

$$I(R, r_1, r_2) = \frac{1}{R} - \frac{2}{|R - r_1| + R + r_1} - \frac{2}{|R - r_2| + R + r_2} + F(R, r_1, r_2) , \quad (2.22)$$

 $F(R, r_1, r_2)$

$$= \begin{cases} \frac{2}{|R-r_1|+R+r_1}, & r_2 < |R-r_1|, \\ \frac{1}{2}\left(\frac{1}{r_1}+\frac{1}{r_2}\right) - \frac{R}{4r_1r_2} - \frac{(r_1-r_2)^2}{4Rr_1r_2}, \\ |R-r_1| < r_2 < R+r_1, \\ \frac{1}{r_2}, & r_2 > R+r_1. \end{cases}$$
(2.23)

In its analytical form, the integral (2.21) can be calculated for a class of the Gauss or Slater orbitals, with all the other terms in Eqn (2.17) being computed numerically. All of them are presented in a single-type form,

$$J = \int [g_t(\rho_1 + \rho_2) - g_t(\rho_1) - g_t(\rho_2)] d^3 r , \qquad (2.24)$$

and are calculated with respect to an ellipsoidal coordinate system. Here $g_t(\rho)$ is the density of the corresponding energy of the electron gas. In Ref. [43] it is shown that for the power form of $g_t(\rho)$ all the contributions to the potential are calculated in elementary functions if the electron density is approximated in a piecewise-exponential form [44]:

$$\rho(r) = \sum_{i=1}^{N} A_i \exp(-a_i r) \left[\theta(r - r_{i-1}) - \theta(r - r_i) \right], \quad (2.25)$$



 $D(r) = 4\pi r^2 \rho(r)$: Hartree-Fock (1); formula (2.25) (2); TFD (3).

where A_i and a_i are parameters, r_{i-1} , r_i are radii of the 'subshells', $\theta(x)$ is a unity step function, and N is the number of 'subshells'. In Ref. [44] it is established that the logarithm of the atomic electron density that corresponds to the HF method, inside the shells, varies almost linearly and therefore in its simplest form the sum given by Eqn (2.25) may consist of several terms. Such a model was constructed in Refs [45, 46], and in Ref. [47] where tables of the parameters for the atoms and ions with $2 < Z \leq 54$ are cited. In calculations, the values for the occupation numbers and the 'subshell' radii calculated by the HF method were taken into account. In Fig. 1 the radial density of the electrons in the Ar atom, which corresponds to Eqn (2.25) for N = 3 [47], as well as the TFD and the Hartree-Fock distributions are shown. It follows from the figure that even for small N the shell structure can be approximated sufficiently well. If necessary, the accuracy can be increased by adjusting Eqn (2.25) for the nodes of the tabulated densities. In solids it is appropriate to take into account the influence of the chemical bonds on the electron distributions. For more details on this aspect see Ref. [326].

Evaluation of the integral (2.24) in Ref. [43] is carried out by the division of the space into domains $\rho_1 > \rho_2$ and $\rho_2 > \rho_1$, with a subsequent series expansion of integrands. The formulas for the IP that were obtained are cited in Refs [43, 46] and have a form sufficiently compact for calculations. This enables us to reduce considerably the time of computation of the potential and eliminates the need for interpolating tabulated densities. In addition, the tables given in Ref. [47] can be used for calculating the potentials in the ion-atom systems, for which there are no quantummechanical electron densities.

The IP in Ref. [48] is expressed by a derivative of the screening function:

$$\frac{\mathrm{d}\boldsymbol{\Phi}}{\mathrm{d}\boldsymbol{r}} = \frac{1}{Z_1 Z_2} \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{r}} \left[\boldsymbol{r} \boldsymbol{V}(\boldsymbol{r}) \right] \,. \tag{2.26}$$

Taking into account Eqns (2.18) and (2.24), the function $\Phi'(r)$ is reduced to a single integral [48], and the IP is calculated with the formula:

$$V(R) = \frac{Z_1 Z_2}{R} \left[1 + \int_0^R \Phi'(r) \, \mathrm{d}r \right] \,. \tag{2.27}$$

Calculations of the potentials based on the method given by Ref. [38] for a great number of atom-atom pairs were carried out in Refs [49, 50]. To facilitate subsequent applications, these results were approximated by a universal screening function obtained by averaging all the calculated potentials [49]:

$$\boldsymbol{\Phi}\left(\frac{R}{a}\right) = \sum_{i=1}^{3} c_i \exp\left(-b_i \frac{R}{a}\right), \qquad (2.28)$$

$$a = 0.8853(Z_1^{1/2} + Z_2^{1/2})^{-2/3} . (2.29)$$

In Ref. [50] an approximation of $\Phi(x)$ was obtained by four exponents, and the screening parameter was modified to the form

$$a = 0.8853(Z_1^{0.23} + Z_2^{0.23}) . (2.30)$$

The contribution of the exchange-correlation energy in Ref. [50a] was calculated separately and presented by the formula $Z = \max(Z_1, Z_2)$

$$\Phi_{\text{exch-cor}}(x) = -0.07Z^{-2/3} \exp(-0.235x^{-2} -0.0738x + 0.0178x^2) . (2.31)$$

In Table 2 a comparison is made between the potentials Ar-Ar calculated with the formulas (2.28)–(2.31) and the corresponding estimations in Refs [38, 44]. As expected, the potentials [38, 44] are in sufficient agreement with each other, but differ noticeably from the 'average' IP [49, 50] which features considerable dispersion. Still greater deviations are obtained for an ion-atom system (see Fig. 2 for the Li⁺-Ne potential). It should be noted that estimation of the exchange energy by means of the screening function [Eqn (2.31)] for the Ar-Ar potential gives very poor results and even for R = 3 the potential becomes negative. An electron gas model is also helpful for predicting the behaviour of the potential curves near the minimum. This is confirmed by the data in Table 3.

Table 2. Ar-Ar potential of interaction.

<i>R</i> /a.u.	V(R)/a.u.							
	Ref. [38]	Ref. [43]	Ref. [50a]	Ref. [49]	Ref. [50b]			
1	24.6	24.7	25.5	17.5	20.1			
2	2.30	2.35	2.91	1.85	1.84			
3	0.395	0.39	0.69	0.351	0.345			
4	0.0758	0.076	0.206	0.088	0.0638			

Note: The contribution of the exchange energy [Eqn (2.31)] is not taken into account in data estimation for the columns 4-6.

In Ref. [52] the relativistic corrections associated with the variance of the atomic electron densities and a modification of the expression for the kinetic energy (for the case of a Hg-Hg system) were taken into account. The data are presented in Table 3. These results show that taking account of the relativistic corrections becomes necessary in the case of heavy atoms. In this connection, note that calculations of the potential which were described in Ref. [50c], without taking into account these factors, are not correct. It is not clear in this case what kind of electron wave functions of the U atom were used by the authors in



Figure 2. Li⁺-Ne interaction potentials: Ref. [38] (solid line); Ref. [43] (dashed line); Ref. [49] (dotted line).

Table 3. The parameters of diatomic molecules.

Molecule	Energy of coupling/	Energy of coupling/10 ⁻¹⁴ erg		Equilibrium distance/A		
	1	2	1	2		
Ne-Ne	0.56	0.63	2.99	3.03		
Ar-Ar	1.75	1.95	3.63	3.70		
Kr-Kr	2.48	2.73	3.89	3.95		
Ne-Ar	0.785	0.93	3.42	3.51		
Ar-Kr	2.03	2.37	3.78	3.80		
Na^+-Cl^-	852	896	2.34	2.36		
K ⁺ -Cl ⁻	798	800	2.56	2.66		
Hg-Hg	5.58	12.2	4.12	4.19		

Note: I—the calculations of Ref. [38]; 2—the experimental data that are cited in Ref. [38]; *the data for Hg–Hg are taken from Ref. [52] (in this case I and 2 are the computations in the nonrelativistic and relativistic approximations).

the method in Ref. [38]. Reference to the calculation of the potential in Ref. [38] is not correct because it has not been carried out there.

It follows from the data in Table 3 that for the light systems the coupling energy of the inert gas molecules is underestimated by 10% - 15% with respect to the experimental values. In this connection, one can think about the possibility of 'improvement' of the IP computation results by introducing the Kirzhnits correction [Eqn (2.13)] into functional (2.7). However, its introduction leads to a dramatic deterioration of the potentials because, as can be seen from Section 2.2, a correction due to the non-homogeneity is approximately $(2/9)U_{exch}$, whereas its value and sign are close to U_{cor} . Taking into account a similar correction of the fourth order provides a negative con-

tribution as well. As a result, the values for the binding energy will increase by a factor of 1.5 to 3 and will considerably exceed the experimental values. Some qualitative justification of this result follows from the decreased degree of nonhomogeneity of the electron gas in the molecular system. Therefore, the corresponding corrections are not as essential as in the case of atoms, where due account for them has led to a conformity of the computed energies with the HF method to within a fraction of a percent [53, 54].

2.4 Rules for combination of potentials

The search for combinational relations for the potentials is supported by the idea that, if we find them, we could dispense with the need for calculating the potentials in heteroatomic pairs, thus dramatically cutting the computation time. Similar combinational relations have already been considered in the early works dedicated to a systematic study of the potentials [55]. The simplest of these are the rules of arithmetic and geometric averaging:

$$V_{\rm AB}(R) = \frac{1}{2} \left[V_{\rm AA}(R) + V_{\rm BB}(R) \right] \,, \tag{2.32}$$

$$V_{\rm AB}(R) = \sqrt{V_{\rm AA}(R)V_{\rm BB}(R)}$$
, (2.33)

where $V_{AA}(R)$, $V_{BB}(R)$, and $V_{AB}(R)$ are the corresponding IP for the homoatomic and heteroatomic combinations. Verification of the relations (2.32) and (2.33), which made use of known theoretical and experimental potentials, is provided in Refs [56, 57]. The rules for combining the long-range potentials were discussed in Refs [58, 59, 76, 77], while those for combining the sum of the short- and long-range potentials were considered in Refs [60–62]. In Ref. [57] the formula (2.32) was modernised by taking into account the difference in the size of the interacting particles:

$$V_{\rm AB}(R) = \frac{1}{2} \left\{ V_{\rm AA}(2r_{\rm A}) + V_{\rm BB}[2(R - r_{\rm A})] \right\}, \qquad (2.34)$$

where the radius of the atom A is determined by searching for an extremum:

$$\frac{\partial V_{AB}(r_A, R)}{\partial r_A} = 0 . (2.35)$$

Calculations that have been carried out in Ref. [57], with the use of formula (2.34) and the Hartree-Fock potential for the inert gases, have shown that the results obtained agree with the exact values of the IP better than the results obtained with relations (2.32) and (2.33). A more detailed analysis of these dependences is carried out in Ref. [63], in which one more combinational rule is proposed:

$$V_{\rm AB}(R) = \frac{1}{2} \left[V_{\rm AA} \left(\frac{2r_{\rm A}R}{r_{\rm A} + r_{\rm B}} \right) + V_{\rm BB} \left(\frac{2r_{\rm B}R}{r_{\rm A} + r_{\rm B}} \right) \right], \quad (2.36)$$

where $r_{A, B}$ are the atom radii according to Pauling [64]. The comparison of the combination formulas (2.32)–(2.36) was made through utilisation of the IP calculated by the electron gas method [63]. Fig. 3 shows the results of such a calculation for the Na⁺-Cl⁻ system, and these results show us that Eqn (2.36) is preferable. Roughly the same results were also obtained for the other ion pairs with widely varying values of the radii [63]. On the contrary, if $r_A \approx r_B$ all the combinational relations give similar results.



Figure 3. The Na⁺-Cl⁻ IP calculated by applying the combinational rules: exact calculation with the electron gas model (solid line); Eqn (2.33) (curve 1); Eqn (2.34) (curve 2); Eqn 2.32 (curve 3); Eqn (2.36) (curve 4).

The method for the separate combination of the separate parts of the potential [Eqn (2.17)] with constant signs is worth considering, since even in the existing form the combination rules are applicable both in the region of repulsion, and (to a greater extent) in the region of attraction. It is evident then that the first term [see Eqn (2.18)] does not require the combination, but the subsequent terms, as well as the potentials $V_{kin}(R)$, $V_{\text{exch}}(R)$, $V_{\text{cor}}(R)$ in Eqn (2.17) can be considered separately as having different signs. Among recent works, Refs [77] and [103] where some new heuristic relations are proposed above all are worth mentioning, connecting the IP with the electron densities of the interacting atoms [77], and with the repulsive forces [103]. In Ref. [334] a universal relation for the repulsive part of the IP of the form $V(R) = r_0 V^*(R/\rho)$ is proposed, where $V^*(x)$ is a universal function, and v_0 and ρ are parameters that correspond to a given atomic pair. In the paper cited, extensive information was used concerning the IP, obtained from the measurements of mobilities of the atoms and ions in gases (see also Refs [297] and the relevant literature). On the whole, in spite of the steady interest in the problem, the problem of justifying the combinational rules suitable for a wide range of interatomic distances and for arbitrary atomic combinations is far from being settled.

2.5 Analytical approximations

In calculations concerning radiation physics, repulsive potentials of the form proposed for the first time by Firsov [65] are most frequently used :

$$V(R) = \frac{Z_1 Z_2}{R} \Phi\left(\frac{R}{a}\right), \qquad (2.37)$$

where $\Phi(x)$ is a screening function, and the parameter (screening length) a is determined by Eqn (2.29). Based on the bilateral variational principles of the TF theory (see Section 2.2), Firsov showed that, within the accuracy range of the TF model, the function $\Phi(x)$ coincides with the solution to the TF equation for an isolated atom. Because of the slow decrease of $\Phi(x)$ for a large R, the potential given by Eqn (2.37) is suitable only if R < 2 a.u. A more precise description of the potential curve for R > 2 a.u. is achieved by means of an exponential approximation of the type given by Eqn (2.28). Moliere [66] was the first to calculate coefficients of this approximation, and the corresponding potential [Eqn (2.37)] was called the Firsov-Moliere potential. Another expression, originally proposed by Lindhard [67], is also frequently employed in calculations for the screening parameter:

$$a = 0.8853(Z_1^{2/3} + Z_2^{2/3})^{-0.5} . (2.38)$$

Approximations similar to Eqn (2.28) and based on the variational solution to the TF equation are obtained in Refs [68, 69], where the function $\Phi(x)$ is represented in the form:

$$\boldsymbol{\Phi}(x) = \left[a \exp(-\alpha x) + b \exp(-\beta x) + c \exp(-\gamma x)\right]^2. (2.39)$$

Formula (2.39) is suitable for computation of the halfinteger powers $\Phi^{n+1/2}$. Parameters for formulas (2.28) and (2.39), which present results of the different authors [49, 50, 68-70], are summarised in Table 4.

Two-exponential approximation parameters [72], the authors claim, are suitable for light atoms with Z < 18. Calculations of the IP of the atoms of inert gases based on Eqns (2.37) and (2.39) have shown [69] that the approximation (2.39) with c = 0 for Z < 18 is in better agreement with the values of the potential obtained experimentally, whereas the complete formula (2.39) is preferable for Z < 18. This result, along with similar conclusions reached in Ref. [72], demonstrates that although the average screening functions given in Refs [49] and [50] are obtained on the basis of a large number of reliable IPs they are not very accurate for calculations of the potentials for arbitrary atomic pairs (also see the data in Table 2).

Table 4. Approximation parameters of the screening function.

Some of the other frequently used approximations include the following: the Lentz-Jensen formula [22],

$$\Phi(x) = (1 + 3.11x^{1/2} + 3.24x + 1.46x^{3/2} + 0.248x^2) \exp(-3.11\sqrt{x}) ; \quad (2.40)$$

the Lindhard formula [70],

$$\Phi(x) = 1 - \left(1 + \frac{3}{x^2}\right)^{-1/2}; \qquad (2.41)$$

the Tietz formula [71],

$$\Phi(x) = \frac{1}{\left(1 + 0.5365x\right)^2};$$
(2.42)

the Firsov formula [25],

$$\Phi(x) = \frac{\sinh^2(\beta c)}{\sinh^2[\beta(c+x)]}, \quad c = 1.76(1 - 1.5\beta^2),$$

$$\beta^2 = 0.16Z^{-2/3}. \quad (2.43)$$

Formula (2.43) presents an approximate solution to the TFD equation (2.11) for a neutral atom. In Ref. [73] on the basis of Eqn (2.37) and the Hartree-Fock-Slater atomic potentials, an IP screening function for the homoatomic pairs was obtained in the form of

$$\boldsymbol{\Phi}(r) = \left\{ H\left[\exp\left(\alpha \frac{r}{r_s}\right) - 1 \right] + 1 \right\}^{-1}, \qquad (2.44)$$

where $H = (4Z - 1)^{0.4} r_s$, $\alpha = 1$ for $Z \le 10$ and $\alpha = 1.13$ for Z > 10, parameters r_s are tabulated as functions of Z. For the heteroatomic pairs in Ref. [74], modifications of the parameters H, r_s of the following form were proposed:

$$H = \left[\left(\sqrt{Z_1} + \sqrt{Z_2} \right)^2 - 1 \right]^{0.4} r'_s ,$$

$$r'_s = \frac{r_s(Z_1) + r_s(Z_2)}{2} ,$$
 (2.45)

where the parameters $r_s(Z_{1,2})$ correspond to individual atoms. Formulas (2.44) essentially postulate new combinational rules, and their validity calls for justification. Therefore, even though Eqn (2.45) takes account of the effects of the shells in an approximate way, it is not likely to be helpful as a universal description of the potentials and, in particular, of the effects of the Z_1 -oscillations for the stopping powers (see Section 3.2 and Ref. [75]). It should also be noted that the model potentials [73] have been criticised for giving an incorrect idea of the asymptotic behaviour for $r \to \infty$ [29].

	R ef. [66]	Ref. [68]*	Ref. [69]*	Ref. [72]	Ref. [49]	Ref. [50a]	R ef. [50b]	Ref. [216]
<i>c</i> ₁	0.1	0.72183	0.52495	1/3	0.0069	0.09	0.18175	0.4841
<i>c</i> ₂	0.55	0.27817	0.43505	2/3	0.1669	0.61	0.50986	0.2829
<i>c</i> ₃	0.35	_	0.04	_	0.8262	0.30	0.2802	0.1589
с	_		_	_			0.02817	0.0741
b_1	6.0	0.17826	0.12062	0.854	0.1318	0.19	3.20	0.6573
b_2	1.2	1.75934	0.84795	0.492	0.3079	0.57	0.942	1.6224
b_3	0.30		6.7469		0.9168	2.0	0.429	0.2994
b	_	_		_	_	_	0.2016	4.4049

*Parameters c_i and b_i (i = 1, 2, 3) correspond to a, b, c and α, β, γ in Eqn (2.39).

