Theory of electronic stopping of heavy ions in metals

I. A. Akhiezer and L. N. Davydov

Khar'kov Physicotechnical Institute, Ukrainian Academy of Sciences
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The physical mechanisms responsible for the slowing down of energetic heavy ions by electrons in matter are discussed for various values of the ion velocity v. The quasiclassical theory of atomic collisions, which determines the energy loss for $v < Z_1^{1/3} v_0$, is presented (Z_1 is the atomic number of the ion; v_0 is the Bohr velocity). Oscillations of the stopping cross section with variation of the atomic numbers of the colliding particles are discussed. Elastic scattering (with respect to the incident ion) is analyzed; it turns out to be dominant for $Z_1^{1/3} v_0 < v < Z_1^{2/3} v_0$. A number of semiempirical formulas for the electronic stopping cross section are discussed.

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CONTENTS

1. INTRODUCTION

It is well known (for example, see Ref. 1) that energetic particles (ions or neutral atoms) passing through solids lose energy as the result of collisions of two types—collisions with electrons of the target material (electronic stopping) and collisions with ionic cores located at crystal-lattice sites (so-called nuclear stopping). The roles of these two types of collisions in the fate of the bombarded material are fundamentally different: collisions with electrons only slow down the moving particle,[1)] while collisions with ionic cores can lead to knockout of the latter from crystal-lattice sites and thereby to the appearance of point defects.

In the region of not too high energies [$\varepsilon < \varepsilon_c$, where ε_c is some characteristic energy, which is different for different (moving ion)–(target atom) pairs] the main role in stopping of the moving particle is played by nuclear stopping. For $\varepsilon > \varepsilon_c$ the greater part of the energy lost by the particle is transferred to the electrons of the medium.

The stopping power of the electrons of the medium is characterized by a stopping cross section; in the literature two different normalizations are used for it:

$$S_e = \int T \frac{d\sigma}{dT} dT, \quad Q_e = m_2^{-1} S_e, \tag{1.1}$$

where T is the energy transferred, $d\sigma/dTdT$ is the cross section for scattering with transfer to the electrons of the medium of an energy in the interval (T, $T + dT$), and m_2 is the mass of the target atom. The cross section $d\sigma$ is normalized per atom (and not per electron) of the medium. The energy loss of the particle (per unit length) is related to the stopping cross section by the equation

$$-\frac{dE}{dx} = nS_e, \tag{1.2}$$

where n is the density of scatterers (for the normalization indicated, n is the number of atoms of the medium per unit volume).

In the high-energy region the stopping cross section is given by the well known Bethe formula (see for example Ref. 3)

$$S_e = \frac{4\pi Z_1^2 Z_2 e^4}{mv^2} \ln \frac{2mv^2}{I}, \tag{1.3}$$

where v is the velocity and Z_1 is the atomic number of the incident particle, Z_2 is the atomic number of the target material, and I is a quantity of the order of the ionization energy (m is the electron mass). We see that in this region the stopping cross section is, roughly speaking, inversely proportional to the energy of the particle.

In the low-energy region the electronic stopping in metals was first investigated by Fermi and Teller.[4] Considering the electrons of the metal as a free degenerate Fermi gas, they obtained a linear dependence of the electronic stopping on the particle velocity. The Fermi-Teller formula can be written in the form

$$S_e = \gamma_F \frac{e^2 a_0}{v_0} v, \quad \gamma_F = 4\pi \frac{a^2}{a_0^2} \frac{v_F}{v_0} Z_2^*, \tag{1.4}$$

[1)] A summary of a large number of experimental and theoretical results on the interactions of particles with the electrons of matter is given in Ref. 2.

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where $v_0 = e^2/\hbar$ and $a_0 = \hbar/mv_0$ are the Bohr velocity and Bohr radius, v_F is the Fermi velocity, Z_2^* is the number of collectivized electrons per target atom, and a^2 is a quantity of the order of the cross section for scattering of the incident particle by an electron (specifically, in the case discussed by Fermi and Teller of stopping of muons the scattering was described by the Rutherford formula and therefore $a^2 \sim (e^2/mv_F^2)^2$. Equation (1.4) describes the contribution from the collectivized electrons of the metal; the region of its applicability is $v \ll v_F$.

The further development of the theory of electronic stopping is based on two models of atomic collisions: The Firsov model[5] and the model of Lindhard and coworkers.[6-10] Both models treat the atom as a classical system; otherwise the physical considerations on which they are based are different. For small v the models lead to a linear dependence of the stopping on the velocity:

$$S_e = Cv, \tag{1.5}$$

with different coefficients C as functions of the atomic number and mass of the incident particle (Z_1, m_1) and of the target atom (Z_2, m_2).

The initial variants of these models describe only the averaged (monotonic) dependence of the coefficient C on Z_1 and Z_2; nevertheless it is clear that, as a consequence of the shell structure of the atom, oscillations of C should arise on variation of the atomic numbers of the target[11-20] and incident particle.[21-32] Sections 2 and 3 are devoted to the quasiclassical models of inelastic scattering and their generalizations which take into account oscillations of the coefficient C.

Until recently it was assumed (see for example Refs. 1 and 33) that proportionality of the stopping cross section to the velocity v is retained right up the velocities of the atomic electrons $v_A \sim Z^{2/3}v_0$, where Z is a quantity of the order of Z_1 or Z_2. This point of view is inconsistent with the experimental data (see Ref. 34), according to which the dependence of S_e on v is substantially nonlinear already at considerably lower velocities.[2)]

Then, in order to match the dependence $S_e = Cv$ with $S_e \sim v^{-2}$, it is natural to assume that the corrections to the function S_e that are nonlinear in the velocity are negative, so that in the intermediate region of velocities we have $S_e(v) < Cv$; however, the same experiments[34] show that at not very high velocities $S_e(v) > Cv$. The question arises of how to explain this behavior of the $S_e(v)$ curve. Sections 4 and 5 are devoted to this question.

Of course, the slowing down of atoms or ions in matter (except perhaps for the single physically transparent case of very high velocities $v \gg v_A$, where the material can be discussed as a gas of electrons and nuclei not interacting with each other, and the incident particle as a bare nucleus) is determined by a large number of different physical processes; therefore the theoretical models used turn out to be too crude to pretend to accurate numerical agreement with experiment. Equally, they cannot encompass at one time the entire range of velocities v. Therefore for practical purposes empirical and interpolation formulas are used; we shall mention some of them in Sec. 6.

A completely special situation arises in the slowing down of ions in a crystal under conditions of channeling. The motion of an ion in a channel obviously cannot be reduced to a sequence of binary atomic collisions—a large number of target atoms take part coherently in the process. Without touching this question (which as the result of its specific nature turns out to be outside the logical scope of the present article), we refer the reader to the review by Gemmel[35] devoted to the subject of channeling.

2. LINEAR DEPENDENCE OF ELECTRONIC STOPPING ON VELOCITY

As we have already noted, at very low velocities ($v \ll v_F$) the electronic stopping in metals follows a linear law $S_e = Cv$ [Eq. (1.4)]. On increase of the velocity the dependence of S_e on v becomes more complicated; in particular, oscillations of S_e as a function of velocity can arise; these reflect the band structure of the electron spectrum. A linear dependence of the stopping cross section is again restored at $v > v_0$, when it is not necessary to take into account the energy gaps between bands.

We shall begin the analysis of electronic stopping in this velocity region with a model extensively used in the literature, due to Firsov.[5] In this model, on collision of two atoms their electron clouds fuse into a single electron cloud. If we introduce the deisgnation Φ for the electron flux through the plane equidistant from the centers of the two colliding atoms (often called the Firsov plane), then obviously the forces acting on the two atoms are equal:

$$\mathbf{F}_1 = -\mathbf{F}_2 = -\Phi m\mathbf{v}. \tag{2.1}$$

The work W done by the force $\mathbf{F}_1$ will depend on the impact parameter b; assuming that the velocity of the atom does not change during the collision, we have

$$W(b) = -mv\int \Phi\, d\mathbf{r}, \tag{2.2}$$

where $\mathbf{r}$ is the radius vector of the moving atom.

Thus, we must first calculate the flux of electrons $\Phi(x)$ through the plane with coordinate $x/2$, using some model for the distribution of atomic electrons (the x axis joins the centers of the colliding atoms). In particular, in the quasiclassical approximation, it is necessary to calculate the quantity

$$\Phi(x) = \tfrac{1}{4}\, n\bar{u}\, dy\, dz, \tag{2.3}$$

where n and $\bar{u}$ are the density and average velocity of the electrons. Then, using (2.2) the integrating over all impact parameters, we obtain the stopping cross section

$$S_e = -2\pi\int W(b)\, b\, db = 2\pi mv\int b\, db\int \Phi\, dr. \tag{2.4}$$

[2)] Recently an experimental paper[68] has appeared which also confirms the nonlinear dependence of S_e on v.

Firsov[5] used the relation between average velocity and density following from Fermi statistics,

$$\bar{u}=\frac{3\hbar}{4m}(3\pi^2 n)^{1/3}. \tag{2.5}$$

If we substitute the Thomas-Fermi density distribution for n for an atom with $Z=Z_1+Z_2$, then the expression for the coefficient C can be represented in the form[3)]

$$C=\gamma_\Phi\frac{e^2a_0}{v_0},\quad \gamma_\Phi=7.51\,\frac{3\pi^2}{32}(Z_1+Z_2). \tag{2.6}$$

We note that the Firsov model (like the model of Lindhard and co-workers discussed below) does not take quantum mechanical effects into account. The condition of applicability of such models is the smallness of the de Broglie wavelength of most of the atomic electrons $\hbar/m\bar{u}$ in comparison with the size of the atom. As is well known, the size of an atom (more precisely, the region occupied by the greater part of the atomic electrons) is $\lambda\sim a_0Z^{-1/3}$; for most atomic electrons $\hbar/m\bar{u}\sim a_0Z^{-2/3}$. Therefore the failure to include quantum-mechanical effects corresponds to a failure to take into account corrections proportional to $Z^{-1/3}$. Thus, quasiclassical models are applicable for description of heavy atoms (for example, for uranium $Z^{-1/3}=0.22$) and are not applicable in the case of light atoms.

Another approach to the electronic slowing down of ions, developed by Lindhard and co-workers,[6-10] is based on the so-called dielectric formalism—description of an atom as a medium with a certain dielectric permittivity. (Comparing the Firsov approach with this approach, many authors speak of the former as a geometrical approach, and the latter as a dynamical approach.)

If a structureless particle with charge Z_1e is slowed down in a uniform medium, then we have for the stopping cross section per electron of the medium in the Born approximation, as is well known (see for example Ref. 36),

$$S_e'=-\frac{Z_1^2e^2}{2\pi^2vn_e}\int\frac{d^3k\,d\omega\,\omega}{k^2}\operatorname{Im}\frac{1}{\varepsilon(\mathbf{k},\omega)}\delta(\omega-\mathbf{kv}), \tag{2.7}$$

where $\varepsilon(\mathbf{k},\omega)$ is the dielectric permittivity and n_e is the density of electrons of the medium. This expression is applicable also in the case of a medium with a slowly varying electron density $n_e(\mathbf{r})$ ($\lambda\gg\hbar/m\bar{v}$, where λ is the characteristic length of inhomogeneity and $\bar{v}$ is the average velocity of the electrons of the medium); in this case it leads to a dependence of S_e' not only on velocity but also on the coordinates, $S_e'=S_e'(v,\mathbf{r})$. Adding the contributions of individual electrons, we obtain

$$S_e(v)=\int d^3r\,S_e'(v,\mathbf{r})\,n_e(\mathbf{r}) \tag{2.8}$$

(the integration is carried out over the volume occupied by one atom of the target material).