Useful expressions for the screening function and the electron density of an ion with an arbitrary ionisation degree were obtained by preserving the coefficients of the exponential approximation of the function (2.28) and by modifying the screening parameter [107]:

$$a_* = 0.8853 N^{-1/3} \left(\frac{N}{Z}\right)^s, \qquad (2.46)$$

where s is an unknown variational parameter, and N is the number of electrons. The screening function of an ion, taking into account Eqn (2.46), is written in the form

$$\Phi_{\rm i}(r) = q + (1-q) \, \Phi\left(\frac{r}{a_*}\right) \,,$$
 (2.47)

where q = 1 - N/Z is the degree of ionisation, and $\Phi(x)$ is defined by Eqn (2.28). The electron density, if we take into account Eqn (2.47) and the Poisson equation, is given by

$$\rho_{\rm i}(r) = \frac{N}{4\pi r a_*^2} \sum_{i=1}^3 c_i b_i^2 \exp\left(-\frac{b_i r}{a_*}\right) \,. \tag{2.48}$$

Substituting Eqn (2.48) in the functional (2.7) (ignoring the exchange term), we get a formula for the ion energy (here the coefficients b_i , c_i correspond to those given in Ref. [68]):

$$E_s(s) = -1.13\sqrt{\pi} N^{4/3} \left[0.911 \left(Z - \frac{N}{2} \right) \left(\frac{N}{Z} \right)^{-s} + 0.345N \left(\frac{N}{Z} \right)^{-2s} - 0.325N \left(\frac{N}{Z} \right)^{-s} \right].$$

Minimising $E_s(s)$ with respect to the parameter s, we get

$$s = \frac{\ln(1.167Z/N - 0.167)}{\ln(Z/N)}, \quad Z = N.$$
 (2.49)

The dependence of s on N/Z is shown in Fig. 4.

Figure 4. Dependence of s on N/Z.

Some other analytical approximations of the IPs and screening functions of the neutral atoms can be found in Refs [321, 328-332]. One of the works, rarely cited today [321], should be mentioned here. This work contains sufficiently simple approximations of the Hartree-Fock electron densities of atoms for $1 < Z \leq 36$. The IP [98] is rather useful in applications:

$$V(R) = 0.45 Z_1 Z_2 \frac{a}{R^2} \,.$$

Using this IP, the authors of Refs [316, 317] successfully described the characteristic radiation Xe(M) that was induced in the channelling of Xe ions in copper, as well as the generation of defects due to this process.

2.6 Nonstationary theories

In the last few years progress in computer science has made possible the solution of the many-particle problems in atomic collision physics, based on the solution of the nonstationary equations of Schrodinger and Hartree-Fock [76-82, 279, 289]. Generally, the systems under consideration contained a small number of electrons (1 or 2), and all the calculations were based on an approximation of the rectilinear trajectories of the moving particles. With this approach to the problem, the calculation of the IP is irrelevant and the problem focuses on the description of time evolution of the electron subsystem. Systems with a larger number of electrons were studied within the framework of the time-dependent Thomas-Fermi theory (TTF), the hydrodynamic version of which is well known [83, 84]. Thus, in Ref. [85] a numerical solution to the TTF equations for the scattering of protons on argon atoms (for proton energies from 27.5 to 2.500 keV) has been obtained. In these cases, the approximation of the rectilinear trajectories has also been used. This last point is, however, not crucial. According to Refs [86, 87] the total energy of the system can be written as:

$$E = \frac{1}{2} \int (\nabla \varphi)^2 \rho(\mathbf{r}, t) \, \mathrm{d}^3 \mathbf{r} + \frac{1}{2} \int \int \frac{\rho(\mathbf{r}, t) \, \rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}^3 \mathbf{r} \, \mathrm{d}^3 \mathbf{r}' + \int V(\mathbf{r}, t) \, \rho(\mathbf{r}, t) \, \mathrm{d}^3 \mathbf{r} + \int G[\rho(\mathbf{r}, t)] \, \mathrm{d}^3 \mathbf{r} , \qquad (2.50)$$

where $V(\mathbf{r}, t)$ is the potential of the nuclei and external fields, the functional $G(\rho)$ includes the sum of the kinetic, exchange, and correlation energies of the electron gas, and $\varphi(\mathbf{r}, t)$ is the hydrodynamics potential of the electron velocities. Hydrodynamics equations are derived from Eqn (2.50) in a standard manner and have the following form [86]:

$$\frac{\partial\varphi}{\partial t} = \frac{1}{2} \left(\nabla\varphi\right)^2 + V(\boldsymbol{r},t) + \int \frac{\rho(\boldsymbol{r}',t)}{|\boldsymbol{r}-\boldsymbol{r}'|} \, \mathrm{d}^3\boldsymbol{r}' + \frac{\delta G}{\delta\rho} \,, \qquad (2.51)$$

$$\frac{\partial \rho}{\partial t} = -\nabla(\rho \nabla \varphi) , \qquad (2.52)$$

with the additional restriction $\partial \phi / \partial n = 0$, where *n* is a normal to the surface that confines the system volume. If we apply Eqn (2.50) to the case of atom-atom scattering, it is evident that, with known $\rho(\mathbf{r},t)$ and $\varphi(\mathbf{r},t)$ and after the subtraction of the energy of the isolated particles, this formula can be viewed as being suitable for a definition of the dynamic interatomic potential. In practice the solution to the system of equations (2.51)-(2.52) can be obtained by splitting it into small time intervals, within each of which the particle trajectories are rectilinear, and then, by calculating U(R,t) and solving dynamics equations for the nuclei (on the same time intervals), with subsequent correction of their positions and velocities before passing on to the next time step. Although in this case the potential cannot be specified outside the trajectory, its calculation remains an important stage in the solution of the dynamics problem and carries additional information on the energy losses of the interacting particles.

2.7 Velocity (energy)-dependent interatomic potentials of interaction

If the ion velocities are $v_1 \leq Z^{2/3}$, which are the typical average velocities of electrons in a TF atom, most of them are still sufficiently strongly bound to the nucleus. On the other hand, it is not difficult to show from Eqn (2.50) that for small variations of the electron density (in the absence of external fields) energy correction will appear only in the second order of the perturbation theory. This is confirmed, for example, by calculations of the time evolution of the function $\rho(\mathbf{r}, t)$ in the system H – Ar [85, 86]. This statement allows for the supposition that the main contribution to IP in the dynamic regime can be calculated in a quasistatic approximation of the electron gas. The idea of such an approach was first proposed in Ref. [48], where corresponding estimates of IP were worked out for the system H-H. The main idea consists in the isolation of the potential (and its modification) from the kinetic energy contribution [the third term in Eqn (2.7)]. It is evident that, for the motion of the atoms with relative velocity v_1 , Fermi spheres of the electrons shift a distance equal to $p_0 = m_e v_1 = v_1$ (see Fig. 5), whereas in a static case they would be concentric. As a result, the variation of the kinetic energy will occur only for those electrons which happen to be in the overlapping part of the Fermi distributions. These electrons, because to the Pauli exclusion principle, will increase their energy by shifting to the free cells of the momentum space. As a new quasiequilibrium electron distribution, in Ref. [48] a Fermi sphere with its centre located in the centre of mass of the system has been adopted, and an approximate estimate of the contribution of kinetic energy in IP has the form

$$V_{\rm kin}(R, E_1) \approx V_{\rm kin}(R) \exp(-0.004\varepsilon) , \qquad (2.53)$$

where $V_{\rm kin}(R)$ is a static value, and ε is the reduced energy defined by the relation

$$\varepsilon = \frac{E_1 a M_2}{Z_1 Z_2 (M_1 + M_2)} \,. \tag{2.54}$$

In this formula, E_1 is the energy of an incident atom with mass M_1 and atomic number Z_1 (M_2 and Z_2 correspond to the target atom), and *a* is a screening parameter given by Eqns (2.29) or (2.38). In Refs [88–92] this model is described in greater detail. It was mentioned in particular

Figure 5. Electron distribution in a volume element d^3R of the momentum space (according to Ref. [48]). On relaxation to the quasiequilibrium distribution with the centre $O_{c.m.}$ at the centre of mass, half the electrons that occupied region A pass to region B.

that for the atoms with a large number of electrons, only a few of them contribute to the formation of the quasimolecular orbitals localised at the centre of mass of the system, with the rest remaining bound to their respective nuclei. Therefore, some other way of calculating the kinetic energy variation should be found, where the centre of a new quasi-equilibrium distribution will match the centres of the initial ones. Let us consider this problem in more detail, following Refs [89, 91].

Let us assume that each atom has a homogeneous distribution of electron density $\rho_{1,2}$, and let us further assume for clarity that $\rho_1 > \rho_2$. Then under quasi-equilibrium conditions the electron distributions in momentum space are Fermi spheres with radii $p_i = (3\pi^2 \rho_i)^{1/3}$, as in the TF theory $\rho_i = p_i^3/3\pi^2$. For the problems of radiation physics, one atom can always be considered as being at rest, and the other as having a velocity of v_1 . If $v_1 \neq 0$, several cases of overlapping for the Fermi distributions shown in Fig. 6 are possible. Even in Fig. 6, it is clear that for $v_1 = p_0 > p_1 + p_2$ there are no variations of kinetic energy of the system (this is also true for the exchange and correlation energies), therefore the potential will include only the Coulomb part [see Eqn (2.17)]. For $p_0 < p_1 + p_2$ the overlapping changes from partial to total. Half the electrons that occupy the overlapping domain should occupy the cells with large values of momenta. The new quasi-equilibrium distributions are shown by a dotted line, and their centres coincide with the centre of the larger sphere because of the minimum energy principle. In cases (a) and (b), a new value for the 'quasi-equilibrium' radius can be determined according to the formula

$$p_{\rm m} = (p_1^3 + p_2^3)^{1/3} ,$$
 (2.56)

which expresses the conservation of the volume of p-space. In the above examples it is not difficult to find the variations of the kinetic and exchange energies. Assuming that the overlapping volume is equal to Ω , the variation of

Figure 6. The same as Fig. 5, but in accordance with Ref. [90]. The dotted lines correspond to quasi-equilibrium distributions of the electrons that were initially located in the shaded domain.

Figure 7. Coordinate system used in the evaluation of the integral (2.58).

the kinetic energy of the electrons which have occupied the Fermi sphere of radius $p_{\rm m}$, can be written as

$$V_{\rm kin} = \frac{2\Omega}{(2\pi)^3} \left[\int_0^{p_{\rm m}} \frac{p^2}{2} 4\pi p^2 \, \mathrm{d}p - \int_0^{p_1} \frac{p^2}{2} 4\pi p^2 \, \mathrm{d}p - \int_{D(p_2)} \frac{p'^2}{2} \, \mathrm{d}^3 p' \right], (2.57)$$

where $D(p_2)$ is the volume of the domain of overlapping for the **p**-space. The first two integrals in Eqn (2.57) are elementary, and the third one can be easily calculated in cylindrical coordinates with the origin in the centre of the smaller sphere (see Fig. 7). From Fig. 7 it can be seen that this integral in Eqn (2.57) is presented in the form

$$\int_{D(p_2)} \frac{p'^2}{2} d^3 p' = \pi \int_0^{p_2} dz \int_0^{\sqrt{p_2^2 - z^2}} r dr [2r^2 + (p_0 - z)^2 + (p_0 + z)^2] = \frac{2\pi}{3} p_0^2 p_2^3 .$$
(2.58)

Substituting Eqn (2.58) in Eqn (2.57), we get

$$V_{\rm kin} = \Omega \left(\frac{p_{\rm m}^5}{10\pi^2} - \frac{p_1^5}{10\pi^2} - \frac{p_2^5}{10\pi^2} - \frac{p_0^2 p_2^3}{6\pi^2} \right) \,. \tag{2.59}$$

The first three terms in Eqn (2.59) correspond to the static result, while the last one is equal to the kinetic energy of the relative motion of the electrons of the second atom, which entered the domain Ω since $\rho_2 = p_2^3/3\pi^2$. Converting p_1 and p_2 to the densities ρ_1 and ρ_2 , we can write Eqn (2.59) in the form

$$V_{\rm kin} = \frac{3}{10} (3\pi^2)^{2/3} \Omega \left[(\rho_1 + \rho_2)^{5/3} - \rho_1^{5/3} - \rho_2^{5/3} - 0.5v_1^2 \rho_2 \right] .$$
(2.60)

The first term in Eqn (2.60) reflects additivity of the electron densities in the domain of overlapping, which is evidently a consequence of the Pauli exclusion principle and the minimum energy principle.

When we turn to nonhomogeneous electron distributions in the atoms, Eqn (2.60) is to be considered as a local relation in the volume d^3r , where $\rho_1 > \rho_2$. The domains $\rho_2 > \rho_1$ are to be taken into account in exactly the same way, with the substitution of $\rho_1 \rightleftharpoons \rho_2$ in Eqn (2.60). Thus in the final form the contribution of kinetic energy to the potential will have the form

$$V_{\rm kin}(R, v_1) = \frac{3}{10} (3\pi^2)^{2/3} \left(\int \left\{ \left[\rho_1(r_1) + \rho_2(r_2) \right]^{5/3} - \rho_1(r_1)^{5/3} - \rho_2(r_2)^{5/3} - \frac{v_1^2}{2} \rho_2(r_2) \right\} \\ \times \theta(\rho_1 - \rho_2) \, \mathrm{d}^3 r + \int \left\{ \left[\rho_1(r_1) + \rho_2(r_2) \right]^{5/3} - \rho_1(r_1)^{5/3} - \rho_2(r_2)^{5/3} - \frac{v_1^2}{2} \rho_1(r_1) \right\} \\ \times \theta(\rho_2 - \rho_1) \, \mathrm{d}^3 r \right).$$
(2.61)

The exchange energy contribution can be calculated in a similar way, considering that its density in unit volume of the configuration space is $-p/\pi$. Finally for the cases (a) and (b) in Fig. 6 we get:

$$V_{\rm ob} = -\Omega \left[\frac{p_{\rm m}^4 - p_1^4}{4\pi^2} - \frac{1}{6\pi^3} \left(2p_0 p_2^3 + 0.4 \frac{p_2^3}{p_0} \right) \theta(p_0 - p_2) - \frac{1}{6\pi^3} \left(\frac{3}{2} p_2^4 + p_2^2 p_0^2 - 0.1 p_0^4 \right) \theta(p_2 - p_0) \right].$$
(2.62)

When we convert from Eqn (2.62) to the volume integral, as in (2.61), this formula should be supplemented with the symmetric terms with the substitution $p_1 \neq p_2$, since Eqn (2.62) pertains only to the domain $\rho_1 > \rho_2$.

With a partial overlapping of the Fermi spheres, the corresponding formulas are also elementary, although more awkward [89, 91]. The radius $p_{\rm m}$ can also be found from a more complex algebraic equation. Since in the TF model the average electron velocity is $1.2Z^{2/3}$, the condition for the IP to become a Coulomb potential can be written in the form:

$$E_1 > E_{\rm cr} = 0.036A_1 (Z_1^{2/3} + Z_2^{2/3})^2 \text{ MeV},$$
 (2.63)

Figure 8. Energy dependence of the screening function of the Ar–Ar IP [90b]: $E = \infty$ (curve 1); E = 10 MeV (curve 2); E = 1 MeV (curve 3); E = 0.1 MeV (curve 4); E = 0 (curve 5).

where A_1 is the mass number of the incident atom. For instance, for Ar-Ar collisions we will get E = 290 MeV. In Fig. 8 the results of calculations of the screening function of the Ar-Ar potential are shown. These calculations were conducted for different energy values E. Electron and atomic densities corresponded to those of the TF model in the approximation [68]. The kinetic energy was calculated in accordance with Eqn (2.61). Fig. 8 shows us that the dynamic effect appears even at $E_1 = 1$ MeV and manifests itself in the region of medium and large interatomic distances. Let us note that Eqn (2.61) somewhat overestimates the value of V_{kin} because it corresponds to the total overlapping of the Fermi spheres. Its correction can be achieved by multiplying those terms in Eqns (2.59) and (2.56) that depend upon p_2 by the coefficient 1/2 [the same is true with respect to Eqn (2.62)].

Variation in the contribution of exchange energy in the total potential is not very noticeable and, as one can see from the numerical results, consists of an extra rise in IP. With p_0 not too small, the second term in Eqn (2.62) is most important, while with small p_0 and large internuclear spacings the main role will be played by the first and third terms.

The theory considered above refers to the case of a weak ionisation of the first particle. With the atom moving in the medium at velocities of ~ $Z^{2/3}$, a significant part of its shell is stripped even at small depths, so the actual degree of ionisation which tends to grow with the growth of velocity should be taken into account in the IP calculation. This factor was taken into account in Ref. [91]. An assumption was also made there that the degree of ionisation corresponds to the equilibrium charge that an ion obtains in a medium. In Fig. 9 the results of calculating the IP for the homonuclear pairs at different velocities are shown. The data on contribution of the kinetic and Coulomb energies (Figs 9a and 9b) and the total potential are presented separately (Fig. 9c). Taking into account Eqn (2.28), the degree of ionisation is equal to

$$q = 1 - \frac{N}{Z} = 1 - \frac{1}{Z} \int_0^{R_1} 4\pi r^2 \rho_1(r_1) dr$$
$$= \sum_{i=1}^3 c_i (1 + b_i x_0) \exp(-b_i x_0) , \qquad (2.64)$$

where $x_0 = 1.13R_1Z^{2/3}$, and R_1 is found from the equation

$$\rho_1(R_1) = \frac{v_1^3}{3\pi^2} \,. \tag{2.65}$$

Formulas (2.64) and (2.65) correspond to the known Bohr stripping criterion, and the factors c_i and b_i are taken from Ref. [68]. From Fig. 9 it follows that a dynamic decrease of the IP occurs at any R if $x_0 > 3$, which corresponds to q < 2/3. The effect is most pronounced at x > 6. Growth of the potential at x < 6 is due to complete depletion of the electron shell of an ion and an increase of the Coulomb interaction. Comparison with the IP calculation for the effect of diminishing of the potential is more evident and takes place at any value of R. If $R \rightarrow 0$, dynamic effects are insignificant, because all the potentials are close to Z_1Z_2/R . For $R > 2R_1$ formula (2.61) can be written in a simpler form,

$$V_{\rm kin}(R, v_1) = V_{\rm kin}^{\rm st}(R) - 0.5v_1^2 \tilde{N}_2 , \qquad (2.66)$$

Figure 9. The universal ion – atom IP of the homonuclear pairs in the quasistatic TF approximation taking into account a degree of ionisation [90c]. Ion 'reduced radius' x_0 is linked with its velocity of movement by relation (2.65): (a) the electrostatic interaction contribution; (b) the kinetic energy contribution; (c) the total IP $(x = 1.13Z^{1/3}R);$ $x_0 = \infty$ (curve 1); $x_0 = 5$ (curve 2); $x_0 = 3.5$ (curve 3); $x_0 = 2$ (curve 4).

where V_{kin}^{st} is a static value of the potential, and \tilde{N}_2 is the number of electrons of the target atom that exist in the electron cloud of an ion (of radius R_1). Thus, in that case a dynamic correction is proportional to the kinetic energy of the particle. This result is not unexpected: a correction,

proportional to the energy, to the long-range potential of interaction of an electron with a hydrogen atom, was obtained in [93], and still earlier a similar result was found by Gombas [22] within the framework of the statistical electron theory and is, in principle, at the foundation of the pseudo-potential theory. Thus Eqn (2.66) may be regarded as a generalisation of these results to an ion-atom potential.