Equations (2.7) and (2.8) can be used directly for description of the slowing down of moving nuclei in material with large Z_2. In fact, in this case $\lambda\gg\hbar/m\bar{v}$, which permits the atom to be discussed as a weakly inhomogeneous electron plasma with some specified electron distribution $n(\mathbf{r})$, for example, a Thomas-Fermi distribution (Lindhard, Scharff, and Winther[8,9]).

A deficiency of this approach is the difficulty of generalization to the case in which the incident particle is not a bare nucleus, but retains all or part of its electrons. Crudely speaking, for such a generalization it is necessary from certain additional considerations to change Eq. (2.8) (in the direction of symmetrization in the atomic numbers Z_1 and Z_2). The most frequently used of the expressions in the literature obtained in this way, for analysis of experiments the formula is that of Lindhard and Scharff,

$$C=\gamma_L\frac{e^2a_0}{v_0},\quad \gamma_L=8\pi Z_1^{7/6}Z_2(Z_1^{2/3}+Z_2^{2/3})^{-3/2}, \tag{2.9}$$

which was published in Ref. 7 without derivation.

Thus, the quasiclassical approaches of Firsov and of Lindhard and co-workers express the stopping cross section $S_e(v)$ in terms of the density of atomic electrons $n(r)$; of course, there is still freedom in the choice of $n(r)$. In the initial variants of these models the Thomas-Fermi distribution was used as $n(r)$, which provided the possibility of tracing the averaged Z-dependence of the stopping cross section. Recent studies have utilized Hartree-Fock distributions, which permit study of a more detailed effect—the oscillations of the cross section with change of Z_1 and Z_2 (in this connection, see the following section). Finally, to obtain simple analytic formulas use is made of model potentials simpler than the Thomas-Fermi potential, for example, the potential[37]

$$V(r)=\frac{Ze^2}{r}\varphi(r),\quad \varphi(r)=[H(e^{r/r_s}-1)+1]^{-1} \tag{2.10}$$

(H and r_s are functions of atomic number).

In concluding this section we call attention to that fact that for $v>v_0$ the incident particle is with a high probability stripped of its outer electrons; however, for heavy atoms for $v<Z_1^{2/3}v_0$ the greater part of the electrons remain in a bound state. Loss of the outer electrons should greatly affect any peripheral processes (for example, processes in which a large role is played by the size of the atom; see Sec. 4). In the deep inelastic process considered here, in which all atomic electrons play comparable roles, the loss of Z_1^* outer electrons makes a small contribution proportional to Z_1^*/Z_1.

3. OSCILLATIONS OF STOPPING CROSS SECTIONS WITH CHANGE OF ATOMIC NUMBER

The quasiclassical approach to atomic collisions, which permits expression of the stopping cross sections in terms of the characteristics of the atom is a continuous medium [in the last analysis in terms of the density of the electron cloud $n(r)$], for all its simplicity and physical clarity, has two important deficiencies. First, the applicability of this approach is limited to large Z; in the best case the small parameter of the

[3)] The expression for the coefficient γ can hardly be considered reliable for accurate numerical calculations. In particular, the values of S_e calculated from Eq. (2.6) for uranium ions for $v<6\cdot10^8$ cm/sec, according to Ref. 34, exceed the measured values. This remark applies equally to Eq. (2.9).

quasiclassical case turns out to be $(Z_1+Z_2)^{-1/3}$. Second, inclusion of effects due to the shell structure of the atom, which is beyond the scope of the first quasiclassical approximation, greatly complicates all formulas, to the detriment of clarity. Nevertheless, the description of one of these effects—oscillations of S_e with change of Z_1 and Z_2—is physically no less interesting than the description of the monotonic (averaged) dependence of S_e on atomic number.

Of the two natural directions of generalization of the quasiclassical model, toward inclusion of Z-oscillations and toward lower values of Z, the former is substantially more attractive for most authors: oscillations in the background of a monotonic Z-dependence are clearly distinguished in analysis of experiments, which facilitates the experimental verification of this or that model. Therefore it is not surprising that most studies generalizing the quasiclassical model are devoted to study of oscillations of the electronic stopping cross section on change of atomic number.

A common feature of all these studies is the attempt to retain physical clarity (even to the detriment of theoretical correctness). The most extreme manifestation of this tendency is in the semiempirical formulas of Refs. 38 and 39.

In generalizing the model based on the dielectric formalism, the authors proceed from Eq. (2.7), substituting into it the electron density $n(r)$ calculated by means of Slater or Hartree wave functions. It is clear that the Z-oscillations of such $n(r)$ distributions will automatically lead to a nonmonotonic dependence of S_e on Z_2. It remains an unanswered question whether or not oscillating terms of the same order are lost in representing the stopping cross section in the form (2.7). This, together with the difficulty in taking into account oscillations of S_e on change of Z_1, is apparently the reason for the relatively small number of papers generalizing the dielectric formalism model.[40-43,20]

A very simple means of introducing oscillations into the Firsov model is used in Ref. 44, whose authors proceed from the expression (2.10) for the atomic potential. Oscillations of the screening radius r_s and of the parameter H with change of Z naturally lead to oscillations of the stopping cross section; the simplicity of the electron distribution used permits closed and easily interpreted analytic expressions to be obtained. The approach of Ref. 45 is somewhat more complicated: the authors start from Eqs. (2.3) and (2.5), substituting the Hartree electron distribution function for $n(r)$.