In Refs [89, 90] the authors used the terminology of the 'velocity-dependent' interatomic potentials. In that case, a rigorous solution of a two-body problem could be obtained with standard methods of classical mechanics. As can be deduced from the results of this Section, however, the effects mentioned here become significant at velocities of the order of $Z^{2/3}$ and are best evident for intermediate and large internuclear distances. In this case, the processes of stopping and scattering at large angles are not sensitive to variations of the potential, as they are defined by its Coulomb asymptotics. Therefore for the practical use of such potentials, the processes of scattering at small angles and channelling might be most suitable when the particle energy (and velocity) is constant in the first approximation. Under these circumstances it is more appropriate to talk about potentials that are parametric energy (velocity) dependent.

3. Interaction of charged particles with solids

The question of the impact of the properties of a solid on the atomic collision processes is a very complicated one. This is in spite of the significant progress made in this area recently. Of primary importance for the subject matter of this review are the classical characteristics of particle motion, when their calculation relies on the application of interatomic and averaged potentials. Some related questions that are beyond the scope of these approximations are considered more briefly.

3.1 Differential cross sections of the ion-atom scattering For most of the ion-atom interactions in matter (except the scattering of H on H₂, He), quantum effects are insignificant, and hence a classical description can be used. In this case, basic relations of the theory and their links with the experimental values are well known [95–97]. Therefore let us consider some practical methods of calculation of the angles and cross sections which are used in radiation physics.

A standard classical expression for the scattering angle in the centre-of-mass system (CMS) has the form [95]:

$$\theta = \pi - 2 \int_{r_{\rm m}}^{\infty} \frac{b^2/r^2}{\left[1 - b^2/r^2 - V(r)/E\right]^{1/2}} \, \mathrm{d}r \,, \tag{3.1}$$

where b is the impact parameter, E is a relative energy of collision, $r_{\rm m}$ is the distance of maximal approach that can be determined from the equation

$$1 - \frac{b^2}{r_{\rm m}^2} - \frac{V(r_{\rm m})}{E} = 0$$
.

In order to eliminate divergence of the integrand in Eqn (3.1), the transformation given in Ref. [98] is used:

$$p = \frac{Z_1 Z_2}{E}, \quad P = \frac{b}{p}, \quad \cos \alpha = \frac{r_{\rm m}}{r}, \quad H = \frac{r_{\rm m}}{p}, \quad (3.2)$$

Taking it into account, we can transform Eqn (3.1) to the form

$$\theta = \pi - \frac{2P}{H} \int_0^{\pi/2} \frac{\sin \alpha \, \mathrm{d}\alpha}{\left[1 - (P/H)^2 \cos^2 \alpha - \cos \alpha \Phi (Hp/\cos \alpha)/H\right]^{1/2}},$$
(3.3)

where $\Phi(x) = rV(r)/Z_1Z_2$ is the screening function of an IP. Typically the angle θ is small, therefore subtraction of two similar quantities in Eqn (3.3) causes large errors. To eliminate them, the transformation given in Ref. [99] is offered:

$$\theta = \pi - \frac{2P}{H} \left\{ \int_0^{\pi/2} y_0(\alpha) \, \mathrm{d}\alpha - \int_0^{\pi/2} \left[y_0(\alpha) - y(\alpha) \right] \, \mathrm{d}\alpha \right\}$$
$$= 2 \operatorname{arccot} \left[\frac{2P}{\boldsymbol{\Phi}(Hb)} \right] + \frac{2P}{H} \int_0^{\pi/2} \left[y_0(\alpha) - y(\alpha) \right] \, \mathrm{d}\alpha \,, \quad (3.4)$$

where

$$y_0(\alpha) = \frac{\sin \alpha}{\left[1 - (P/H)^2 \cos^2 \alpha - \cos \alpha \Phi(Hb)/H\right]^{1/2}}$$

and $y(\alpha)$ coincides with the integrand in Eqn (3.3). An integral in Eqn (3.4) is easy to calculate with the Simpson formula. For $\theta \ll 1$ a small-angle approximation [95] is also used:

$$\theta = -\frac{b}{E} \int_{b}^{\infty} \frac{\mathrm{d}V}{\mathrm{d}r} \frac{1}{\sqrt{r^2 - b^2}} \,\mathrm{d}r \,, \qquad (3.5)$$

it is advisable to calculate this integral using the Gauss-Christoffel quadrature formula [100]:

$$\int_{-1}^{1} \frac{f(x) \, \mathrm{d}x}{\sqrt{1 - x^2}} \approx \frac{\pi}{n} \sum_{i=1}^{n} f(x_i) \,, \quad x_i = \cos\left[\frac{\pi}{n} \left(i - \frac{1}{2}\right)\right] \,, \quad (3.6)$$

where f(x) is a function without singularities. Taking into account Eqns (3.5) and (3.6), we have

$$\theta E = -\frac{\pi}{2n} \sum_{i=1}^{n} r_i \left(\frac{\mathrm{d}V}{\mathrm{d}r}\right)_{r=r_i}, \quad r_i = b \left| \cos\left[\frac{\pi}{n} \left(i - \frac{1}{2}\right)\right] \right|^{-1}.$$
(3.7)

Usually even with n = 20-30, Eqn (3.7) guarantees high precision. Lindhard and coauthors [101] proposed a modification of Eqn (3.5) for large angles, using the representation of V(r) by means of a TF screening function. Then, taking into account Eqns (2.37), (2.54), and (3.5), we get

$$\varepsilon\theta = F\left(\frac{b}{a}\right)\,,\tag{3.8}$$

$$F(x) = -x \int_{x}^{\infty} \frac{\mathrm{d}}{\mathrm{d}y} \left[\frac{\boldsymbol{\Phi}(y)}{y} \right] \frac{\mathrm{d}y}{\sqrt{y^{2} - x^{2}}} \,. \tag{3.9}$$

Extrapolation of Eqn (3.8) to large angles consists in substitution of θ by $2\sin(\theta/2)$. Next we introduce a dimensionless scattering parameter $\sqrt{t} = \epsilon \sin(\theta/2)$, and obtain

$$\sqrt{t} = 0.5F\left(\frac{b}{a}\right). \tag{3.10}$$

Solution of Eqn (3.10) with respect to b/a will give us a universal relation,

$$b = a\Psi(\sqrt{t}) , \qquad (3.11)$$

where $\Psi(\sqrt{t})$ is the function that is inverse with respect to F(z). Taking into account Eqn (3.11), we present the scattering cross section as

$$d\sigma = 2\pi b \, db = \pi a^2 \, \frac{d}{dt} \left[\Psi^2(\sqrt{t}) \right] = \frac{\pi a^2}{2} \frac{f(\sqrt{t})}{t^{3/2}} \, dt \,, (3.12)$$

where $f(\sqrt{t})$ is a universal scattering function [101] which depends upon the potential through $\Phi(x)$. For the TF potential, the function $f(\sqrt{t})$ is approximated in the form [102a]:

$$f(\sqrt{t}) = \lambda t^{0.5-m} \left[1 + (2\lambda t^{1-m})^q \right]^{-1/q} , \qquad (3.13)$$

where $\lambda = 1.309$, q = 2/3, m = 1/3. For other screening functions, similar parameters are cited in Ref. [102b]. If the cross section is calculated based on an exact formula describing the scattering angle, then, setting Eqn (3.12) equal to $2\pi b \, db$ and taking into account the relation $t = \epsilon^2 \sin^2(\theta/2)$, we get the scattering function in a general form [103]:

$$f(\sqrt{t}, \varepsilon) = \frac{4\varepsilon}{a^2} b[\theta(t)] \left[\frac{\mathrm{d}b}{\mathrm{d}\theta} \tan \frac{\theta}{2} \sin \frac{\theta}{2}\right]_{\theta=\theta(t)}.$$
 (3.14)

Thus in the general case f depends not only upon the universal parameter t, but also upon the energy ε , where ε enters also $f(\sqrt{t}, \varepsilon)$ through b [104]. In Ref. [105] a 'magic' formula for $\theta(b)$ is proposed. This formula is convenient for simulation of ion transport in the medium with an error of about 1%. The corresponding code called TRIM (Transport of Ions in Matter) is widely used in radiation physics.

Comparison of some theoretical approximations for the scattering functions calculated with various potentials (screening functions) with and without a large angle approximation had been carried out in Ref. [104, 107]. In Fig. 10 the results of the computation are shown [104]. Curve 3 corresponds to Eqn (3.13), i.e. to the TF potential; curve 2 approximates the experimental results for the ranges [142]; curve 1 corresponds to the computation in the wide angle approximation for an average potential [49]; and the dashed curves to the exact computations with Eqn (3.14) for the same case. The points of the cut-off of the curves at the large t end correspond to the values of ε under consideration. As follows from Fig. 10, the form of the potentials used influences mainly the scattering function (compare curves 1 and 3). A large angle approximation leads to 5% – 10% deviations of $f(t^{1/2}, \varepsilon)$ with respect to $f(t^{1/2})$ when $\varepsilon > 10^{-2}$. The scattering functions for the energy-dependent potentials were calculated in Refs [106, 107]. In Fig. 11 the results of the computation [106] carried out by means of the wide angle approximation are shown. Curve 1 was plotted for the static potential, curve 2 for the 'bare' electrostatic one, and curve 3 for the velocity $v_1 = 0.24Z_1^{2/3}$ (a case of a homoatomic pair taking into account ionisation of a moving ion was under consideration). The parameters of the screening function (2.28) corresponded to those in Ref. [72]. Fig. 11 shows us that taking into account the energy dependence of an IP dramatically decreases the scattering cross sections at $\sqrt{t} < 1$, i.e. at middle to large internuclear distances.

Figure 10. The reduced scattering functions $f(\sqrt{t})$ corresponding to the various approximations and IP [104]: dashed lines — calculation of $f(\sqrt{t}, \varepsilon)$ by (3.14) for the IP [49] for different ε (values of $\sqrt{t} = \varepsilon$ at the curves' breaks correspond to the values of ε under consideration); 1, 2, 3 — calculation of $f(\sqrt{t})$ in the large angle approximation [1 — the [49] IP, 2 — the experimental data [142], 3 — according to the Formula (3.13)].

Figure 11. A scattering function for the velocity dependent IP of the homoatomic pairs [106]: the static IP (curve 1); the electrostatic IP (curve 2); for $v_1 = 0.24Z_1^{2/3}$, the ionisation being taken into account (curve 3); according to Eqn (3.13) (curve 4).

3.2 Elastic and inelastic energy losses and ion ranges in solids

Energy loss mechanisms of nonrelativistic ions in matter are most typically linked with elastic and inelastic effects. Fundamental stopping parameters are stopping losses per unit length and stopping cross sections S. For elastic scattering, by definition

$$\frac{\mathrm{d}E}{\mathrm{d}z} = NS_{\mathrm{n}} = N \int T \,\mathrm{d}\sigma \,, \qquad (3.15)$$

where $T = T_{\text{max}} \sin^2(\theta/2)$ is the energy transferred to a target atom in a single collision,

$$T_{\max} = 4M_1M_2 \frac{E}{(M_1 + M_2)^2}$$

is the maximum transferred energy, θ is the scattering angle in CMS, N is the density of the target atoms, and $d\sigma$ is the differential scattering cross section. The specific values of S_n are defined by the form of an interaction potential. After introduction of a dimensionless unit of a range [101]

$$\rho = 4\pi a^2 N z \; \frac{M_1 M_2}{\left(M_1 + M_2\right)^2} \,, \tag{3.16}$$

where z is the length of an ion range in matter (other variables have the usual meaning). Substitution of Eqn (3.12) in Eqn (3.15) and taking into account Eqn (2.54) will give us

$$\frac{\mathrm{d}E}{\mathrm{d}z} = NT_{\max} \frac{\pi a^2}{2} \frac{1}{\varepsilon^2} \int_0^{\varepsilon} \frac{f(\sqrt{t})}{\sqrt{t}} \,\mathrm{d}t$$
$$= \frac{4\pi M_1 Z_1 Z_2 a N}{(M_1 + M_2)} \frac{1}{\varepsilon} \int_0^{\varepsilon} f(x) \,\mathrm{d}x \qquad (3.17)$$

or, taking into account Eqn (3.16),

$$s_{\rm n}(\varepsilon) = \frac{\mathrm{d}\varepsilon}{\mathrm{d}\rho} = \frac{1}{\varepsilon} \int_0^\varepsilon f(x) \,\mathrm{d}x$$
 (3.18)

Eqn (3.18) has a general character regardless of whether a large angle approximation was used or not in order to define f(x). Recently in the calculation of ranges, the approximations of cross sections based on 'average potentials' have become widespread (see Refs [49, 50]):

$$s_{\rm n}(\varepsilon) = \frac{0.5\ln(1+\varepsilon)}{\varepsilon + 0.1412\varepsilon^{0.4206}},$$
 (3.19)

$$s_{\rm n}(\varepsilon) = \frac{0.5 \ln(1 + 1.383\varepsilon)}{\varepsilon + 0.0132\varepsilon^{0.2123} + 0.19594\varepsilon^{0.5}} \,. \tag{3.20}$$

Both Eqns (3.19) and (3.20) satisfy the passage to the limit for $\varepsilon \ge 1$, when a cross section becomes the Rutherford cross section. In this case, it is not difficult to show that the exact result is $s_n = 0.5 \ln \varepsilon/\varepsilon$.

A cross section of electron (inelastic) stopping S_e is defined by

$$\frac{\mathrm{d}E}{\mathrm{d}z} = NS_{\mathrm{e}} \ . \tag{3.21}$$

The theory of electron stopping power has not yet taken its final form, despite a large number of existing approximations. Numerous reviews and monographs have been written on the various aspects of the subject [75, 108–112], therefore we shall restrict ourselves to the analysis of only some recent results. For the velocities $v_1 > Z_2v_0$, the basic approximation is the Bethe-Meller-Bloch theory [22, 75], where $S_e \propto v_1^{-2}$. For $v_1 < Z_1^{2/3}v_0$, mostly $S_e \propto v_1$, but in the case $v_F < v_1 < Z_1^{2/3}v_0$, where v_F is the Fermi velocity, the domain of the quadratic dependence $S_e \propto v_1^2$ also exists [110, 111]. S_e theory in the domain of the maximum for the case of light particles was considered in Ref. [211]. For $S_e \propto v_1$ two approaches are generally accepted: the Firsov model [113] (which treats stopping as a sequence of individual acts of the ion-atom interactions), and the model of Lindhard with coauthors [114–117] which is based on dielectric

formalism. In their initial form both models have predicted the monotonic dependence of S_e upon Z_1 and Z_2 . Their modification for the purpose of description of the Z_1 and Z_2 oscillations has been elaborated in several works. The main versions of the modernised Firsov theory are presented in Refs [75, 118-122]. Although on the whole this approach gives an approximate description of the oscillation effects, as has been mentioned in Ref. [111], generalisations of the phenomenological theory [119] reveal a great deal of arbitrariness, especially where it is concerned with the definition of the location of the Firsov plane and the flux of electrons through it. A dielectric approach did not develop so actively, and was primarily concerned with the description of the Z_2 oscillations [123-125]. Introduction in the dielectric theory of the Z_1 effect is achieved at a sacrifice of the model of a structureless particle. In this case, stopping losses can be written in the form [126, 127]

$$\frac{\mathrm{d}E}{\mathrm{d}z} = \frac{2}{\pi v_1^2} \int_0^\infty \frac{\mathrm{d}k}{k} |\rho_{\mathrm{ne}}(k)|^2 \int_0^{k v_1} \mathrm{d}\omega \,\omega \,\mathrm{Im} \left[-\frac{1}{\varepsilon(k,\omega)}\right] \quad , \quad (3.22)$$

where $\rho_{ne}(k)$ is a form factor of the charge distribution of the particle, and $\varepsilon(\mathbf{k}, \omega)$ is a dielectric function. It is essential that from this formula we can get both limit relations for S_e : $S_e \propto v_1$ for $v_1 \ll v_F$ and $S_e \propto v_1^{-2}$ for $v_1 \gg v_F$.

It is believed [128, 129] that the linear dielectric theory [Eqn (3.22) has been derived within its framework] cannot be applied in the case of $v_1 \ll v_F$, this opinion being based on the absence of the Z_1 oscillations in calculations [127]. However, in the latter work a rough atomic model was employed that does not take into account the shell structure of the atoms. In Ref. [130] identical calculations have been carried out with a piecewise-exponential approximation [Eqn (2.25)] for the atoms with $Z_1 < 18$, which have shown the presence of the Z_1 effect. Therefore there are reasons to expect that the results could be noticeably improved with the use of the more exact form factors. Using Eqn (3.22), we can also derive the dependence of the energy transferred in one collision on the impact parameter *b*:

$$T_{\rm e}(b) = 2 \int_{r_{\rm m}}^{\infty} \frac{\mathrm{d}E}{\mathrm{d}z} \frac{\mathrm{d}r}{\left\{1 - (b^2/r^2) - [V(r)/E]\right\}^{1/2}}, \qquad (3.23)$$

where the main parameter of a dielectric function, namely plasma frequency, depends on the density of the electrons of a target atom, $\omega_p = \sqrt{4\pi\rho_2(r)}$. In this case it is evident that the Z_2 effect is introduced into the theory through the function ω_p . Calculation based on Eqn (3.23) has not, however, yet been done in this form. Quantum generalisation of Eqn (3.23) for the structureless particles was made in Ref. [75], but because of the awkwardness of the final formulas this approach has not been widely applied and has only been used to describe the stopping of the light, channelled particles. To simulate ion-atom collisions in solids, the calculation methods that divide electrons into the strongly and weakly bounded ones [112, 131-133] are used as well.

In Refs [128, 129, 134, 135] the nonlinear S_e theory based on the known formula of Massey and Burhop was developed. The generalisation of this formula can be written in the form

$$S_{\rm c} = \frac{4\pi n}{v_{\rm F}^2} v_1 \sum_{l=0}^{\infty} (l+1) \sin^2(\delta_l - \delta_{l+1}) , \qquad (3.24)$$

nsity of the Fermi**3.3 Multiple scattering**fts of the electron
tential. The most
out in Refs [128,The basic tool in the theory of multiple scattering is the
method based on application of the Bethe kinetic equation
[148], a general solution to which, suitable for arbitrary

method based on application of the Bethe kinetic equation [148], a general solution to which, suitable for arbitrary ion-target combinations, has been found by Kompaneets [149]. According to these studies, a function of the angular distribution of the particles after having penetrated a film of thickness l and atomic density N is given by

$$f(\theta) = \frac{1}{2\pi} \int_0^\infty u J_0(u\theta) \, \mathrm{d}u \exp\left\{-Nl \int \, \mathrm{d}\sigma \left[1 - J_0(u\theta')\right]\right\},$$
(3.29)

where $d\sigma$ is a differential cross section, $J_0(x)$ is the Bessel function. Eqn (3.29) links the angular profile $f(\theta)$ with the interaction potential through the cross section $d\sigma$. Meyer [150] presented the cross section in the form of Eqn (3.12), introduced the optical depth $\tau = N\pi a^2 l$ and the reduced scattering angle $\eta = \epsilon \theta/2$. Eqn (3.29) was then transformed into a dimensionless form (the angles θ and Ω are related to the laboratory coordinate frame):

$$f(\theta) d\Omega = \eta d\eta \int_0^\infty x J_0(x \eta) \exp\left[-\tau \Delta(x)\right] dx , \qquad (3.30)$$

where the function $\Delta(x)$ is $[f_s(y)$ is a scattering function given in Eqn (3.12)]:

$$\Delta(x) = \int_0^\infty \frac{f_s(y)}{y^2} \left[1 - J_0(xy) \right] dy .$$
 (3.31)

In actual fact, however, in such a transformation the upper limit of the integration in Eqn (3.31) should be equal to ε and thus take into account the asymptotics of $f_s(y)$ for $y \ge 1$; this result is correct only for $\varepsilon \ge 1$. In addition, the scattering function $f_s(y)$ itself (see Section 3.1) depends upon ε and therefore angular distributions, generally speaking, cannot be represented in a universal form even for the TF potentials. Numerical results for the angular distributions according to Eqns (3.30) - (3.31) are tabulated Refs [150, 151] for the thickness in ranges $10^{-3} < \tau < 2 \times 10^3$. In these calculations, the TF potentials with different screenings as well as the power series ones were used. The results of Ref. [151] show that the use of different kinds of potentials for $\tau < 1$ leads to a variation of several orders in the angular half-width of the distribution profile. On the contrary, for $\tau > 1$ the results are similar because scattering is caused by the Coulomb part of the potential.

In Refs [152–154] the authors assumed that particles which penetrated the film at the angle close to $\theta = 0$ have undergone collisions only when the scattering angles do not exceed the angular half-width of the distribution for all the particles penetrated, $\eta_{1/2}$. Thus the elastic energy losses of such particles are supposed to be limited, while the value of the angle $\eta_{1/2}$ is connected to the thickness τ by the relation

$$\tau \rho \varepsilon_* s_n(\varepsilon_*) = c \eta_{1/2}^2, \quad \varepsilon_* = \frac{\varepsilon \psi_{\max}}{2}, \quad (3.32)$$

where ψ_{max} is the maximum scattering angle in CMS, $s_n(\varepsilon)$ is the reduced cross section of the slowing down losses, c is a numerical coefficient close to unity (in Refs [151–153] it was assumed that c = 1, and in Ref. [157] that c = 1.4). In Ref. [155], to develop these ideas it was shown that, under the assumptions made, a simpler dependence exists:

$$\eta_{1/2} = \varepsilon_* = 0.5\varepsilon \psi_{\max} . \tag{3.33}$$

where $v_{\rm F}$ and *n* are the velocity and density of the Fermi electron gas, and δ_l are the phase shifts of the electron scattering on a self-consistent ion potential. The most accurate calculations have been carried out in Refs [128, 129], where in order to determine an ion potential the method of the electron density functional was applied. The results of these calculations for Z_1 oscillations of the stopping cross sections are in good agreement with experimental data (although only ions with $Z_1 \leq 18$ were considered). The semiempirical trend of the theory of electron stopping is based on the concept of the Bohr effective charge [94, 137]

$$S_{e}(Z_{1}, Z_{2}, v_{1}) = Z_{1eff}^{2}(v_{1}) S_{e}(1, Z_{2}, v_{1}) , \qquad (3.25)$$

where $S_e(1, Z_2, v_1)$ is the stopping cross section of a proton, and Z_{1eff} is an effective charge of the stopping proton. Several types of approximations for Z_{1eff} are cited in Refs [137, 138, 140, 141], among others—the analytic approximations describing the effects of oscillations of the cross sections are described in Refs [50, 140, 141].

The basic approximation used in the theory of ranges, beginning with the fundamental work [101], is based on the assumption of independence of elastic and inelastic stopping mechanisms, with the resulting cross section $s = s_n + s_e$, the reduced range $\rho(\varepsilon)$, and the relative energy straggling given by [101]:

$$\rho(\varepsilon) = \int_0^{\varepsilon} \frac{\mathrm{d}\varepsilon'}{s_{\mathrm{n}}(\varepsilon') + s_{\mathrm{e}}(\varepsilon')}, \qquad (3.26)$$

$$\frac{\langle \Delta \rho^2 \rangle}{\rho^2} = \frac{\gamma}{\rho^2} \int_0^{\varepsilon} \frac{W(\varepsilon')}{\left[s_{\rm n}(\varepsilon') + s_{\rm e}(\varepsilon') \right]^3} , \qquad (3.27)$$

$$W(\varepsilon) = \frac{1}{2\varepsilon^2} \int_0^{\varepsilon} f(\sqrt{t}) \sqrt{t} \, \mathrm{d}t \,, \qquad (3.28)$$

where $\gamma = 4M_1M_2/(M_1 + M_2)^2$, and $f(\sqrt{t})$ is a scattering function. With $\varepsilon \ll 1$, if the Z_1 and Z_2 effects are not taken into account, it is usually assumed that $s_e = 0.15\sqrt{\epsilon}$. Most probably, all the values considered are eventually related to the scattering potential.

A comparison of the ranges and the parameters of their distributions from the point of view of the IP role was carried out in Refs [49, 104, 143]. Depending on the potentials used, ρ , $\langle \Delta \rho^2 \rangle / \rho^2$, and the other parameters at $\varepsilon < 0.1$ in these studies differ significantly, by several times, when we pass to the higher moments of distribution, which indicates clearly the dependence upon the potential being used.

More precise calculations of the profiles of the distribution for the penetrated ions are carried out by the Monte Carlo methods along with the transport equation methods (see Refs [143-145] and references cited there), but the main factors that determine the results of calculations remain unchanged.

In Ref. [146] a modification of the TRIM code [105] is reported, with the approximation $s = s_n + s_e$ being sacrificed. Inelastic losses are directly taken into account in the collision integral. This made it possible to improve the agreement of the theoretical and experimental values of the ranges for $\varepsilon < 10^{-2}$. A similar method within the bounds of the small angle approximation was proposed somewhat earlier in Ref. [147]. This result directly follows from the relations

$$\varepsilon = \frac{aM_{2}E_{1}}{Z_{1}Z_{2}(M_{1} + M_{2})}, \quad \eta = \frac{E_{1}a\theta}{2Z_{1}Z_{2}},$$

$$\theta = \frac{M_{2}}{M_{1} + M_{2}}\psi, \qquad (3.34)$$

where θ is a scattering angle in the laboratory system, ψ is a scattering angle in CMS, the rest of the designations being standard. Taking into account Eqns (3.32)–(3.33) for c = 1 we have [155]

$$s_{\rm n}(\eta_{1/2}) = \frac{\eta_{1/2}}{\tau}$$
 (3.35)

Eqn (3.35) was verified by means of simulation with the TRIM code [105] with the Moliere potential. In the case of an analytical calculation, the cross sections $s_n(\varepsilon)$ derived for this potential were approximated in the form (3.19), where the numerical coefficients in the denominator were substituted for 0.052 and 0.32. In addition, a similar approximation was used for the potential Kr-C, calculated according to the electron gas model (with the coefficients of 0.11 and 0.38). The results of the calculation of dependences $\eta_{1/2}(\tau)$ based on the proposed formula and those obtained by simulation are compared in Fig. 12. As would be expected, the dependence obtained with the simulation agrees better with Eqn (3.35) for the function $s_n(\varepsilon)$ corresponding to the Moliere potential. In Ref. [155] the authors see the significance of these results in the possibility of extracting the elastic contribution from the total energy losses, since a simple method of estimating the electron stopping does not exist as yet. Let us note that Eqn (3.35) can be obtained directly from Eqn (3.29) if we limit the integration in the exponent (3.29) by the value $t = \varepsilon_*^2$ [the cross section is expressed by means of a

Figure 12. The reduced function of the angular width profile of the multiple scattering [155]: calculation according to Eqn (3.35) for the Moliere potential (curve 1); according to Ref. [150] (curve 2); the same as for curve 1 but for the Kr–C potential (curve 3); according to Ref. [151] for the TF and Lentz–Jensen potentials (curve 4, 5); according to Ref. [153] (curve 6).

scattering function from Eqn (3.12), with the subsequent consideration of the relation (3.18)] and if we further use for the Bessel function the expansion $J_0(u\theta') \approx 1 - u^2 \theta'^2/4$, and do a substitution of $t = \varepsilon^2 \theta'^2/4$ for θ' , bearing in mind that $\theta' \leq 1$.

Based on direct summing up of the small angular deviations, the Moliere theory [156] is also being used for the interpretation of the experiments in multiple scattering. It is less convenient for practical use as a specific potential-oriented theory, since it tolerates only variation of the screening parameters and the effective particle charges. A comparison of the angular distribution of Moliere [156] and Meyer [150] was carried out in Ref. [75] (see also the corresponding references), where it was shown that for $\tau \ge 1$ the results are close, and for $\tau \ll 1$ the agreement is poor.

As follows from Sections 3.1 and 3.2, differential cross sections are most sensitive to the form of a scattering potential when \sqrt{t} , $\varepsilon < 1$. Thus for a correct comparison of the experimental data with the IP we should calculate angular distributions according to Eqn (3.30) without further simplifications. The case with $\tau < 1$ is of particular interest. The use of Eqn (3.35) gives us a possibility of investigating the potential for $\tau > 1$ as well.

In conclusion we would like to note that in Refs [108, 151, 109] the formulas that directly link angular distribution functions with the differential cross sections were obtained but they have not been widely used so far.

3.4 Dynamic screening of potentials

When ions move in the plasma of a solid, their electric field is further screened and thus the effectiveness of their interaction with the atoms should decrease. The degree of screening should decrease with the increase of the ion velocity, and when $v_1 \ge v_F$ it approaches zero because the screening charges have no time 'to catch up' with the particle. The importance of this effect was described in Ref. [158]. General formulas for the potential of a 'bare' electric charge moving in plasma with the velocity v_1 were obtained in Refs [159-165] within the scope of the linear dielectric theory. In Ref. [163] the formulas for the density fluctuations of the induced charge surrounding an ion were also derived. Detailed presentation of topics related to the mechanisms of forming the ionic charge states is given in the review Ref. [327]. In Refs [91, 107, 166-168] general expressions are obtained for the short-range part of the screened potential (taking into account its own electrons), and further on the potentials of interaction with the individual atoms of the solid. Following Refs [91, 166, 167], let us write a general expression for an ion potential

$$\boldsymbol{\Phi}(\boldsymbol{r},t) = \frac{1}{2\pi^2} \int d^3\boldsymbol{q} \int \frac{\exp\left[i(\boldsymbol{q}\cdot\boldsymbol{r}-\omega t)\right]}{q^2 \varepsilon(\boldsymbol{q},\omega)} \,\rho(\boldsymbol{q}) \,\delta(\omega-\boldsymbol{q}\cdot\boldsymbol{v}_1) \,d\omega \;,$$
(3.36)

where $\rho(q)$ is a form factor of the charge distribution and $\varepsilon(q, \omega)$ is the dielectric function. It is convenient to use an expression for $\rho(q)$ that corresponds to an approximation of the electron density with Eqn (2.48):

$$\rho(q) = Z_1 - N_1 + \sum_i \frac{c_i (qa_*/b_i)^2}{1 + (qa_*/b_i)^2} \,. \tag{3.37}$$

In order to simplify Eqn (3.36), one either integrates directly with respect to the frequencies [163, 164], or

introduces a cylindrical coordinate system in the *p*-space with the *z* axis in the direction of the vector v_1 [160], and then integrates with respect to the angular variable and the *z* component of the vector. In this case we have [160]:

$$\boldsymbol{\Phi}(\boldsymbol{r},t) = \frac{1}{\pi v_1} \int_0^\infty J_0(\rho x) x \, \mathrm{d}x \int_{-\infty}^\infty \frac{\exp\left[\mathrm{i}\omega(z/v_1-t)\right] \rho(q)}{\varepsilon(\boldsymbol{q},\omega) \left(x^2 + \omega^2/v_1^2\right)} \, \mathrm{d}\omega,$$
(3.38)

where $q^2 = x^2 + \omega^2 / v_1^2$. When we integrate Eqn (3.38) with respect to the frequency, we apply analytical properties of the function $\varepsilon(q, \omega)$. If plasmon damping is absent, its poles are real, and integration with respect to a complex contour including the real axis, leads to the potential known as a 'wake' [159, 160, 163], which describes the polarisation 'track' of a particle. This potential and the possibility of formation in it of the quasi-bounded states of the 'escort' electrons have been discussed in detail in the cited works and are beyond the scope of this paper. Note that the space period of the 'wake' potential is equal to v_1/ω_p and that it is localised behind the particle. Taking into account the absorption in the function $\varepsilon(q, \omega)$ leads to the diminishing of the oscillation amplitude with the moving away from the ion [163]. The short range part of the ion field is due to the poles $\omega = \pm i x v_1$ for a 'bare' charge and the poles of the form factor $\rho(q)$ for the electron contribution [91, 167]. In the first case, a specific dependence of $\varepsilon(q, \omega)$ upon q is not significant, because q = 0. Then (in the case of $N_1 = 0$) we get [163, 167]:

$$\Phi(\mathbf{r},t) = \frac{Z_1}{\sqrt{\rho^2 + z'^2}} - Z_1 \frac{\omega_p}{\nu_1} \int_0^\infty \frac{J_0(\rho y \omega_p / \nu_1)}{1 + y^2} \\ \times \exp\left[-\frac{\omega_p}{\nu_1} |z'|y\right] dy , \qquad (3.39)$$

where ω_p is the plasma frequency, $z' = z - v_1 t$, ρ and z' are the cylindrical coordinates of a point with respect to the location of an ion at the instant t. From Eqn (3.39) it follows that the correction to the Coulomb ion field at the point $\mathbf{r} = 0$ is equal to

$$\Delta \Phi(0) = -Z_1 \frac{\pi \omega_{\rm p}}{2v_1}$$

If we consider it as the first term of an expansion of the screened potential $Z_1 \exp(-\alpha r)/r$, it is evident that $\alpha = \pi \omega_p/2v_1$. Actually, the integral in Eqn (3.39) diminishes somewhat more slowly. In Refs [91, 165] it is calculated in an analytical form and then represented by an expansion with respect to the Legendre polynomials as the functions of $\cos \theta$, where θ is an angle between r and v_1 . The spherical part of the expansion is nicely approximated by the following equation [91, 168]:

$$\Delta \Phi_0(r) \approx \frac{Z_1}{r} \left[1 - \exp\left(-1.064 \frac{\omega_p}{\nu_1} r\right) \right]. \tag{3.40}$$

Anisotropy of the potential $\Delta \Phi$ due to the taking into account of the angular terms is not too large; in the direction of the z axis the potential is somewhat larger than in the perpendicular direction. These dependences are shown in Fig.13 for the potential of H⁺ in aluminum for $v_1 = 3v_0$ ($\omega_p = 0.56$ a.u.).