We call attention to that fact that generalization of the Firsov formula involves considerably greater arbitrariness than the generalization of Eq. (2.7). In fact, as long as we are interested in the averaged Z-dependence it is natural to describe the electron distribution in the fused electron clouds by the Thomas-Fermi function for $Z=Z_1+Z_2$. However, in the description of the oscillations of S_e there are no general physical or experimental reasons to assume that this quantity depends only on the sum Z_1+Z_2 or any other previously known combination of Z_1 and Z_2. Therefore most authors

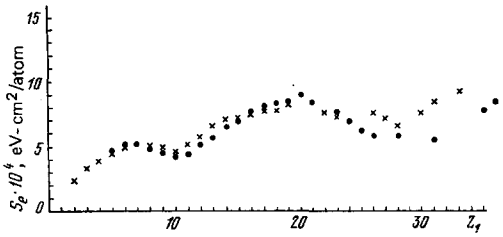

FIG. 1. Dependence of electronic stopping cross section in carbon on Z_1 (Ref. 46). ●—experiment,[27] ×—theory (Ref. 46). The ion velocity is $1.38\cdot 10^8$ cm/sec.

attempt to introduce oscillations into the Firsov model not at the level of the density $n(r)$, but at an earlier level—for the flux Φ which enters into Eq. (2.4).

The main difficulty arising in this procedure is due to the quantum mechanical generalization of the expression (2.3) for the flux of electrons through the Firsov plane. Most authors follow Cheshire *et al.*,[46] who postulated the following expression for the quantity Φ entering into (2.4):

$$\Phi(x)=\frac{1}{4}\int\left[\sum_i \bar{u}_i|\psi_i|^2+\sum_j \bar{u}_j|\psi_j|^2\right]dy\,dz; \tag{3.1}$$

here the indices i and j enumerate the wave functions ψ of the electrons of the moving atom (i) and the target atom (j), and therefore the quantities $|\psi_i|^2$, $|\psi_j|^2$ describe the contributions of the individual electrons to the function $n(r)$ (on the assumption that the electron shells are not deformed in the collision). The quantities $\bar{u}_i$ and $\bar{u}_j$ are chosen in the form

$$\bar{u}_i=\sqrt{\frac{2}{m}\varepsilon_i},\quad \bar{u}_j=\sqrt{\frac{2}{m}\varepsilon_j}, \tag{3.2}$$

where ε_i, ε_j are the average values in the states i and j of the kinetic energy operator $\hat{\varepsilon}=-(\hbar^2/2m)\Delta$.

References 46–49 (see also Refs. 50 and 51) are devoted to the description of Z-oscillations of the stopping cross section in a Firsov model generalized in this way; one of these studies succeeds in carrying out the calculation analytically.[47]

As an illustration of the results obtained in this way, we present a comparison of the theoretical[46] and experimental[27] dependences of S_e on Z_1 (see the figure). The plot is taken from Ref. 46.

Of course, from the point of view of theoretical correctness the generalization presented above for the Firsov model has the same deficiencies as the generalized model of Lindhard and co-workers: it is far from obvious that Eq. (3.1) actually determines the quantum-mechanical flux through the Firsov plane.

The generalization of the Firsov model based on a correct quantum-mechanical determination of the flux is due to Brice.[52] Following this work, we introduce a wave function $\psi_+(\mathbf{r})$ of an electron crossing the Firsov plane in a definite direction. Separating from the wave function of the atomic electron $\psi(\mathbf{r})$ the harmonics with $k_x>k_0$, we have

$$\psi_+(\mathbf{k})=\int\frac{d^3k}{(2\pi)^3}e^{i\mathbf{kr}}\psi(\mathbf{k})\,\Theta(k_x-k_0), \tag{3.3}$$

where $\hbar k_0/m$ is the velocity of the Firsov plane and

$$\psi(\mathbf{k})=\int d^3r e^{-i\mathbf{k}\mathbf{r}}\psi(\mathbf{r}),\quad \Theta(x)=\begin{cases}1, & x>0,\\ 0, & x<0.\end{cases} \tag{3.4}$$

Knowing the functions $\psi_+(\mathbf{r})$, we can find the contribution Φ' of an individual electron to the quantity Φ:

$$\Phi'=-\frac{\hbar}{2m}\int\left[i\left(\psi_+^*\frac{\partial\psi_+^*}{\partial x}-\psi_+\frac{\partial\psi_+}{\partial x}\right)+2k_0|\psi_+|^2\right]dy\,dz. \tag{3.5}$$

The first two terms in the integrand describe the quantum-mechanical flux through the stationary plane; the last term is due to the additional flux arising from motion of the Firsov plane.

Using the wave function of the $1s$ state of a hydrogen-like atom (with charge Ze) as ψ,

$$\psi(r)=\frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\exp\left(-\frac{Zr}{a_0}\right), \tag{3.6}$$

Brice obtained the following expression for the contribution of one electron to the stopping cross section:

$$S_e'=\frac{16e^2a_0}{5Zv_0}v\xi\left(\frac{v^2}{4Z^2v_0^2}\right), \tag{3.7}$$

where ξ is a function of the velocity (which goes to unity at $v=0$),

$$\xi(x)=\frac{21+74x+83x^2+30x^3}{24(1+x)^3}+(1+10x)\frac{\operatorname{arctg}\sqrt{x}}{8\sqrt{x}}. \tag{3.8}$$

For $v\ll Zv_0$ this formula leads to a linear dependence of the energy loss on velocity; here the proportionality coefficient differs (not only numerically, but also in the Z-dependence) from both the Firsov coefficient and the Linhard coefficient. In this sense the Brice model, which uses a rigorous quantum-mechanical determination of the flux density and the very simple wave function (3.6) for the atomic electrons, can be considered an attempt (the only one known to us) to generalize the quasiclassical models to small Z.

4. STOPPING BY A FREE FERMI GAS

Having considered electronic stopping of heavy ions in the region of low velocities where the stopping cross section is linear in the ion velocity, let us turn to analysis of stopping at high velocities. We note first of all that the initial formulas of both quasiclassical models (2.4) and (2.7) contain v only in odd powers. This can easily be seen by observing that Φ, $\mathrm{Re}\varepsilon(k,\mathbf{kv})$, and $\mathbf{kv}\,\mathrm{Im}\varepsilon(k,\mathbf{kv})$ are even functions of the velocity (more precisely, of the ratio v/v_A, where $v_A\sim Z^{2/3}v_0$ is the average velocity of the atomic electrons). Equations (2.7) and (3.8) lead to a similar dependence of S_e on v (in the case of a hydrogen-like atom $v_A\sim Zv_0$). Nevertheless, there are no physical reasons to assume that significantly higher corrections (proportional to v^2 but not v^3) are lacking in the expression for S_e. We reach the conclusion that the terms that are quadratic in velocity in the stopping cross section have been lost at an earlier stage and cannot be extracted from the formulas of Secs. 2 and 3.

In this connection it is interesting to trace the transition in the simplest model from the dependence $S_e\sim v$ at low velocities to $S_e\sim v^2$ at higher velocities. As such a model we shall consider the stopping of a particle by a free electron Fermi gas. This problem is a generalization of the work of Fermi and Teller[4] to the case of particle velocities that are not small in comparison with the Fermi velocity.[4)]

Of course, on taking into account the identity of the scatterer particles (in particular, in the problem of stopping by a Fermi system at $v\ll v_F$), the energy loss of the incident particle is not expressed in terms of the sum of stopping cross sections for each scatterer. As before we shall use the concept of the (effective) stopping cross section, determining it by means of Eq. (1.2) (In Eq. (1.4) above we had just this quantity in mind.)

The particle energy loss per unit path in a Fermi gas is determined by the obvious relation

$$-\frac{dE}{dx}=\frac{1}{v}\int\frac{p'^2-p^2}{2m}n_F(p)[1-n_F(p')]\,dw_{\mathbf{p}\to\mathbf{p}'}\,d\tau_{\mathbf{p}}, \tag{4.1}$$

where p and p′ are the momenta of an electron of the medium before and after the scattering, n_F is the Fermi distribution function, and $dw_{\mathbf{p}\to\mathbf{p}'}$ is the probability of scattering of the electron into an element of phase space $d\tau_{\mathbf{p}'}$.

We shall dwell first on the case of slow particles ($v<v_F$) and short-range forces ($R<\hbar/m_rv_r$, where R is the range of the forces, v_r is the relative velocity of the colliding particles, and m_r is the reduced mass, which in the case of the heavy particles of interest here coincides with the electron mass). In this case, according to the well-known Bethe formula (see for example Ref. 3), the elastic-scattering cross section is isotropic and does not depend on the velocity:

$$d\sigma'=a'^2\,do, \tag{4.2}$$

where $d\sigma'$ is the differential scattering cross section for one scatterer (electron) and a' is the corresponding scattering length. Converting from cross sections to transition probabilities, we have, in accordance with Eqs. (1.2) and (4.1),

$$S_e'=4\pi a'^2mvv_F \tag{4.3}$$

(as in Ref. 4, we set $v_F>v>mv_F/m_1$).

If, like Fermi and Teller, we proceed from an unscreened Coulomb potential and consequently from the Rutherford scattering cross section, instead of (4.3) we obtain[4]

$$S_e'=2\pi a_0^2mvv_Ff\left(\frac{v_F}{v_0}\right),\quad f(x)=x^{-4}\ln x. \tag{4.4}$$

If we take into account that $v_F\sim v_0$ and $a'\sim a_0$, we see that Eqs. (4.3) and (4.4) differ only by a factor of the order of unity. We note that in a real metal $R\sim\hbar/mv_F$; therefore we have a case intermediate between Rutherford scattering and scattering by a short-range potential. We shall not give the corresponding awkward expressions, which differ from (4.3) and (4.4) only by a factor of order unity.

In the case of fast particles ($v>v_F$), assuming the potential to be short-range, we obtain from (4.1) and (1.2)

[4)] To explain the slowing down of very slow ions in a metal it has been necessary to generalize the results of Fermi and Teller[4] in another direction—inclusion of Fermi-liquid effects in the system of conduction electrons.[52]

$$S_e' = 4\pi a'^2 m v^2. \quad (4.5)$$

We see that the linear dependence of the stopping cross section on the velocity of the particle is replaced for $v > v_F$ by a quadratic dependence.

Let us now see which features of the actual scattering of fast ions ($v > v_0$) by electrons are reflected by the model discussed. For this purpose we shall break down the electrons of the incident particle and the target atom into two groups—electrons of the outer shells (outer electrons) and electrons of the inner shells (inner electrons, electrons of the ionic core). The stopping of the ion obviously receives contributions from scattering of the ionic core of the moving particle by both the ionic core and the outer electrons of the target atom. (In regard to the outer electrons of the moving ion—in the case when the ion still retains them—, their interaction with the target material for $v > v_0$ is more likely to lead to charge exchange of the ion than to its slowing down.)