For the ions with partial ionisation, the potential given by Eqn (3.38) was calculated in Refs [107, 168]. The

Figure 13. Dynamic electric potential of the H⁺ ion in aluminum at $v_1 = 3v_0$ [168]: Eqn (3.40) (curve 1); Eqn (3.39) at $\rho = 0$ (along the direction of motion) (curve 2); similar to curve 2 at z' = 0 (in the perpendicular direction) (curve 3).

dielectric function was taken in the form proposed from Refs [127, 163]:

$$\varepsilon(\boldsymbol{q},\omega) = 1 + \frac{\omega_{\rm p}^2}{\omega_{\rm g}^2 + 0.6v_{\rm F}^2 q^2 + 0.25q^4 - \omega^2}, \qquad (3.41)$$

where ω_g is the energy gap width. Substitution of Eqns (3.41) and (3.37) into Eqn (3.38) leads us to the following result

$$\Phi(\rho, z') = \frac{Z_1 - N_1}{\sqrt{\rho^2 + z'^2}} - \frac{N_1}{\sqrt{\rho^2 + z'^2}} \sum_i c_i$$

$$\times \exp\left(-\frac{\sqrt{\rho^2 + z'^2}}{a_*} b_i\right) - k(Z_1 - N_1)$$

$$\times \int_0^\infty \frac{J_0(k\rho y) \exp(-k|z'|y)}{1 + y^2} \, dy + \frac{N_1 \omega_p^2}{a_*} \sum_i \frac{c_i}{b_i}$$

$$\times \int_1^\infty \frac{J_0(\rho b_i \sqrt{t^2 - 1}/a_*)}{A_i + v_1^2 b_i^2 t^2 / a_*^2} \exp\left(-t|z'| \frac{b_i}{a_*}\right) \, dt \,, (3.42)$$

$$A_i = \omega^2 + \frac{b_i^2}{2} \left(v_i^2 - v_i^2 + \frac{b_i^2}{2}\right) \qquad (3.43)$$

 $A_{i} = \omega_{g}^{2} + \frac{v_{i}}{a_{*}^{2}} \left(v_{1}^{2} - v_{F}^{2} + \frac{v_{i}}{4a_{*}^{2}} \right), \qquad (3.43)$

where $k = (\omega_p^2 + \omega_g^2)/\omega_p$. It is evident that the first two terms in Eqn (3.42) represent the static electric potential of the ion at the point $r = \sqrt{\rho^2 + z'^2}$, and the two last terms are connected with the screening effect. It is not difficult to show that the second integral is, as a rule, essentially smaller than the first one. Majorising them by the corresponding values at $\rho = z' = 0$ and assuming that c_i and b_i are equal to the Moliere coefficients, we can write the ratio of the second integral to the first one as

$$s \approx 1.6 \, \frac{Z_1 - N_1}{N_1} \frac{v_1}{\omega_p a_*} \,.$$
 (3.44)

Since usually $\omega_p \simeq 0.5$ a.u. and $a_* \approx 0.2-0.3$, then for $v_1 > v_0$ and for $Z_1 - N_1$ not too small we have $s \ge 1$. The case $Z_1 \approx N_1$ is not really important because there the screening due to the electrons of the atoms predominates. Thus in cases important in practice the last term in Eqn (3.42) can be ignored, and for the third term we can

use Eqn (3.39) with the substitution of Z_1 for $Z_1 - N_1$. The sphere of applicability of Eqns (3.39)–(3.42), as noted in Ref. [167], is limited to the distances $r < v_1/\omega_p$, when the high-frequency harmonics of the potential are essential. This case can be considered as a limit for the weak screening, because the ion field at the point \mathbf{r} varies rapidly during the time of flight (in comparison with the plasma oscillation period). On the contrary, for $r > v_1/\omega_p$ the variation of the field is small and screening is close to that in the static case. Then in the limit $\omega \to 0$ the dielectric function can be presented in the form [169, 170]

$$\varepsilon(\boldsymbol{q},\omega) = \frac{1}{q^2 D^2} + \frac{2i\omega}{q^3} , \quad q \leq 2k_{\rm F} , \qquad (3.45)$$

where D is the Debye radius. The potential of the 'bare' charge Z_1 , which can be obtained by substituting Eqn (3.42) into Eqn (3.36), is equal to [91, 166, 167]:

$$\begin{split} \varPhi(\mathbf{r},t) &= \frac{Z_1}{r} \exp\left(-\frac{r}{D}\right) r - \frac{Z_1 D^3 v_1^2}{4} \sin^2 \theta \left(1 + \frac{r}{D}\right) \\ &\times \exp\left(-\frac{r}{D}\right) + 4Z_1 v_1^2 D^3 \left(1 - \frac{3}{2} \sin^2 \theta\right) \\ &\times \left[\frac{2}{x^3} - \left(\frac{3}{8} + \frac{x}{8} + \frac{1}{x} + \frac{2}{x^2} + \frac{2}{x^3}\right) \exp(-x)\right], (3.46) \end{split}$$

where θ is an angle between the vectors \mathbf{r}_1 and $\mathbf{r} - v_1 t$, $r = [|\mathbf{r} - v_1 t|^2]^{1/2}$, x = r/D. From Eqn (3.46) it follows that at large distances

$$\boldsymbol{\Phi}(\boldsymbol{r},t) \sim \frac{v_1^2}{r^3} \left(1 - \frac{3}{2} \sin^2 \theta \right) \,.$$

In the case of partial ionisation of the particle, if we apply the form factor [Eqn (3.37)] for $\Phi(\mathbf{r}, t)$, it is not difficult to obtain an analytical formula, but it looks more awkward. The potential of interaction of a 'bare' screened ion with a separate target atom is equal to [91, 167]:

$$U(\boldsymbol{R},t) = \boldsymbol{\Phi}(\boldsymbol{R},t)Z_2 - \int \boldsymbol{\Phi}(\boldsymbol{R},t)\rho(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}'\,,\qquad(3.47)$$

where $\rho(\mathbf{r'})$ is the density of the electrons of the target atom which, generally speaking, should be taken without considering the collective part of the electrons (at least for metals). Substituting Eqn (3.40) into Eqn (3.47) and taking account of $\rho(\mathbf{r'})$ in the form given by Eqn (2.48), we have

$$U(R) = \frac{Z_1 Z_2}{R} \exp(-\tilde{a}R) - \frac{Z_1 N_2}{R} \sum_i \frac{c_i b_i^2}{(\tilde{a}a_*)^2 - b_i^2} \times \left[\exp\left(-\frac{b_i R}{a_*}\right) - \exp(-\tilde{a}R) \right], \quad (3.48)$$

where, as usual, *R* is the interatomic distance, and $\tilde{a} = 1.064 \omega_p / v_1$. If an ion retains a part of its shell, the main result for the static case [Eqn (2.18)] can be easily modified. If, as noted above, we ignore the last term in Eqn (3.42), then, as follows from this equation, our taking into account the dynamic screening gives corrections $-\Delta \Phi$ to the potential of a point charge Z_1 , and $(N_1/Z_1)\Delta\Phi$ to the potential of the electron cloud, where $\Delta\Phi$ is determined by the second term in Eqn (3.39) with the substitution $\omega_p \rightarrow (\omega_p^2 + \omega_g^2)^{1/2}$. Thus, we must introduce a correction term in Eqn (2.18):

$$\Delta U(\mathbf{R}) = -\Delta \boldsymbol{\Phi} \, \frac{Z_2}{R} + \int \Delta \boldsymbol{\Phi}(\mathbf{R}) \left(1 - \frac{N_1}{Z_1}\right) \rho_2(\mathbf{r}') \, \mathrm{d}^3 \mathbf{r}' \, . \quad (3.49)$$

Eqns (2.18) and (3.49) are of a general nature, irrespective of the model used for the calculation of $\rho_2(\mathbf{r}')$. The contributions to the IP which are linked with the electron density functional should be calculated in a conventional way. Evidently, in such a case we do not take into account the influence of the screening upon the corresponding terms of the potential. For $v_1 = 0$ this influence, as was shown in Refs [171, 172], is absent, i.e. the screening alters only the electrostatic interaction of the particles. For $v_1 \neq 0$ the analogous result has not yet been established, but the general considerations (decrease of the screening role with the increase of velocity) allow us to assume that the variation of the IP is due only to the potential $\Delta U(R)$. In Ref. [107] calculations of $\Delta U(R)$ were carried out with respect to Eqn (3.49) with the use of $\rho_2(r)$ in the approximation given by Eqn (2.25). Moreover, in Refs [107, 168] an expression for an ion-atom potential is obtained for the case of the light ions that retain 1-2

electrons in a bonded state. In Fig. 14 the results of the calculation of the potential H – Al for $v_1 = 1.2v_0$ are shown [168] with or without taking into account the bonded electron. Fig. 14 shows us that the screening essentially alters the IP for R > 2 a.u. For heavy particles influence of the dynamic screening is expressed to a lesser extent and manifests itself at larger internuclear distances.

Figure 14. The H-Al IP at $v_1 = 1.2v_0$: ignoring the screening (curve *l*); taking the screening into account (curve 2); taking into account the screening and a bonded electron of H (curve 3).

3.5 Continuous potentials of atomic chains and planes in channelling

In the theory of the orientation effects that are connected with penetration of the charged particles through the crystals in directions close to the crystallographic axes (planes) directions, one of the basic concepts is the continuous potential (CP), which was introduced for the first time in Refs [173–175, 70]. This potential is characteristic of the coherent small angle scattering of a particle on a large number of atoms of a chain (plane) that interact with it within a small segment of its trajectory. In this case, the processes of scattering at large angles as well as noncoherent multiple scattering tend to be suppressed, and the characteristic angles of the particle velocities with respect to the directions of the channels do not exceed the critical values θ_{cr} . For the classical particles a CP approximation is valid beginning from the keV energy range, if the ion impact parameters with respect to the chain (plane) do not exceed the quantity $(u_{\perp}^2 + a^2)^{1/2}$ (where u_{\perp} and a are correspondingly the thermal oscillations amplitude and a screening parameter). In the case of relativistic lepton channelling, a CP model is valid beginning from the MeV energies, provided that at least several levels are generated in the potential well formed by the channel walls. The wave functions of the transverse motion of these particles are obtained from the Schrodinger equation which contains a CP, and which is modified here by replacement of the electron rest mass with a relativistic one. In the case of the isolated atoms of the chain and the plane, the CP is equal to

$$U_{\rm ch}(r) = \frac{1}{d} \int_{-\infty}^{\infty} V\left(\sqrt{z^2 + r^2}\right) {\rm d}z , \qquad (3.50)$$

$$U_{\rm pl}(x) = 2\pi n_{\rm s} \int_0^\infty V\left(\sqrt{\rho^2 + x^2}\right) \rho \,\mathrm{d}\rho \,\,, \tag{3.51}$$

where V(r) is an atom – atom IP, d and n_s are the distance between the atoms of a chain and the surface concentration of atoms of a plane, respectively, and r and x are the coordinates that are perpendicular to a chain (a plane). It is not difficult to show that these relations determine the zero coefficients of the Fourier expansions of the sum of interactions of a particle with all the atoms of a chain (a plane). In initial studies on the calculation of channelling of positive particles [173 – 178], the total potential acting on an ion in the channel was chosen in the form of the CP from a few neighboring chains (planes). The approximations used [Eqn (2.37)] contained the screening functions of Lindhard [70] and Moliere [66] [see Eqns (2.41) and (2.28)]. The well-known expressions of the CP [176] follow from Eqns (3.50)–(3.51).

(a) In the case of a chain:

$$U_{\rm ch}^{\rm L}(r) = \frac{2Z_1 Z_2}{d} \ln \left[1 + \frac{3a^2}{r^2} \right]^{1/2}, \qquad (3.52)$$

$$U_{\rm ch}^{\rm M}(r) = \frac{2Z_1 Z_2}{d} \sum_{i} c_i K_0 \left(\frac{b_i r}{a}\right) \,. \tag{3.53}$$

(b) In the case of a plane:

$$U_{\rm pl}^{\rm L}(x) = 2\pi n_{\rm s} Z_1 Z_2 a \left[\left(\frac{x^2}{a^2} + 3 \right)^{1/2} - \frac{x}{a} \right], \qquad (3.54)$$

$$U_{\rm pl}^{\rm M}(x) = 2\pi n_{\rm s} Z_1 Z_2 a \sum_{i} \frac{c_i}{b_i} \exp\left(-\frac{b_i x}{a}\right) \,. \tag{3.55}$$

Here *a* is a screening parameter and $K_0(x)$ is a modified Bessel function. In Refs [177, 178] the values of 'thermal' CPs within the bounds of the Debye approximation for the displacements of the atoms from their positions of equilibrium were obtained. In the absence of mutual correlations, the probability distributions of the displacements of the atoms for the axial and plane cases are equal to [178]:

$$f_{\rm ch}(\Delta r) = \frac{1}{\pi u_{\perp}^2} \exp\left(-\frac{\Delta r^2}{u_{\perp}^2}\right), \qquad (3.56)$$

$$f_{\rm pl}(\Delta x) = \frac{1}{\sqrt{2\pi}u_1} \exp\left(-\frac{\Delta x^2}{2u_1^2}\right), \qquad (3.57)$$

where u_1 and u_{\perp} are one- and two-dimensional $(u_{\perp} = \sqrt{2} u_1)$ mean square amplitudes for the thermal oscillations of the lattice atom, Δr and Δx are displacements from the chain and plane. Taking into account Eqns (3.56) and (3.57), we can present the 'thermal' CP in the form:

$$U_{\rm ch}^{\rm t}(r) = \int_0^\infty \Delta r \,\mathrm{d}(\Delta r) \int_0^{2\pi} \mathrm{d}\theta f_{\rm ch}(\Delta r)$$
$$\times U_{\rm ch} \left\{ \left[r^2 + (\Delta r)^2 - 2r \,\Delta r \cos \theta \right]^{1/2} \right\}, \qquad (3.58)$$

$$U_{\rm pl}^{\rm t}(x) = \int_{-\infty}^{\infty} d(\Delta x) f_{\rm pl}(\Delta x) U_{\rm pl}(|x - \Delta x|) . \qquad (3.59)$$

Averaging the plane potential [Eqn (3.55)] will give [177, 178]:

$$U_{\rm pl}^{\rm t}(x) = \pi n_{\rm s} Z_1 Z_2 a \sum_i \frac{c_i}{b_i} \exp\left(\frac{b_i u_1^2}{2a^2}\right) \\ \times \left\{ \exp\left(-\frac{b_i x}{a}\right) \operatorname{erfc}\left[\frac{1}{\sqrt{2}}\left(\frac{b_i u_1}{a} - \frac{x}{u_1}\right)\right] \\ + \exp\left(\frac{b_i x}{a}\right) \operatorname{erfc}\left[\frac{1}{\sqrt{2}}\left(\frac{b_i u_1}{a} + \frac{x}{u_1}\right)\right] \right\}, \quad (3.60)$$

where

$$\operatorname{erfc}(t) = \frac{2}{\sqrt{\pi}} \int_{t}^{\infty} \exp(-y^2) \,\mathrm{d}y$$

Similarly, for an axial CP determined by Moliere [179]:

$$U_{\rm ch}^{\rm t}(r) = \frac{Z_1 Z_2}{d} \sum_i c_i \exp(q_i^2) \int_0^1 \exp\left(-\frac{r^2 t}{u_{\perp}^2} - \frac{q_i^2}{t}\right) \frac{\mathrm{d}t}{t}, \ (3.61)$$

where $q_i = b_i u_\perp/2a$. Formulas (3.60) and (3.61) and the analogous formulas for the other potentials [187] are inconvenient for numerical calculations that include a sum of the CPs for a large number of planes (chains). Therefore, in Ref. [183] for the resulting potential of a crystal, which acts on a particle of charge Z_1 and moving in the channelling regime, the following formula was proposed:

$$U(\boldsymbol{\rho}_{\perp}) = \frac{Z_1}{\Omega} \sum_{\boldsymbol{g}_{\perp}} v_{\boldsymbol{g}_{\perp}} \exp(\mathrm{i}\boldsymbol{g}_{\perp}\boldsymbol{\rho}_{\perp}) S(\boldsymbol{g}_{\perp}) \exp(-0.5g_{\perp}^2 u_{\perp}^2), (3.62)$$

where p_{\perp} is a transverse coordinate, $v_{g_{\perp}}$ is a Fourier transform of an atomic potential, $S(g_{\perp})$ is a structure factor, Ω is a volume of an elementary cell, g_{\perp} is a transverse component of the inverse lattice vector, $u_{\perp} = u_1$ for a plane case, and $u_{\perp} = \sqrt{2} u_1$ for an axial case. For a monoatomic crystal, the 'lattice' has the simplest basis in the transverse direction , and thus $S(g_{\perp}) = 1$. In the case of the crystals of a complex composition, Eqn (3.62) can easily be generalised by introducing an additional summation with respect to the differing components [186]. Formula (3.62) seems evident for $u_{\perp} = 0$, i.e. in the case of a static lattice. However, its identity in the case of $u_{\perp} \neq 0$ with a generalised potential expressed as a sum of the individual CP of the type given by Eqns (3.60) and (3.61) appears to need justification, because the Debye-Waller factor is included in Eqn (3.62) by analogy with a formula for an x-ray scattering amplitude. Let us first

consider the planar case by rewriting Eqn (3.59) in the form [187]:

$$U_{pl}^{t}(x) = \frac{1}{\sqrt{2\pi}u_{1}} \int_{0}^{\infty} U_{pl}(z) \left\{ \exp\left[-\frac{(z+x^{2})}{2u_{1}^{2}}\right] + \exp\left[-\frac{(z-x)^{2}}{2u_{1}^{2}}\right] \right\} dz . (3.63)$$

Taking into account that the total potential acting upon a particle due to all the planes is equal to

$$U(x) = \sum_{n = -\infty}^{\infty} U_{pl}^{t}(x + nd_{p}) , \qquad (3.64)$$

where d_p is the interplanar distance, and expanding Eqn (3.64) into the Fourier series, we get $(g_n = 2\pi n/d_p)$:

$$U(x) = \sum_{n} U(g_n) \exp(ig_n x) . \qquad (3.65)$$

The expansion coefficients $U(g_n)$, taking into account Eqn (3.51), are equal to

$$U(g_n) = \frac{2}{d_p} U_{p1}(g_n) \exp(-0.5g_n^2 u_1^2) . \qquad (3.66)$$

On the other hand, if the atomic potential V(R) is spherically symmetric, the corresponding form factor is equal to

$$v_g = 4\pi \int_0^\infty \frac{\sin(gr)}{gr} V(r) r^2 \,\mathrm{d}r \;. \tag{3.67}$$

Integrating Eqn (3.67) by parts, and taking into account the asymptotics of V(R) and Eqn (3.51), we obtain:

$$v_g = \frac{2}{n_s} U(g_n) . (3.68)$$

Since in this case $\Omega = d/n_s$, from Eqns (3.65)–(3.68) it can be seen straightaway that Eqns (3.65) and (3.62) are equivalent, because $g_{\perp} = g_n = 2\pi n/d_p$ and $u_{\perp} = u_1$. In the axial case, analogously with Eqns (3.65) and (3.66), the Fourier expansion coefficient is equal to

$$U(\boldsymbol{g}_{\perp}) = \frac{1}{\Omega_2} \int \exp(-\mathrm{i}\boldsymbol{g}_{\perp} \cdot \boldsymbol{\rho}_{\perp}) U_{\mathrm{ch}}^{\mathrm{t}}(\boldsymbol{\rho}_{\perp}) \,\mathrm{d}^2 \boldsymbol{\rho}_{\perp}$$
$$= \frac{1}{\Omega_2} U_{\mathrm{ch}}(\boldsymbol{g}_{\perp}) \exp(-0.5g_{\perp}^2 u_1^2) , \qquad (3.69)$$

$$U_{\rm ch}(g_{\perp}) = 2\pi \int_0^\infty U_{\rm ch}(r) \, r J_0(g_{\perp}r) \, \mathrm{d}r \;, \qquad (3.70)$$

where $J_0(x)$ is the Bessel function. On further transformation of the form factor, we obtain:

$$v_g = \int \exp(-\mathbf{i}g \cdot \mathbf{r}) V(r) d^3 r$$

= $2\pi d \int_0^\infty r U_{\rm ch}(r) J_0(gr) dr = dU_{\rm ch}(g) .$ (3.71)

Taking into account that $\Omega_2 = \Omega/d$, we again return to Eqn (3.62). However, the Debye–Waller factor, as in the case of a plane potential, is equal to $\exp(-0.5g_{\perp}^2u_1^2)$, as opposed to the result obtained in Ref. [183]. Thus, in (3.62) both in the plane and axial cases $u_{\perp} = u_1$. When we calculate the potential for the channelling of heavy particles, it is evident that, in Eqn (3.62), instead of Z_1v_g

we should substitute the Fourier transform of the ion – atom IP.

In Refs [180-182] in order to calculate the radiation spectra of the relativistic channelled electrons and positrons, the approximation of quantum-mechanical atomic factors was used from the work of Doyle and Turner [184]:

$$v_g = 2\pi f(s) = 2\pi \sum_{i=1}^4 a_i \exp(-b_i s^2)$$
, (3.72)

where $g = 4\pi s$, and a_i and b_i are the tabulated coefficients. Inverting it, we obtain the Doyle–Turner atomic potential

$$V(r) = \frac{2}{\sqrt{\pi}} \sum_{i=1}^{4} \left(\frac{a_i}{B_i}\right)^{3/2} \exp\left(-\frac{r^2}{B_i}\right), \qquad (3.73)$$

where $B_i = b_i/4\pi^2$. Eqns (3.73) and (3.74) are convenient, because if we take into account Eqns (3.50), (3.51), (3.58) and (3.59), they will provide us with the simple equations for the 'thermal' CP of a chain [181, 185] and a plane [182]:

$$U_{\rm ch}^{\rm t}(r) = \frac{2Z_1}{d} \sum_{i=1}^{4} \frac{a_i}{B_i + u_1^2} \exp\left(-\frac{r^2}{B_i + u_1^2}\right), \qquad (3.74)$$

$$U_{\rm pl}^{\rm t}(x) = 2\sqrt{\pi} \, n_{\rm s} Z_1 \sum_{i=1}^{4} \frac{a_i}{\left(B_i + 2u_1^2\right)^{1/2}} \exp\left(-\frac{x^2}{B_i + 2u_1^2}\right) \,. \tag{3.75}$$

Note that although the potentials given by Eqns (3.74) - (3.75) are usually considered to be quantum-mechanical ones [180–182], such identification is not quite correct. This follows from the fact that Eqn (3.73) does not reproduce the asymptotics of the atomic potential for $r \rightarrow 0$. Moreover, the electron density that corresponds to Eqn (3.73) does not describe the shell structure. In that sense, the CP obtained on the basis of a piecewise exponential model [Eqn (2.25)] and an analytical HF model [321] are more justified. The corresponding equations for the static and 'thermal' potentials are cited in Refs [45, 187]. A comparison of the different approximations for the channelled particles is given in Section 4.6.

The potential given by Eqn (3.62) can be generalised when a crystal consisting of several kinds of atoms (ions) of type *i* is deformed by a field of a transverse ultrasonic (electromagnetic) wave with a frequency ω_s (ω_e) [277]. If x_i is an amplitude of the atomic displacements that are induced by this field, then the averaged (with respect to the plane) particle-crystal potential will be

$$U(x,t) = 2\sum_{i} \sum_{m=1}^{\infty} c_{im} J_0(g_m x_i) \cos(g_m x) + 4\sum_{i} \sum_{m=1}^{\infty} \sum_{p=1}^{\infty} c_{im} J_{2p}(g_m x_i) (-1)^p S_{im} \cos(g_m x) \times \cos(2p\Omega t) + 4\sum_{i} \sum_{m=1}^{\infty} \sum_{p=1}^{\infty} c_{im} J_{2p-1}(g_m x_i) \times (-1)^p S_{im} \sin(g_m x) \sin[(2p-1)\Omega t] , \qquad (3.76)$$

where $g_m = 2\pi m/d_{pi}$ is a vector of an inverse lattice, $\Omega = (c/v_s)\omega_s$ for an ultrasonic wave, and $\Omega = (n-1)\omega_e$ for an electromagnetic wave (v_s is the velocity of sound, c is the velocity of light in vacuum, and *n* is an optical refraction index); S_{im} depends on the channel type [in the case of (100) and (110) NaCl, for example, $S_{im} = 1$, and for (111) NaCl, $S_{im} = (-1)^m$]; $J_k(x)$ is the Bessel function of the *k*th order; coefficients c_{im} are equal to

$$c_{im} = \frac{n_{si} d_{pi}}{\pi m^2} \left[Z_i - \rho_i(g_m) \right] \exp\left(-\frac{g_m^2 u_i^2}{2}\right) \,. \tag{3.77}$$

In Eqn (3.77), n_{si} and d_{pi} are the surface density and the interplanar distance for the sublattice of the ions of type *i*; $\rho_i(g_m)$ is the form factor of the electron density; and u_i are the corresponding amplitudes of the thermal oscillations.

The problem of taking into account the dislocation effects is similar to the problem of influence of an external periodic field on a CP. The former is considered in Refs [315, 316] with the model potentials.

3.6 Surface effects

When a charged particle moves near the surface of a solid, the role of the plasma effects essentially increases. As is shown in Refs [188, 189], in this case the stopping losses are connected with excitation of the surface plasmons and, in addition, a dynamic-induced surface potential appears, similar to the potential in a volume [see Eqn (3.36)]. In the conditions of a sliding interaction with a surface on a section of the trajectory after reflection [245], the surface 'wake' potential attracts a positive ion, and this may give rise to its spasmodic motion [190]. The other effect is connected with the possibility of orientational influence of the surface on the motion of a diatomic molecule or a cluster, which causes a rotation of the line perpendicular to the surface of the nuclei [112, 191]. In Ref. [192] the influence of the 'wake' interactions on multiple scattering was also considered. In particular, an emergence of the coherence of the scattering for the small angles between the direction of the velocity vector and the molecule axis was mentioned.

There are two main approaches most often used in the theory of dynamic surface potentials (and of the stopping power): a dielectric method based on the model of a specular reflection [193–199], and the method of an effective Hamiltonian in the representation of surface plasmons [188–190, 200]. The trajectory of a particle before and after deflection is assumed to be rectilinear. The most general equations for the induced dynamic potential are obtained in Ref. [199]. In particular, when a charge (having velocity components v_{\parallel} and v_{\perp} parallel and normal to the surface) moves outside a solid, the induced potential is equal to

$$\boldsymbol{\Phi}^{\text{ind}}(\boldsymbol{r},t) = \frac{Z_1}{2\pi^2} \int d^2 \boldsymbol{k} \int d\omega \, \frac{v_{\perp} \exp(-k|z|)}{(\omega - v_{\parallel} \cdot \boldsymbol{k})^2 + v_{\perp}^2 k_z^2} \frac{kI_0 - \pi}{kI_0 + \pi} \\ \times \exp\left[-\mathrm{i}(\boldsymbol{k} \cdot \boldsymbol{v}_{\parallel} - \omega) t\right], \qquad (3.78)$$

where $\mathbf{k} = (\mathbf{k}_2, k_z)$, z is the distance from the surface, and I_0 is defined by the expression

$$I_0 = \int_{-\infty}^{\infty} \frac{\mathrm{d}k_z}{(k^2 + k_z^2)\,\varepsilon(\boldsymbol{k},\omega)} \,. \tag{3.79}$$

With regard to Eqn (3.78), the stopping losses per unit path length are equal to

$$\frac{\mathrm{d}E}{\mathrm{d}x} = \frac{1}{v_1} \frac{\mathrm{d}E}{\mathrm{d}t} = \frac{Z_1}{v_1} \left(-\frac{\partial \boldsymbol{\Phi}^{\mathrm{ind}}}{\partial \boldsymbol{r}} v_1 \right) \,. \tag{3.80}$$

Taking into account that, for the rectilinear motion $\mathbf{r} = v_1 t$, we have

$$\frac{\mathrm{d}E}{\mathrm{d}x} = -\frac{Z_1}{v_1} \left(\frac{\partial \boldsymbol{\Phi}^{\mathrm{ind}}}{\partial t}\right)_{\boldsymbol{r}=v_1 t}.$$
(3.81)

In Ref. [199] the equations for calculations of dE/dx with the different approximations of a dielectric function are cited. The case of the 'dressed' ions has not been considered so far. It is evident that sufficiently far away from the surface $Z_1 \Phi^{ind}(\mathbf{r}, t)$ may be considered as a potential resulting from the ion-solid interaction. However, for z < 1.2 a.u. one should take into account pair interactions, and so far it is not clear how this can be made compatible with the dielectric approach. As a rougher alternative model the use of a 'continuous' potential of the surface of the form given below was proposed [202, 203]:

$$U(x) = N \int_{x}^{\infty} dz \int_{0}^{\infty} 2\pi r V \left(\sqrt{z^{2} + r^{2}} \right) dr , \qquad (3.82)$$

where N is the density of the target atoms, z is the distance from the surface, V(R) is the pair IP of a particle with an atom of the medium. In the computer simulation of the sliding reflections, all the known codes, such as TRIM [105], MARLOWE [204], and the like [205, 206] deal with the usual IPs, with collisions being considered according to a binary scheme.

In conclusion let us note that in a number of works the dynamic effects due to interaction of the neutral particles with surfaces have also been studied. In particular, in Refs [207, 208] such effects have been considered for the van der Waals interactions of neutral atoms with cylindrical and plane surfaces. In Ref. [208] it was shown that, for nonrelativistic motion of an atom that moves parallel to the surface, apart from the attracting force, a stopping force of a comparable value and, under some conditions, even an accelerating force acting in the direction of motion of the particle and caused by the energy exchange of the particle with the surface plasmons may appear. Some other effects related to the small angle reflection of ions from the surface are considered in Ref. [245].

3.7 Characteristic features of interactions at high energies

In this Section we shall discuss briefly a number of recent results connected with taking into account the effects that are beyond the scope of the standard approximations for pair and averaged potentials. Thus, in radiation effects that appear in the interaction of relativistic electrons and positrons with the crystal lattice, a significant role is played by the noncoherent processes of gamma radiation generation with the simultaneous birth or absorption of crystal excitations [304, 306, 307, 317]. Radiation transitions accompanied by the transfer of the longitudinal momenta of the order of $2\pi n/d$ to the lattice (d is an interatomic distance in a chain) can be considered by taking into account only the discreteness of the atomic chains (and their potentials) in the longitudinal direction. This mechanism is especially significant in the regime that is transient from the plane to axial channelling. In the case of motion of electrons with angular momenta that are small with respect to the chains, it is necessary to take into account the variation of their kinetic energy due to longitudinal oscillations of period d/c, which is achieved by adding an additional term to a CP associated with this

energy [304]. The effect of a rainbow scattering of electrons appears in thin crystals [313, 314] because of the coherent addition of the amplitudes of scattering to the same angle for the momenta of different particles with respect to a single atomic chain. On the contrary, a similar effect in the scattering of positive particles (protons) [310, 311] was interpreted within the concept of the interference of the contributions of scattering from several chains.

In review [309] the phenomenon of dynamic chaos due to combined action of the crystal fields and noncoherent effects upon the oriented motion of the particles was considered. In particular, the idea of an atomic plane as a system of crystal axes was developed.

In order to take into account scattering of the particles by the field originating from the lattice polarisation, the optical (complex) potentials for the electrons and heavy particles are used [112, 318]. Within the scope of this approach, the stopping power functions and coefficients of 'absorption' of the heavy channelled ions were obtained.

In Refs [305, 319] the authors discussed induced-dispersion interaction of the particles with the lattice, which consists in the fact that on the atom that is moving in longitudinal-periodic field of a crystal lattice, an electric (and in a magnetic lattice — a magnetic) moment $p = \alpha E$ is induced, that interacts with the field generating that moment, during the whole period of the particle's flight. This effect accompanies the known phenomenon of the resonance excitation of the atom discovered by Okorokov [320]. One more work [305] deals with the potentials of magnetic interaction of neutrons with the magnetic field

$$\boldsymbol{H} = \frac{1}{c} \boldsymbol{v} \cdot \boldsymbol{E}$$

induced in their rest system, where v is the neutron velocity and E is the electric field of the lattice.

4. Experimental results

I would like to point out that, owing to the limitations of space and time, the analysis of the experimental results is not in the least exhaustive. In the process of selection of this material we put the emphasis on such topics, the theoretical interpretation of which within the bounds of description of the models still calls for elaboration. Discussion of the characteristic radiation in channelling is restricted to a plane case, where only those positions of the lines of the detected radiation which are directly connected with the potentials are considered. Other subjects can be found in monographs and reviews [10, 11, 112, 306-310, 314].

4.1 Energy losses and ranges of the low-energy ions

Over the last 15 years, significant progress has been made in describing the stopping of low-energy ($\varepsilon \ll 1$) ions and their ranges, when the main mechanism of energy losses is nuclear stopping. The universal theoretical model of Lindhard et al. [101] is at the base of these achievements. This model is based on application of the relations (3.16)–(3.18) for the cross sections of elastic slowing down, as well as the equation $s_e = 0.15\sqrt{\varepsilon}$ for the inelastic ones and the assumption of their independence. The result of the development of this concept is justification of the universal 'range-energy' dependence [50b, 50c, 142, 209, 210], which agrees with the experimental dependence $\rho_{exp}(\varepsilon)$ obtained for the amorphous silicon targets with a deviation of several percent (on the average). At a semi-empirical level, the introduction of the effects of Z_1 and Z_2 oscillations for the cross sections of slowing down was successfully achieved [50b, 50c, 211]. It further encouraged the successful development of the theoretical description of the processes of sputtering of solids due to ion bombardment [210-212]. Deviations from the universal dependence for the metal [213] and ion-crystal targets [214, 215] have been overcome by modification of the screening parameters of IPs [216] and by taking into account ion-ion components of interaction of a particle with a target [214, 215]. However, there is so far no adequate theoretical description of the Z_1 and Z_2 dependences of the stopping cross sections and variables related to them. This gap in the theory was known already at the level of differential cross sections of elastic scattering. Their oscillation, although observed in experiments [217, 218], could not be described even with the most precise interatomic IP calculated with respect to the electron gas model (a detailed discussion of these experiments and the results of calculations is given in Refs [48, 75]). The situation became even more complicated when a significant effect of the Z_1 oscillations of the ranges in amorphous semiconducting targets and its absence in metal targets was discovered [219-221]. Since at the energies of the order of 1 keV a.m.u.⁻¹, typical for these experiments, the ratio of the elastic and inelastic losses is about 10:1, the assumption was made that the range oscillations were due to the elastic cross section oscillations, and, finally, to the shell-effects of an IP. To this end, calculations of the ranges were carried out on the basis of application of the potentials that were calculated by means of the electron gas model [222-225], and which, as could be expected, were not in agreement with the experimental results. This can be seen from Fig. 15, where theoretical [225] and experimental dependences $\rho(\varepsilon)$ for the ions of Au, Yb, and Eu in amorphous silicon [220] are shown. Oscillations of the stopping cross sections were also observed on gaseous targets [218, 226]. In this work a suggestion was made that the effect was due to the oscillation of the cross section S_e of electron stopping. In that case, the corresponding amplitudes should be of the order of 200% of the mean values of $0.15\sqrt{\epsilon}$. Experimental results of the measurements of electron stopping [227] apparently disprove this conclusion, as they show that the amplitude of the Z_1 effect in carbon does not exceed 20%. Note that from the initial experiments concerning Z_1 oscillations it was known that their amplitudes in carbon are especially large [228, 229]. Thus, this effect is probably due to elastic stopping. Theoretical difficulties seem most serious so far as gaseous targets are concerned since the potentials of interaction of the free atomic particles in this case are more adequate for the experiments. As an alternative, factors responsible for the oscillations of differential cross sections, an impact of inelastic effects on the one hand [231] and generation of the quasimolecular states [48, 218] on the other, were suggested but these ideas have not been developed to a proper extent.

The problem of the absence of Z_1 oscillations of the ranges in metal targets remains unsolved as well. A working hypothesis was proposed in Refs [220-225] that the electron gas screening the ion 'masks' the details of the shell structure. General considerations suggest, however, that for a large ion size a screening electron cloud should

Figure 15. Ion ranges in reduced units. Open circles denote the experimental data [220], and solid circles the theoretical calculations [225]. Solid lines are for the purpose of demonstration of the dependence.

also be large enough, so the peripheral electron distribution around an ion should be very close to the distribution that corresponds to a neutral atom, and therefore the fact of suppression of the Z_1 effect seems doubtful. On the whole, these matters have still not been clearly understood.

4.2 Multiple scattering

A detailed review of multiple scattering considering the relation between theory and experiments up to 1980 is given in Ref. [75], where the corresponding references are cited. A number of recent results can be found in Refs [233-239]. On the whole it can be said that, for the large reduced target thicknesses $(T \gg 1)$, see Section 3.3), a good agreement between the theory and experiments is evident. However, for 'slow' ions with energies between 3 keV and 1 MeV, in a number of cases essential divergences were noted [240–242]. In Ref. [241] Z_1 oscillations of the angular half-width of the scattered particle distribution were observed. In scattering on the polycrystal targets with grain sizes over 100 A, the experimental angular half-width is sometimes only 25% of the theoretical half-width [243]. This difference was attributed to the influence of channelling. Experimental angular distributions (especially for thin targets) are, as a rule, narrower that the theoretical ones, which indicates a weaker scattering potential. However, in the interpretation of the angular distributions of the Li ions scattered on V, Cr, Fe, Co, and Ge targets [240], on the contrary, it was necessary to decrease the screening parameter by 20% - 30% in order to improve the agreement with the experimental results, i.e. the scattering potential was higher than the theoretical one.