Equation (4.2) for the scattering of slow particles by a short-range potential is applicable to collisions between electrons and neutral atoms for $v < Z_1^{1/3} v_0$. Leaving aside for a minute the question of up to what values of uncompensated charge $Z_1^* e$ the ion can be treated as a neutral atom, we see that the necessary condition for applicability of Eq. (4.5) is the inequality $v < Z_1^{1/3} v_0$.

We shall therefore limit ourselves to the region of velocities $v_0 < v < Z_1^{1/3} v_0$. Here if $Z_1 \sim Z_2$, then (even outside this region, up to $v \sim Z_1^{2/3} v_0$) we can apply the quasiclassical model of atomic collisions to the ionic cores of both colliding particles, using the expressions (1.5) and (2.6) [or (2.9)] for the contribution of the cores to the stopping cross section.

If there were a sharp boundary between the binding energies of the outer electrons of an atom (I_p) and the inner electrons (I_c), then, by choosing a velocity in the interval $\sqrt{I_p/m} \ll v \ll \sqrt{I_c/m}$, we could directly apply Eq. (4.5) to the analysis of the contribution of the outer electrons. Adding the contributions of the inner and outer electrons to the stopping cross section, we obtain

$$S_e = Cv + 4\pi a'^2 Z_2^* m v^2, \quad (4.6)$$

where Z_2^* is the number of outer electrons. Of course, there is no distinct boundary between the outer and inner electrons; therefore Z_2^* must be considered a phenomenological parameter which increases with increasing velocity. Equation (4.6) has been used for analysis of experiments[34,54] in Ref. 55.

In concluding this section we shall evalute the conditions under which collisions of electrons with an ion do not differ greatly from collisions with a neutral atom. For this purpose let us compare the scattering length a' for scattering by an electron of a neutral atom with the length a_c' for scattering by an electron of an uncompensated charge $Z_1^* e$ moving in a medium. These quantities, as is well known, have the form

$$a' = \frac{Z_1 \overline{r^2}}{3a_0}, \qquad \overline{r^2} = Z_1^{-1} \int r^2 n \, d^3 r, \quad (4.7)$$

$$a_c' = \frac{2e^2 Z_1^* a_0^{-1}}{q^2 + r_s^{-2}}, \qquad \hbar q = 2mv \sin\frac{\vartheta}{2}, \quad (4.8)$$

where n is the density of atomic electrons, ϑ is the scattering angle in the c.m.s., and r_s is the charge-screening radius due to the medium ($r_s \sim a_0$). Taking into account that $\overline{r^2} \sim Z_1^{-2/3} a_0^2$, we see that $a_c' < a'$ if

$$Z_1^* < Z_1^{1/3} \max\left(\frac{v^2}{v_0^2}, \frac{a_0^2}{r_s^2}\right). \quad (4.9)$$

Thus, the condition $Z_1^* < Z_1^{1/3}$ is sufficient that we need not take into account the distinction between an ion and a neutral atom for all values of its velocity.

5. NONLINEAR DEPENDENCE OF ENERGY LOSS ON VELOCITY

The contribution of elastic scattering (with respect to the incident atom) by free electrons, discussed in the preceding section, is in principle not difficult to calculate for all velocity values if we know the structure of the incident particle, described by its elastic form factor. Knowledge of the elastic form factors (determined experimentally, for example from scattering of electrons by atoms, or calculated theoretically, for example by the Hartree-Fock method or on the basis of the Thomas-Fermi model) permits tracing the dependence of the stopping cross section on the ion velocity up to $v \sim Z_1^{2/3} v_0$. For further increase of the velocity, a knowledge of the elastic form factors turns out to be insufficient, since with increase of the velocity there are opened an increasing number of inelastic channels which contribute to the slowing down of the ion (channels not involving charge exchange). For $v \gg Z_1^{2/3} v_0$ it is possible to carry out a summation of the contributions of all these channels, which leads to the Bethe formula (1.3).

For a target with large Z_2 this approach would not permit going beyond a qualitative description of the slowing down of ions, since the electrons of a heavy material for $v < Z_2^{2/3} v_0$ cannot in any way be considered a free-electron gas. The situation is different in the case of a target with low Z_2 and consequently a low total-ionization energy I_2. For such a target there can exist a velocity region

$$\left(\frac{I_2}{m}\right)^{1/2} < v < Z_1^{2/3} v_0, \quad (5.1)$$

in which the model of elastic collisions between free electrons and a particle having an internal structure adequately describes the electronic stopping of a heavy ion.

Thus, we shall discuss the electronic stopping of a heavy ion in a light material in the velocity range (5.1). Using the well known expression for the elastic-scattering differential cross section (see for example Ref. 3),

$$d\sigma' = \left(\frac{e^2}{2mv^2}\right)^2 [Z_1 - f(q)]^2 \frac{do}{\sin^4(\vartheta/2)}, \quad (5.2)$$

we obtain

$$S_e = \frac{Z_2 e^4}{2mv^2} \int \frac{do}{\sin^2(\vartheta/2)} [Z_1 - f(q)]^2, \quad (5.3)$$

where $f(q)$ is the atomic form factor, which is connected with the electron distribution in the atom by the relation

$$(q) = \int d^3 r n(r) \exp(-i\mathbf{qr}). \quad (5.4)$$

It is well known that for $Rq \gg 1$ (R is the size of the scattering system), we have $f(q) \to 0$. We see that for $v \gg Z_1^{2/3} v_0$ the expression (5.3) behaves like the exact expression (1.3), which takes into account the contribution of the inelastic channels in addition to elastic scattering, provided that we ignore the factor under the logarithm sign.