Recently, interest in multiple scattering had increased because of the correlation that was discovered between the energy losses and the angle of escape of a particle leaving the film. For ions, this effect was noted in Refs [232-234], and for electrons in Refs [235-236]. In these studies, an increase in the stopping losses of particles with an increase in the angle of the outgoing particle was observed with subsequent saturation of dependence. Intensification of the effect with the increase of Z_2 was noted. In the case of penetration of the protons with energy 100 keV [234], the effect was observed up to the outgoing angles of $\alpha = 15^{\circ}$. The practical significance of these investigations is stipulated by the necessity of increasing the accuracy of measurements of the energy losses of proton beams used for calibration in studies of the radiation stability of materials (in particular, biological tissues). The interpretation of experiments [232-234] is not completely clear so far (see, for example Refs [237, 238]). While at the energies of E < 1 MeV in the angular range $0^{\circ} - 3^{\circ}$ one might expect the influence of the channelling effect for a part of the beam [234], for the angles of $10^{\circ} - 15^{\circ}$ it is certainly not the case, and therefore the experimental results cannot be explained by this effect (although it diminishes energy losses). The same can be said about experiments [232, 233], where the proton energy was 7 MeV. The saturation of the dependence was observed at the angles $3^{\circ}-4^{\circ}$, which exceed the critical angles of channelling by an order of magnitude. In Ref. [237] it was noted that although the simulation results [233] agreed with the experimental dependences, the stopping powers that were used in calculations and that depended upon an impact parameter, were three times the stopping losses calculated in the local electron density approximation, which was considered reliable enough at these energies. Calculations of the slowing down made by means of the semiclassical model [238] with separation of the contributions of the inner and outer electrons led to still lower values of the energy losses (for the impact parameters close to zero).

The investigation of multiple scattering of the partially 'stripped' ions, with specific processes of charge exchange and screening, or when there is *E*-dependence of an IP, is of particular interest. For light ions with $Z_1 < 10$, the first two effects are most important. In Ref. [239] angular distributions of the ¹⁴N and ¹⁶O ions with energies 30-330 keV a.m.u.⁻¹ scattered on metal films were measured. The authors of Ref. [239] achieved a consistency between the measured and theoretical (according to Moliere) angular distributions, on the condition that the effective ion charges responsible for multiple scattering are 1.5-1.8 times as high as the effective 'stopping' charges. Hence, it was concluded that a multiple scattering process occurs at smaller impact parameters than that of stopping. This conclusion seems to contradict the idea of correlation of energy losses with the scattering angle, which has been discussed earlier. In order to clarify this point, in Ref. [107] calculations of the angular distributions were made with respect to the Moliere theory modified with an interaction potential taking into account the experimental values of the

Figure 16. Angular distributions of the ¹⁶O ions that penetrated an Al film with the thickness $l = 0.3 \,\mu\text{m}$; • and • — experiment [239] for E = 1.25 and 1.77 correspondingly; *l* and 2 — theoretical calculations that ignore the dynamic screening [108]; *3* and 4 — taking into account the screening and degree of ionisation.

degree of ionisation and dynamic screening. The results of computation of angular distributions of the ions scattered on the aluminum films are compared with the experimental ones in Fig. 16. The value of the plasma frequency is assumed to be equal to 0.57 a.u. From Fig. 16, it follows that the application of a more correct potential can explain experimental dependences without additional assumptions concerning 'special' impact parameters.

4.3 Critical angles of channelling

In the Lindhard model [70], a critical channelling angle θ_{cr} is directly connected with the value of a scattering potential. In the axial case, θ_{kr} can be found from the equation

$$U_{\rm ch}(\theta_{\rm cr}d) = E\,\theta_{\rm cr}^2\,\,,\tag{4.1}$$

where $U_{ch}(r)$ is a continuous potential (CP) of the atomic chain that is defined by Eqn (3.50), d is the distance between the atoms of the chain, and E is the particle energy. For a CP (3.52) from (4.1) the well known formulas for θ_{cr} at high and low energies [176] follow

$$\theta_{\rm cr} = \begin{cases} \sqrt{\frac{2Z_1Z_2}{dE}}, & E > \frac{2Z_1Z_2d}{a^2}, \\ \left(\frac{3Z_1Z_2a^2}{d^3E}\right)^{0.25}, & E < \frac{2Z_1Z_2d}{a^2}, \end{cases}$$
(4.2)

where a is a screening parameter. The value of the energy,

$$E = \frac{2Z_1 Z_2 d}{a^2} \,,$$

in the case of proton channelling in (110) Ge is 170 keV. In experiments, the angular half-width of the backscattering dip $\psi_{1/2}$ proportional to $\theta_{\rm cr}$ is measured rather than $\theta_{\rm cr}$ itself [178, 244, 246]. The dependences $\psi_{1/2} \propto E^{-1/2}$ and

 $\psi_{1/2} \propto E^{-1/4}$ that follow from Eqn (4.2) at high and low energies are nicely verified in experiments, although the low-energy range (E < 0.5 MeV a.m.u.⁻¹) is less studied [247-250] because the experiments are complicated by the dependence of $\psi_{1/2}$ on the scattering depth, by the necessity of a detector with better energy resolution, and by other factors. I would like to stress, however, that the dependence $\psi_{1/2} \propto E^{-1/2}$ is good for any form of potential, where a relation $\psi_{1/2} \propto E^{-1/4}$ is specific only for the Lindhard potential given by Eqn (3.52). In the general case, solution of Eqn (4.1) leads us to function $\theta_{\rm cr}(E)$ of a more complicated form which has been noted for the first time in Ref. [251], where the 'fall' of the dependence $\theta_{\rm cr}(E)$ (from the low-energy part) in channelling of the protons of the keV energies in tungsten has been studied. Experimental confirmation of this result was reported in Ref. [252].

In the event of plane channelling at both low and high energies, relation $\theta_{\rm cr} = \sqrt{U_{\rm B}/E}$ is valid, where $U_{\rm B}$ is the height of the potential barrier, and therefore the energy dependence (if any) of the value of $\psi_{1/2}\sqrt{E}$ unambiguously indicates a variation in CP. This fact was noted for the first time in Refs [91, 166, 167], where it was shown that an E dependence of an IP or its variation due to influence of dynamic screening and variation in the charge state could induce an increase (decrease) of $\psi_{1/2}$ in comparison with the expected values by a factor of 10% - 15%. A decrease in the recorded angles of capture of Br and I ions in the plane channels of an Au crystal with the increase of energy have been noted in Ref. [253], where the channelling of ions with the energies of 20-80 Mev has been studied. Unfortunately, there are no other experimental data available. It should also be noted that the form of a CP also influences the angular profile of the backscattering dip [176]. However, this phenomenon did not attract the attention of those who tried to find a more precise definition of a potential.

4.4 Measurement of the trajectories and potentials in the planar channelling of heavy particles

The planar channelling of ions, in contrast to the axial type (and also to the channelling of electrons and positrons), is specified by a marked periodic motion of particles at small depths (in this case the effects of multiple scattering are still small). This effect results in oscillations of the back-scattering yield and the secondary processes concurrently with the approach of the particles to the atomic planes. The stopping the moving ions generates energy 'scanning' of the backscattering spectrum, its oscillations being due to the reflection of particles at depths that are multiples of the trajectory half-wave $\lambda/2$. The distance between adjacent maxima *a* and *b* of the energy spectrum is given by [254]

$$\Delta E_{ab} \approx \frac{\lambda}{2} \left[S_{\rm r}(k^2 E_0) \frac{\cos \theta_{\rm in}}{\cos \theta_{\rm out}} + \gamma k^2 S_{\rm r}(E_0) \right], \qquad (4.3)$$

where E_0 is the initial energy, k is a kinematic factor of the backscattering, θ_{in} and θ_{out} are the angles of incidence and emergence from a crystal which are estimated from the normal to the surface, $S_r(E)$ is the stopping power of a nonoriented motion, γ is the ratio of the stopping power of the particles with a large oscillation amplitude, contributing to the scattering, to S_r . Measuring ΔE_{ab} gives information related to λ and a potential, on the one hand, and to the energy losses, on the other hand. In most known experiments [255-263], such spectra have been measured for different ratios of $\cos \theta_{\rm in} / \cos \theta_{\rm out}$ (the so-called 'cosine method' [254]), and the value of λ has been determined from Eqn (4.3) by means of the tabulated values of $S_{\rm r}$ [50b]. Barrett [264] proposed a 'q-method', where the $\psi_{\rm m}$ angle corresponding to the maximum of backscattering could be found by scanning the angle of inclination of the beam with respect to the planes. The value of $\psi_{\rm m}$ is related to $\lambda/2$ by the expression

$$q = \frac{\lambda}{2} \psi_{\rm m} d_{\rm p} , \qquad (4.4)$$

where d_p is the interplanar distance, q is a constant of the order of unity, which is typical for the given energy and plane. Eqn (4.4) is derived by computer simulation and has a clear physical meaning: if a particle that starts moving from the centre of a channel at the angle of ψ_m with respect to a plane moves along a straight line, then it would intersect the plane at the depth $\Delta z = \lambda/4$. In this case we would have q = 1. In reality, its trajectory is curvilinear, which increases the values of λ and q. Ref. [254] shows in particular that, for the He ions with the energies 1-2 MeV which are channelling in a germanium crystal, 1.39 < q < 1.43. The param-eters λ and ψ_m are connected with a CP in an obvious way:

$$\psi_{\rm m} = \sqrt{\frac{U_{\rm B}}{E_0}}\,,\tag{4.5}$$

$$\lambda = 4\sqrt{\frac{2E_0}{M_1}} \int_0^{d_p/2} \frac{\mathrm{d}x}{\sqrt{U_\mathrm{B} - U(x)}} \,, \tag{4.6}$$

where x is counted from the middle of the channel, $U_{\rm B} = U(d_{\rm p}/2) - U(0)$ is the barrier height of the potential, M_1 is the mass of the particle. Comparison of the theoretical [calculated with Eqns (4.5) and (4.6) and by simulation] and experimental values of λ and $\psi_{\rm m}$, determined by the 'cosines method' and by the 'qmethod', shows us [254] that there is an agreement between them with a 3%-10% deviation, where the He-Ge IP should be 'weaker' than the Moliere potential having a screening parameter given by Eqn (2.29). This is probably due to the influence of the screening with respect

Figure 17. Relative yield of the backscattered helium ions with the energy 2 MeV as a function of the depth while channelling in (110) Ge [254]. The points correspond to the experimental values, and the solid line to the simulation.

to a bonded He electron and the electron gas of the crystal. In Fig. 17 the experimental and simulated spectra of the yield of the backscattered particles are shown as a function of the depth, the resolution with respect to the latter (in experiment and in simulation) being 12-13 nm.

Another trend in the empirical evaluation of potentials has been initiated by the works of Robinson [265]. It is based on the application of empirical dependence of stopping losses upon the frequency of oscillations of the ions in a channel (α and β are empirical constants typical of a given type of an ion and channel):

$$S(\omega) = \frac{\mathrm{d}E}{\mathrm{d}x}\Big|_{E=E_0} = \alpha + \beta\omega , \qquad (4.7)$$

where ω is the frequency of oscillations which can be determined by the formula (x_{max} is an oscillation amplitude)

$$\omega^{-1} = 2 \int_0^{x_{\max}} \frac{\mathrm{d}x}{\left[U(x_{\max}) - U(x)\right]^{1/2}} \,. \tag{4.8}$$

Factor $\sqrt{2M_1}$ in Eqn (4.8) is omitted, because it is included in the coefficient β in Eqn (4.7). Robinson proposed a model expression for the stopping power of the form

$$S(x,E) = S_0 + S_1[\sigma(x) - 1], \qquad (4.9)$$

where x is an ion coordinate in a channel, S_0 and S_1 depend on the energy, and $\sigma(0) \equiv 1$.

Assuming that an ion has made an integer number of half-oscillations, after averaging Eqn (4.9) with respect to the period of motion and taking into account Eqn (4.7), we will get:

$$\alpha = S_0 - S_1 , \qquad (4.10)$$

$$\beta = 2S_1^{x_{\max}} 0 \,\sigma(x) \,\frac{dx}{\left[U(x_{\max}) - U(x)\right]^{1/2}},$$

$$0 \le x_{\max} \le \frac{d_p}{2}.$$
 (4.11)

Solution to the integral equation (4.11) with respect to $\sigma(x)$ has the form

$$\sigma(x) = \frac{\beta}{\pi S_1} \frac{d}{dx} \left[U(x) - U(0) \right]^{1/2}, \quad 0 \le x \le \frac{d_p}{2}.$$
(4.12)

Taking into account the parity of U(x) and the condition $\sigma(0) = 1$, from Eqn (4.12) it follows that

$$U''(0) = 2\pi^2 \frac{(S_0 - \alpha)^2}{\beta^2}.$$
(4.13)

One more relation is obtained by averaging Eqn (4.9) with respect to the coordinate x. Taking into account Eqns (4.7)–(4.11) and Eqn (4.12), we get

$$S_{\rm r}(E) = S_0 + S_1 \left[\frac{2}{d_{\rm p}} \int_0^{d_{\rm p}/2} \sigma(x) \, \mathrm{d}x - 1 \right]$$

= $\alpha + \frac{2\beta}{\pi d_{\rm p}} \left[U\left(\frac{d_{\rm p}}{2}\right) - U(0) \right]^{1/2}$. (4.14)

The variables α , β , S_0 , and $S_r(E)$ are found directly from experiment. Inner consistency of the model is verified by the closeness of the values of $S_r(E)$ obtained from Eqn (4.14) for different channels by means of different CP. When CP is specified in an appropriate parametric form, Eqns (4.13)-(4.14) allow us to find approximation parameters making use of the data for several channels. In Ref. [265] this method was used for estimating the IP of H, He, O, and I ions with Si and Au atoms. In the case of H and He ions, empirical potentials agreed well with the Hartree–Fock IP but not very well with the Moliere IP. For I ions the agreement was poor (in each case it was assumed that an ion is a bare particle with an effective charge corresponding to a given velocity).

In Ref. [266], Eqns (4.9) and (4.12) were used for calculating the energy losses of α particles in the plane channels of Ta with different approximations of CP. A weak dependence of the form of the resulting spectra from CP was detected. In Ref. [267] functions S(x, E) were calculated with Eqn (4.9) for a plane potential of the form

$$U(x) = 2\pi Z_1 Z_2 N d_p \sqrt{3}a^2 \times \left(\frac{1}{0.5d_p + a - x} + \frac{1}{0.5d_p + a + x}\right),$$
(4.15)

where standard designations were used. Parameters S_0 and S_1 necessary for the calculations were taken from the experiment [268]. The calculation results were compared with the computational ones for S(x, E) which were carried out with respect to the local electron density model [for α particles in the channels of (100) and (110) Si]. The agreement of the S(x, E) functions close to the channel walls was interpreted as a proof of adequacy of the CP [Eqn (4.15)] for the given case. In particular, an agreement was observed of the experimental values,

$$\sigma'_{\rm exp} = (S_{\rm r} - \alpha) \, \frac{\pi}{\beta} \, ,$$

with the theoretical ones,

$$\sigma_{\rm th}' = \frac{2}{d_{\rm p}} \left[U\left(\frac{d_{\rm p}}{2}\right) - U(0) \right]^{1/2},$$

within a deviation of 7% - 8% ($\sigma'_{th} < \sigma'_{exp}$). It is quite obvious, however, that the temperature influence, ignored in Eqn (4.15), will cause an additional decrease in the height of a potential barrier of at least 10%. Thus the total deviation of the value of $U(d_p/2) - U(0)$ from its experimental value will be ~ 35 %, so that the advantage of the potential [Eqn (4.15)] is dubious. One more method of estimating the plane potentials was used in Ref. [270]. The basic relations are of the following form (x is a coordinate, U is a CP):

$$\begin{aligned} x(U) &= \frac{1}{(8\pi M_1 \nu_1)^{1/2}} \int_0^U \lambda_{\rm ch}(E_\perp, U) \frac{\mathrm{d}E_\perp}{\sqrt{U - E_\perp}} \,, \\ E_\perp &= E \psi_{\rm in}^2 \,, \end{aligned}$$
(4.16)

where $\lambda_{ch}(E_{\perp}, U)$ is a 'wavelength' of particle oscillations with transverse energy E_{\perp} , ψ_{in} is an initial 'ingoing' angle with respect to the planes. In this case, the experimental parameters are λ_{ch} and ψ_{in} [see Eqns (4.3) and (4.6)]. It is pretty obvious that Eqn (4.16) is the inverse of Eqn (4.6) and is a special case of the known equation of the reconstruction of the potential by the period of motion in a one-dimensional potential field [95].

4.5 Dependence of energy losses of heavy ions on the frequency of oscillations in planar channelling

In Refs [91, 92] some essential details of experiments in which the dependence of energy losses [Eqn (4.7)] was studied are presented. This has not, however, attracted

Figure 18. A diagram of the ion motion in a plane channel for different CPs. The turning points *i*, *j* and *i'*, *j'* correspond to the oscillation frequencies ω and $\omega + \Delta \omega$.

sufficient attention. Moreover, the dependence given by Eqn (4.7) itself was not given a thorough theoretical explanation. Its main peculiarity is increase of the coefficient β with the increase of the ionic energy. Following Ref. [91], we will show that this fact is directly connected with the decrease of the planar CP due to the energy dependence of the interaction potential. This is illustrated through Fig. 18, where the turning points i-iand j-j of an ion having the same frequency of oscillations ω but moving in different potential wells are shown schematically. Owing to the greater steepness of curve 2, the points j-j are located further from the channel walls than the points i-i. With an increase in the oscillation frequency of $\Delta \omega$, the new turning points i' - i' will be displaced relative to the channel walls to a greater degree than the points j' - j' because the potential curves are less steep. This suggests that, for ions having different energies but the same stopping power, the energy losses of the particles moving in a less steep CP will be higher since the ions move in the domain of a higher density of the electrons and nuclei of the crystal. Comparing this supposition with the experimental dependence [Eqn (4.7)], we can conclude that potential curve 2 in Fig. 18 corresponds to a lower energy. On the contrary, for a CP which increases with an increase in energy, the coefficient of inclination β would decrease. Quantitative calculations confirming these conclusions were reported in Refs [107, 333]. Fig. 19 presents experimental and computational dependences $S(\omega)$ for the I ions with energies of 15 and 60 Mev for channelling in (111) Au. In the calculations of an I-Au IP, an electrostatic interaction with respect to Eqn (2.18) was taken into account as well as the contribution of the kinetic energy of the electron gas with respect to Eqn (2.61), and the densities of the Au and I electrons were obtained from Eqn (2.48) taking into account the experimental values of an ionisation degree of the I ions for the given energy $(Z_1 - N_1 = 13$ for E = 15Mev and $Z_1 - N_1 = 22$ for E = 60 MeV [272]). The coefficients c_i and b_i in Eqn (2.48) corresponded to the

Figure 19. Stopping powers of 127 I ions while channelling in (111) Au as the functions of the oscillation frequencies and energy: solid lines represent experimental values; dashed lines represent the values of calculation in the quasistatic approximation [333]; dotted lines represent the values of calculation for the potential given by Eqn (4.17).

approximation in Ref. [68]. The IPs calculated in this way were averaged by a standard method taking into account the thermal oscillations. The resulting CPs are shown in Fig. 20 along with the potentials of Moliere type for the effective ion charges $Z_{1\text{eff}} = 13$ and $Z_{1\text{eff}} = 22$, respectively. In the second case, the I-Au IP is

$$V(R) = \frac{Z_{1\text{eff}}Z_2}{R} \Phi\left(\frac{R}{a_2}\right), \qquad (4.17)$$

where $a_2 = 0.8853Z_2^{-1/3}$ is a screening parameter of an Au atom, and the function $\Phi(x)$ corresponds to that given in Ref. [68]. Fig. 20 shows us that the dynamic decrease of the potential is most dramatic in the middle part of a channel.

Figure 20. A CP for the I ions for channelling in (111) Au: curves 1, 2 represent an 'effective charge' approximation [Eqn (4.17)]; curves 3, 4 represent a quasistatic approximation [107, 333].

On the contrary, Eqn (4.17) leads to an increase of CP when the particle energy increases.

In order to find a theoretical dependence $S(\omega)$, the oscillation frequencies with respect to Eqn (4.8) were calculated followed by elimination of the amplitudes x_{max} by means of the coordinate dependence of the stopping losses averaged with respect to the period of motion and taken in the form

$$S(x,E) = 0.034 Z_{\text{leff}}^2(E) \left(1 + \frac{16}{d_p^2} x^2\right) \text{ MeV } \mu \text{m}^{-1}$$
 . (4.18)

Eqn (4.18) provides an approximation of the results of theoretical calculation of the stopping losses [273] for He and I ions in an Au crystal. As can be seen from Fig. 19, the theoretical calculation (dotted curves) correctly shows the main feature of the experiment: increase of the steepness β with the increase of energy. Some overestimation of the oscillation frequencies of ions can be accounted for by the errors in calculation of the potentials. Analogous calculations for a CP [Eqn (4.17)] which are shown by dotted and dashed lines show a decrease of steepness of β with the energy increase. One more consideration in support of this theory arises when the stopping powers of I ions for a disoriented crystal are compared. Thus, for the energies of 15 and 60 MeV, the corresponding experimental values were 9 and 23.9 Mev μm^{-1} [274], i.e. they increased by a factor of 2.65. At the same time, the square of the charge of the ions increased by a factor of $(22/13)^2 = 2.9$. In accordance with Eqn (4.14) this discrepancy can be related to the decrease of the potential barrier height by 10-15% owing to the energy dependence of the IP. This fact conforms with the agreement between the theoretical and experimental estimates of $S_r(E)$ which occurs with the energy increase [265], since the theoretical values for the stopping losses were estimated for the potential [Eqn (4.17)] which grows with the energy. In this case, the rise in $S_r(E)$ in accordance with Eqn (4.14) occurs more rapidly than in the dependence $\propto Z_{\text{leff}}^2$, which follows from Eqn (4.18) and is averaged with respect to the coordinate x; and thus the stopping 'deficit' observed at E = 15 MeV decreases at E = 60 MeV (see the data of Table 3 in Ref. [265b]). Thus the dependence $S(\omega) = \alpha + \beta \omega$ is defined, on the one hand, by dynamics of the motion of ions in the channel which is determined by the CP, and, on the other, by dependence of the stopping upon the coordinate Eqn (4.18). Let us note that, for sufficiently high energies, when an IP begins to rise (see Section 2.7), the parameter β in Eqn (4.7) decreases down to its asymptotic value which corresponds to the potential [Eqn (4.17)] for $Z_{1\text{eff}} = Z_1$. Therefore estimates of β for different energies could give valuable information for the more precise definition of the energy dependence of an IP.

4.6 Characteristic radiation of the channelled electrons and positrons

When the relativistic leptons are channelled, the wave function of the bonded motion satisfies the Schrodinger equation [275-277]:

$$-\frac{1}{2\gamma}\Delta_{\perp}\Psi(\mathbf{r})_{\perp} + \left[U(\mathbf{r}_{\perp}) - E_{\perp}\right]\Psi(\mathbf{r}_{\perp}) = 0 , \qquad (4.19)$$

where γ is the Lorentz factor,

$$\Delta_{\perp} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \,,$$

r(x, y) is a transverse projection of the radius vector to a plane xy that is perpendicular to the direction of the longitudinal motion, $U(\mathbf{r}_{\perp})$ is a continuous potential (in the case of planar channelling, $\Delta_{\perp} = d^2/dx^2$). It is shown in Refs [112, 275, 278] that for the electrons with energies E < 50 MeV for planar channelling and E < 10 MeV for the axial type the energy levels E_{\perp} are discrete. The radiation lines that correspond to the spontaneous transitions between them, taking into account the relativistic transformation of the frequency, conform to the energies

$$E_{\gamma} = 2\gamma^2 \Delta E_{\perp} . \tag{4.20}$$

Nonequidistance of the E_{\perp} levels leads to emergence of some isolated peaks in the spectrum, which allows us to estimate the spatial location of the radiating particles. The spectrum of the transverse energies and gamma quanta is in all probability determined only by the form of a CP.

Comparison of the experimental and theoretical values of the energies E_{γ} that have been calculated for the specific potentials allows us to assess their quality. On the other hand, the experimental information can be used for various purposes, i.e. diagnostics of the potentials, in the analysis of the electron density in channels, in the measurement of Debye temperatures, in the study of the anisotropy of the thermal oscillation of the lattice atoms, etc. [11, 280, 281, 186, 306, 307].

Electron radiation in axial channelling in diamond and silicon crystals was reviewed in Refs [283, 284], in planar channelling in Refs [285, 287, 288], and for positrons in Refs [288, 290, 291]. Radiation in a LiF crystal was investigated in Refs [292, 293], and in some other crystals of a complex type in Refs [285, 294, 295]. In the calculations of spectral lines, potentials of the Doyle-Turner type were most often used [Eqns (3.74) - (3.75)], and the Schrodinger equation (4.19) was solved by the plane waves method. In Refs [296, 187, 298] a quasiclassical approximation was used, and for positrons the classical method was used, because for energies E > 50 MeV the number of levels of coupled motion is sufficiently large. In these studies, a planar potential that corresponds to the model given by Eqn (2.25) was used. In Ref. [299] a variational method of solving the Schrodinger equation with a Doyle-Turner potential was used. The results of the theoretical calculations of the energies of the radiation peaks agree well with each other and with the experimental data. In Refs [287, 296, 187], however, it was noted that the frequencies corresponding to the maxima of the positron radiation for the Doyle-Turner (DT) potential exceeded the experimental values by approximately 7% - 10%, whereas for the electron deviations they exceeded the experimental values by 1% - 5%. In this respect, a CP for the piecewise exponential model (PEM) given by Eqn (2.25) proves to be more universal, which is confirmed by the data of Tables 5 and 6. Calculations with the Moliere potential have a poorer agreement with the experimental data. Note that the initial calculated values of a CP with the application of the PEM were overestimated [187] [in Eqn (14) of this work the last term must have a positive sign].

Data in Tables 5 and 6 show that the DT potential is responsible for the higher energy values of the peak of positron radiation and for the higher energies of the separate lines for the electrons [especially in the case of transition 1-0 in (100) and (110) Si]. On the contrary, a

Table 5. Energies of the gamma quanta in the maximum of a radiation peak of the channelled positrons. In columns 3-5, the results of calculations corresponding to the PEM, the Moliere potential, and the DT potential, respectively, are given.

Plane	γ	Calculated values	Experimental values			
	Refs [296, 187]		Ref. [187]	R efs [290, 291]	R efs [290, 291]	
(110) Si	111	42	40	44.2	42.5	
(110) Si	107.4	38	37	41.6	38.8	
(100) Si	111	45	45	46-51	46.7	
(110) C	107.4	64	60	69.2	65.3	
(110) Ge	107.4	49.5	_	52.2	48.1	

PEM approximation leads to smaller energies of the 1-0 transition. These deviations cannot be related to the inaccuracy of the quasi-classical approximation used in Refs [296, 187], because it was shown [187] that the error of this method in determining the levels of transverse motion does not exceed 1% even for energies of 5-10 MeV. An additional test of the potentials allows comparison of the sums of energies for the separate transitions. Table 7 lists the values corresponding to the potentials in Tables 5 and 6 and shows that eventually the sums of the PEM differ from the experimental values by only 1% - 2%. This fact is due to a compensation of the energy 'deficit' for the transitions from the lower levels by a corresponding 'excess' for the higher levels. In the case of the DT potential, deviations are somewhat larger and reach 2.5% - 3%

These results make it possible to evaluate somewhat differently an attempt to define more precisely the Debye temperature of the silicon crystal in Ref. [285b], where in order to achieve consistency between theoretical and experimental values of the energies of quanta in the 1-0line, the value of 495 K was taken instead of 543 K (the commonly used value corresponding to the data of x-ray diffraction [302, 303]). More precise calculations in Ref. [312] resulted in the values of $\theta_{\rm D} = 504$ K for T = 298 K, and $\theta_D = 514$ K for T = 110 K. Note that a deviation of $\theta_{\rm D}$ influences only the 1–0 transition, and does not influence the other levels. On the contrary, if we try to achieve such an agreement for the PEM potential, $\theta_{\rm D}$ will have to be increased to up to 575 K, which will result in a noticeably poorer agreement between the theoretical and experimental values of $\sum E_{\gamma}$. Thus, the Debye temperature values cannot be revised without the critical choice of a CP.

Similar remarks can be made in connection with the use of the radiation spectra of the channelled particles for determination of the electron densities in a channel [283] based on the Poisson equation

$$\rho_{\rm e}(\mathbf{r}_{\perp}) = \frac{1}{4\pi} \,\Delta_{\perp} V(\mathbf{r}_{\perp}) \,. \tag{4.21}$$

The method used here consists in correcting the theoretical values of the form factor of the potential in Eqn (3.62) to attain conformity between the theoretical and experimental spectra. This procedure is not quite correct mathematically, because the Fourier transform of the atomic factor, represented by a sum of Gaussian exponents [Eqn (3.72)], does not present correctly the shell distribution of the potential and the electron density which would

Plane	γ	Transition	Calculated values	*		Experimental values	
			Refs [296, 187]	Ref. [300]	Refs [291, 180]	R efs [291, 292]	
(110) Si	110.6	1 - 0	122.4	139.1	134	128	
, ,		2 - 1	94.8	101.4	96	94	
		3 - 2	70.6	75.5	69	68	
		4-3	53.8	58.2	53	52	
		5-4	43.6	45.4	41	42	
(110) Si	55.8	1 - 0	38.7	44.8	_	40	
		2 - 1	26.8	28.9	_	25	
		3-2	19.0	19.8	_	17	
(100) Si	110.6	1 - 0	95.2	109.1	_	99	
		2 - 1	66.3	72.3	_	64	
		3 - 2	45,3	50.3	_	39	
(100) Si	55.8	1 - 0	29.5	34.3	_	31	
		2 - 1	17.6	17.3		21	
(110) C	106.7	1 - 0	158.4	161**	163.8	161.8	
		2 - 1	104.3	100**	108.3	104.4	
		3 - 2	78.2	72**	79.0	78.4	
		4-3	56.3	49**	60.4	58	
(100) C	106.7	1 - 0	116.9	117**	120.6***	120	
. /		2 - 1	65.1	57**	65***	65.4	

Table 6. Energies of the gamma quanta radiated by the channelled electrons in the 'forward' direction.

*The results of calculations in columns 4-6 correspond to the same potentials as in Table 5 (columns 3-5).

**These values are taken from Ref. [276].

***These values are taken from Ref. [301].

 Table 7. Total values of the gamma-quanta energies of the planar channelling of the electrons.

Plane	γ	Calcula	ted values	Experimental values	
		(1)	(2)	(3)	, and b
(110) Si	110.4	385.2	417.6	393	384
(110) Si	55.8	84.5	93.5		82
(100)Si	110.6	206.8	231.7		202
(110) C	106.7	397.2	382	411.5	402.6
(100) C	106.7	182	174	185.6	186.3

*Data in the columns (1), (2), and (3) correspond to those of the columns 4-6 in Table 6.

correspond to the Hartree–Fock distribution. In addition, when we make a correction of the form factors by the value of $\Delta V_{\rm g}$, the corresponding function can be determined only for a finite number of vectors. Therefore, the reciprocal which is an inverse Fourier transform for the atomic potential and electron density in a crystal, is not unique. As a result, there is an entire class of functions of the electron density distributions and Debye temperatures for which it is possible to reach an agreement between the theoretical and experimental data [306]. I believe that a more consistent approach would be to apply the analytical Hartree–Fock approximations of the PEM type or the Bonham–Strand model [321] rather than the DT model, where a correction function $\Delta V_{\rm g}$ should ensure fulfillment

of the standard normalising conditions that are imposed upon the atomic potential and electron density. The models mentioned above provide correct initial approximations for the solution of this problem.

In Refs [292, 293] a form factor correction was also used in calculations of the radiation spectra in a LiF crystal, where the amplitudes of the thermal oscillations of the Li⁺ and F^- ions corresponded to different values of Debve temperatures. Thus, in Ref. [292] the ratio of the amplitudes was equal to 1.28 instead of 1.65; this latter value followed from the relation $k_{\rm B}\Theta_{\rm D} \sim M_{\rm i}u_{\rm i}^2$ (M_i is an ion mass, $k_{\rm B}$ is the Boltzmann constant). This fact, together with the disagreement of the values of $\Theta_{\rm D}$ used by different authors (especially for the crystals and alloys of a complex composition), makes the comparison and interpretation of results rather difficult. Thus, the authors of Refs [285, 293] came to the conclusion that the amplitude of thermal oscillations of a F^{-} ion in a LiF crystal is underestimated by a factor of 2, and in a LiH crystal the amplitudes of H are twice as high as those of D in LiD. It was noted (see also Ref. [306]) that this conclusion is supported by Fig. 21, where the experimental radiation spectra of the electrons with the energy of 54.5 MeV in the (100) channel of the LiH and LiD crystals are shown. The conclusion is based on the apparent shift of the radiation lines into the lower frequency domain for a LiH crystal. However, it follows from the theory that variation of the Debye temperature (and in the thermal oscillations amplitude as well) influences noticeably only the frequency of the 1-0 transition, whereas in Fig. 21 one can see the shift of all the lines. Besides, at a higher

Figure 21. Radiation spectra of the electrons of 54.5 MeV channelled in the (100) plane of the LiH and LiD crystals [239, 295].

amplitude of the thermal oscillations the line width should be greater for a LiH crystal (for example, the impact of the temperature upon the spectra shown in Fig. 7 in Ref. [306]), which also does not agree with the data given in Fig. 21. Thus, we arrive at opposite conclusions.

It is shown in Ref. [186] that comparison of the intensities of the first maxima of the coherent bremsstrahlung radiation (CBR) can give us significant information on the values of the ionic charges of the crystal atoms (in the case of planar channels that consist of the planes with the ions of different CBR signs [for example, (111) NaCl]. This can be explained by the presence of harmonics with the periods of d_p and $2d_p$ in a CP (d_p is the distance between the planes with the ions of different signs), where the Fourier harmonics of the larger period are proportional to the ionic charges of the crystal atoms. In my opinion the possibilities of diagnostic application of the CBR spectra have not yet been fully understood, whereas the CBR peak amplitudes are directly related to the separate Fourier harmonics of the crystal potential, in contrast to the radiation spectra in channelling which are formed by the total potential.

It is useful to note a number of works related to the spectral characteristics of the radiation of channelled particles taking into account the dislocation effects [315-316] and the influence of the external periodic fields [277, 305, 307], as well as works dealing with direct reconstruction of the potentials through their spectra [322-323]. The latter problem is a complicated one and needs additional analysis.

In conclusion it may be said that although the theory is successful in explaining the characteristic features of the observed radiation spectra, application of these data in the framework of a new diagnostic method will impose rigid requirements concerning the quality of the potentials required for the calculation models. At present, these requirements are not fully satisfied.

5. Conclusions

It can be seen from this review that the concept of interatomic potentials is widely used in the study and

interpretation of numerous phenomena associated with the penetration of beams of the charged particles in matter. Many of these phenomena (such as sputtering, phase transitions due to irradia-tion, interaction with surfaces, energy losses in channelling, dechannelling, etc) were considered only briefly, or completely omitted, here. Progress in experimental techniques over the last 10-15years enables one to carry out measurements of various values pertaining to a particle beam with an accuracy of several percent (including the values for energy losses and ranges, angular and energy distributions, radiation spectral lines in channelling, etc.). The experimental results promoted the formation of the modern ideas concerning the physical nature of the processes of stopping and channelling of particles in matter, radiation in channelling, and the yield in secondary processes. These achievements have led to the creation of new experimental methods of measurement of IPs and some other variables, the information related to them being a powerful tool for the probing of solids.

At the same time, there are still problems which, along with the interpretation of experiments (they are, first of all, Z_1 and Z_2 oscillations of the scattering cross sections, stopping, and ranges), also involve the need for obtaining the correct theoretical potential curves for a wide range of internuclear distances both in a gaseous phase and in solids. As can be seen from this review, one of the probable trends of development in the theory of radiation effects is a possibility of introducing the concept of a particle-solid IP not only by way of summation of the separate independent contributions, but also by taking into account the ion charge states, the effects of dynamic screening, correlation due to separate interactions in the small-angle scattering and channelling, as well as the electron structure of the target atoms. In the case of small-angle scattering and channelling, the energy dependence of the potential that produces changes in the stopping losses through the trajectories of motion may become sufficiently great. Thus, solid state effects can be taken into account at an earlier stage by including them in the potentials. For the successful development of this trend, additional experiments are necessary on dynamic screening and energy dependences of an IP for heavy ions.

Another theoretical topic that is only briefly discussed in this review is the possibility of taking into account the inelastic channels in the processes of elementary acts of ion-atom interaction through their inclusion in the potentials. Doing so within the framework of a model of continuous slowing down will give fresh impetus to the development of the theory.

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