In the case of not very high velocities of the moving particle, $v < Z_1^{1/3} v_0$, we have $Rq < 1$; here

$$Z_1 - f(q) = \tfrac{1}{6} q^2 \int d^3 r n r^2 + Z_1^*. \tag{5.5}$$

In this case [at least, if $Z_1^* < Z_1^{1/3}$; see the inequality (4.9)] there is isotropic scattering in a short-range potential with the scattering length (4.7), characterized by the stopping cross section (4.5). Since $\overline{r^2} \sim Z_1^{-2/3} a_0^2$, the stopping cross sections of different atoms in the same material for not very high velocities should be related as $Z_1^{2/3}$ [in the case $v \gg Z_1^{2/3} v_0$ these cross sections are related, according to Eq. (1.3), as Z_1^2].

In Refs. 34 and 54, experiments are described on the slowing down or bromine ions in carbon at a velocity $v = 15 \cdot 10^8$ cm/sec, which fits satisfactorily into the interval (5.1). Substituting the Hartree-Fock form factor of the bromine atom (see for example Ref. 56) into (5.3) and integrating, we find, in complete agreement with experiment, $Q_e \approx 50$ keV-cm$^2/\mu$g.

At lower velocities Eq. (5.3) is more suitable as a convenient language for interpretation of experimental results than it is for their numerical explanation. In this case we can assume only part of the electrons of the target material to be free; this can be taken into account by replacing Z_2 in Eq. (5.3) by some function of velocity $Z_2^*(v)$. A corresponding analysis of the experiments of Refs. 34 and 54 is given in Ref. 57.

Equation (5.3) permits comparison of the stopping cross sections for different ions in the same material even in the case when the condition $v > \sqrt{I_2/m}$ is not satisfied. In fact, the empirical parameter Z_2^* characterizing the target material cancels in comparison of the stopping cross sections for different ions; therefore the cross sections should be proportional to the integrals entering into Eq. (5.3).

It is especially simple to carry out this comparison for $v < Z_1^{1/3} v_0$, when the stopping cross sections are determined by Eqs. (4.5) and (4.7) and consequently are related as $Z_1^{2/3}$. For example, for ions of uranium, iodine, and bromine we have

$$S_e(\mathrm{U}) : S_e(\mathrm{I}) : S_e(\mathrm{Br}) = 20.4 : 14.1 : 10.7. \tag{5.6}$$

Unfortunately the inequality $v < Z_1^{1/3}$ on the one hand and the requirement of dominance of elastic scattering $S_e > Cv$, on the other, limit the region of applicability and the accuracy of relations such as (5.6). Nevertheless, as can be judged on the basis of the experiments of Refs. 34 and 54, for $v = 8 \cdot 10^8$ cm/sec the relation (5.6) is satisfied with good accuracy.

6. SEMIEMPIRICAL FORMULAS

As we have already remarked, a large number of different physical processes contribute to the electronic slowing down of heavy ions. Therefore theoretical models, however correct they may be from the point of view of theoretical physics, cannot encompass all aspects of the phenomenon and therefore can hardly pretend to accurate numerical agreement with experiment or to give reliable quantitative predictions. Nevertheless, in the analysis of experimental data one can note a number of empirical regularities[5)] which turn out to be very useful for practical calculations.[34,39,52,58-66]

As an illustration of the approaches used for the physical interpretation of such regularities, we present the derivation of the three-parameter Brice formula.[52] The author starts with Eq. (3.7), which takes into account the contribution of quantum effects in the Firsov model. In this model, as we have seen, an electron crossing the Firsov plane in the direction from atom A to atom B changes its affiliation, transferring its entire energy to atom B. Since at high velocities of the colliding atoms the electron does not succeed in transferring its entire energy, Brice introduces into the stopping cross section a cutoff factor

$$f_c(v) = \left[1 + \left(\frac{av}{v_0}\right)^n\right]^{-1}, \tag{6.1}$$

where a and n are empirical parameters. It is then proposed to consider the quantity Z in Eq. (3.7), for S_e' as an empirical parameter. As a result, adding the contributions of the individual electrons, we arrive at the formula[52]

$$S_e(v) = (Z_1 + Z_2)\, S_e' f_c(v), \tag{6.2}$$

which satisfactorily fits the experimental stopping cross sections for a number of pairs (Z_1, Z_2).

Another widely used approach is based on the concept of effective charge. (This concept, in particular, was already used in Niels Bohr's 1948 monograph.[67]) The physical considerations on which this approach is based can be made clear as follows.

In the Born approximation the differential cross section $d\sigma$ for scattering of an ion is easily related to the differential cross section $d\sigma_0$ for a "standard" process (as which we have chosen the scattering of a hydrogen atom in the 1s state) in the same material with identical transfers of momentum $\hbar q$ and energy $\hbar\omega$. We obtain

$$d\sigma = Z_1^2 \Psi\, d\sigma_0, \tag{6.3}$$

where Ψ is some function of q and ω which characterizes the ion being scattered. Substituting this relation into (1.1), we find

$$S_e = Z_1^2 \int \hbar\omega \Psi \frac{d\sigma_0}{do}\, do. \tag{6.4}$$

The quantities ω and q are functions of the relative velocity v and the c.m.s scattering angle ϑ; we can therefore write here $\Psi \equiv \Psi(v, \vartheta)$.

Using a well known mathematical relation (the theorem of the mean), we rewrite (6.4) in the form

$$S_e = Z_1^2 \Psi(v, \vartheta_1)\, S_{e0}, \tag{6.5}$$

[5)] Semiempirical tables of electronic (and also nuclear) stopping cross sections can be found in Ref. 58.

where S_{e0} is the stopping cross section in the case of the hydrogen atom,

$$S_{e0} = \int \hbar\omega \frac{d\sigma_0}{do}\, do, \tag{6.6}$$

and ϑ_1 is some angle (which is, of course, different for different Z_1).

Thus, the stopping cross section can be represented in the form

$$S_e(v) = (Z_1\gamma(v))^2 S_{e0}(v), \tag{6.7}$$

where γ is a function of the velocity and the atomic number Z_1. The quantity $Z_1\gamma(v)e$ is called the effective charge.

If we limit ourselves to inclusion of only elastic scattering (which according to Sec. 5 is dominant in the velocity range $Z_1^{1/3}v_0 < v < Z_1^{2/3}v_0$), then the function Ψ is expressed in terms of the elastic form factor $f(q)$:

$$\Psi = (1 - Z_1^{-1}f(q))^2. \tag{6.8}$$

From this we obtain for the effective charge[57]

$$\gamma^2(v) = \left(8\pi \ln\frac{v}{v_0}\right)^{-1} \int [1 - Z_1^{-1}f(q)]^2 \frac{do}{\sin^2(\vartheta/2)} \tag{6.9}$$

(we have substituted the form factor of the $1s$ state of the hydrogen atom in explicit form for $a_0 q \gg 1$, which corresponds to $v \gg v_0$).

In principle the function Ψ, and consequently the effective charge, is determined by the contribution of both the elastic channel and all inelastic channels (which do not lead to charge exchange). Therefore it is desirable not to calculate the function γ from theoretical considerations, but to consider it as empirical.

Any reasonable parametrization of the function $\gamma(v)$ must reflect the fact that for $v \gg v_A$ the electrons of the moving particle do not take part in its slowing down; therefore for $v \gg v_A$ $\gamma(v) \to 1$. Most authors express $\gamma(v)$ in the form

$$\gamma(v) = 1 - C_1 \exp\left(-\frac{v}{Z_1^{2/3}v_1}\right), \tag{6.10}$$

where C_1 and v_1 are constants.

As $q \to 0$, as is well known, the form factor of a neutral atom vanishes; therefore we can choose $C_1 = 1$ and consider only the quantity v_1 as an empirical constant. In this way we arrive at the formula of Pierce and Blann[62]:

$$\gamma = 1 - \exp\left(-0.95 Z_1^{-2/3}\frac{v}{v_0}\right), \tag{6.11}$$

where v_0 is the Bohr velocity.

A somewhat different parametrization is used by Brown and Moak[34]:

$$\gamma = 1 - 1.034 \exp\left(-Z_1^{-0.688}\frac{v}{v_0}\right). \tag{6.12}$$

It must be kept in mind that the usefulness of the effective-charge concept is related to the possibility of representing the differential scattering cross sections in the form of a product of two factors, one of which depends only on the properties of the incident ion, and the other—only on the properties of the medium. This factorization exists in the Born approximation, the region of applicability of which is limited by the requirement $(e^2/\hbar v)[Z_1 - f(\bar{q})] < 1$ ($\bar{q}$ is the characteristic momentum transfer). In addition, factorization exists at high velocities, when the electrons of the medium can be considered free. Therefore for heavy ions (in the case of a heavy target material, where the electrons of the latter cannot be considered free) the usefulness of the effective-charge concept is destroyed for $v < Z_1^{1/3}v_0$ and is again restored for $v > Z_2^{2/3}v_0$.

7. CONCLUSIONS

1. In the low-energy region the electronic cross section for slowing down of heavy ions is proportional to the velocity:

$$Q_e = \varkappa \frac{e^2 a_0}{m_H}\left(\frac{\varepsilon}{\varepsilon_0}\right)^{1/2}, \quad \frac{e^2 a_0}{m_H} = 0.46 \text{ keV-cm}^2/\mu g, \tag{7.1}$$

where ε is the energy of the ion, $\varepsilon_0 = (1/2)m_H v_0^2 = 24.97$ keV is the energy corresponding to the Bohr velocity, and $\varkappa$ is a numerical coefficient (m_H is the proton mass).

2. Simple and frequently used theoretical models give the following values for the coefficient $\varkappa$:
the Firsov model[5]:

$$\varkappa = \eta_\Phi (Z_1 + Z_2)^{-1} A_2^{-1} A_1^{-1/2}, \quad \eta_\Phi = 6.95; \tag{7.2}$$

the Lindhard-Scharff model[7]:

$$\varkappa = \eta_L Z_1^{7/6} Z_2 (Z_1^{2/3} + Z_2^{2/3})^{-3/2} A_2^{-1} A_1^{-1/2}, \quad \eta_L = 25.13. \tag{7.3}$$

(A is the atomic weight). These models determine the averaged (monotonic) dependence of the stopping cross section on Z_1 and Z_2.

The literature contains generalizations of these models which also permit the tracing of the oscillations of the coefficient $\varkappa$ with change of atomic number.

3. Strictly speaking, the region of applicability of Eq. (7.1) is limited on the low side by the Bohr velocity v_0 and consequently by the energy ε_0 per nucleon.

The upper limit of the region of applicability of this formula for heavy ions is the energy $\varepsilon_1 \sim Z_1^{2/3}\varepsilon_0$ per nucleon. With further increase of the ion energy the stopping cross section rises more rapidly than $\varepsilon^{1/2}$, reaches a maximum, and begins to fall off according to the well known Bethe law: $Q_e \sim \varepsilon^{-1}\ln\varepsilon$.

4. A comparatively clear physical picture of electronic stopping in the energy region $\varepsilon > \varepsilon_1$ exists for the case of heavy ions moving in a light material (see Sec. 5). For heavy ions in a heavy material it is possible to take into account accurately only one of the scattering channels and to explain only qualitatively the experimentally observed rise of the stopping cross section at $\varepsilon \sim \varepsilon_1$.

5. In the literature there are a number of semiempirical formulas which are in good agreement with experiment [for example, Eqs. (6.2), (6.9), and (6.10)].

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