Quasihydrodynamic behavior of linear atomic collision cascades

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A self-similar solution is found of a time-dependent spatially homogeneous transport equation describing a linear atomic collision cascade. This solution is used to provide a physical description of the development of a cascade as a pattern of consecutive generations of knocked-out atoms and to obtain a system of quasihydrodynamic equations describing the evolution of the cascade in space and time.

INTRODUCTION

The well-known 1955 paper of Kinchin and Pease[1] was the starting point of the theory of atomic collision cascades. Many theoretical papers have since been published (the most recent review can be found in Ref. 2). However, we must admit that the progress has been mainly due to numerical solution of transport equations or computational modeling of the relevant processes,[3] whereas the number of analytical results is small (see, for example, Refs. 4–12) and most of them have been obtained for the spatially homogeneous steady-state case. Therefore, we are still facing the problem of developing an analytical theory of cascades.

Our aim will be to show that the theory of linear cascades has self-similar solutions which make it possible, firstly, to provide a clear physical description of the development of a cascade as a pattern of consecutive generations of knocked-out atoms and, secondly, can be used as the basis of a quasihydrodynamic description of a cascade. In dealing with quasihydrodynamics we must stress that, in contrast to ordinary hydrodynamics, where a system is described by a local Maxwellian distribution, in the case of a linear cascade the local description is different and it is given by the self-similar solution mentioned above.

FORMULATION OF THE PROBLEM

A solid consisting of A atoms is bombarded with B atoms or ions which knock out A atoms from their equilibrium positions. Each primary knocked-out A atom is a source of a collision cascade knocking out other A atoms from their equilibrium positions.

It is assumed that the density of the bombarding particles is low, so that the number of moving atoms is small and we have to allow only for collisions of moving atoms with those at rest, whereas collisions between moving atoms can be ignored (linear cascade case[2]). We shall also assume that collisions between atoms can be regarded as occurring in pairs. Let $f_\mathbf{k}$ be the distribution function of the momenta of B atoms and $f_\mathbf{p}$ be the distribution function of moving A atoms. Then, the situation under discussion is described by the following system of transport equations. For the B atoms we have

$$\frac{\partial f_\mathbf{k}}{\partial t} = -\mathbf{v}_\mathbf{k}\nabla f_\mathbf{k} + \sum_\mathbf{k} (f_{\mathbf{k}'} w_{\mathbf{k}'\to\mathbf{k}} - f_\mathbf{k} w_{\mathbf{k}\to\mathbf{k}'}), \tag{1}$$

$$w_{\mathbf{k}\to\mathbf{k}'} = \sum_\mathbf{p} w_{\mathbf{k}\to\mathbf{k}',\mathbf{p}}. \tag{2}$$

Here $w_{\mathbf{k}\to\mathbf{k}',\mathbf{p}}$ is the probability that a B atom moving in a medium of A atoms at rest is scattered from $\mathbf{k}$ to $\mathbf{k}'$ giving rise to a moving A atom with a momentum $\mathbf{p}$. For the A atoms we have

$$\frac{\partial f_\mathbf{p}}{\partial t} = -\mathbf{v}_\mathbf{p}\nabla f_\mathbf{p} + \hat{\mathrm{S}}\{f_\mathbf{p}\} + \hat{\mathrm{C}}\{f_\mathbf{k}\}, \tag{3}$$

$$\hat{\mathrm{C}}\{f_\mathbf{k}\} = \sum_{\mathbf{k},\mathbf{k}'} f_\mathbf{k} w_{\mathbf{k}\to\mathbf{k}',\mathbf{p}}, \tag{4}$$

$$\hat{\mathrm{S}}\{f_\mathbf{p}\} = \sum_{\mathbf{p}'} (f_{\mathbf{p}'} w_{\mathbf{p}'\to\mathbf{p}} - f_\mathbf{p} w_{\mathbf{p}\to\mathbf{p}'} + f_{\mathbf{p}'} \tilde{w}_{\mathbf{p}',\mathbf{p}}), \tag{5}$$

$$w_{\mathbf{p}\to\mathbf{p}'} = \sum_{\mathbf{p}''} w_{\mathbf{p}\to\mathbf{p}',\mathbf{p}''}, \qquad \tilde{w}_{\mathbf{p},\mathbf{p}'} = \sum_{\mathbf{p}''} w_{\mathbf{p}\to\mathbf{p}'',\mathbf{p}'}. \tag{6}$$

Here $w_{\mathbf{p}\to\mathbf{p}',\mathbf{p}''}$ is the probability that after a collision between an A atom characterized by a momentum $\mathbf{p}$ and an A atom at rest the momentum of the latter is $\mathbf{p}''$ and the former atom has a momentum $\mathbf{p}'$. Next, $w_{\mathbf{p}\to\mathbf{p}'}$ is the scattering probability of an A atom in an undisturbed medium, whereas $w_{\mathbf{p},\mathbf{p}'}$ is the probability that after the scattering of an A atom with a momentum $\mathbf{p}$ a new moving A atom with a momentum $\mathbf{p}'$ appears in the undisturbed medium.

Equation (1) for $f_\mathbf{k}$ can be solved independently and then $\hat{\mathbf{C}}$ in Eq. (3) becomes a known source for $f_\mathbf{p}$ and the solution of Eq. (3) reduces to finding the Green's function $G(\mathbf{p},\mathbf{p}_0;\mathbf{r},\mathbf{r}_0,t)$, which satisfies the equation

$$\partial G/\partial t = -\mathbf{v}_\mathbf{p}\nabla G + \hat{\mathrm{S}}\{G\} + \delta_{\mathbf{p},\mathbf{p}_0}\delta(t)\delta(\mathbf{r}-\mathbf{r}_0). \tag{7}$$

The function G is the distribution function in the case when one primary knocked-out A atom with a momentum $\mathbf{p}_0$ appears at time $t=0$ at a point $\mathbf{r}_0$ in a normalization volume L^3. Our aim will be to find this function.

We shall ignore the crystal structure of the medium and the anisotropy of the probability w relative to the crystallographic axes. We shall write down the transport equations ignoring electron deceleration, i.e., neglecting excitation and ionization of atoms as a result of collisions. We shall regard the motion of atoms as classical.

POTENTIALS AND CROSS SECTIONS

The decisive stage in the solution of Eq. (7) is the selection of the scattering probability w, i.e., the selection of the interatomic interaction potential $U(r)$. In a rough approximation we can use an interaction potential characterized by

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certain amplitude U_0 and a radius of action a. The characteristic energy transfer ω as a result of a collision of a moving atom of energy ε with an atom at rest can be estimated to be $\omega\sim\varepsilon$, if $\varepsilon\ll U_0$, and $\omega\sim U_0^2/\varepsilon$, if $\varepsilon\gg U_0$ (it is asumed that the masses of atoms are of the same order of magnitude). If we exclude the situation when $\varepsilon\sim U_0$, we find that we always have $\omega\ll U_0$. Therefore, irrespective of the energy of the bombarding B atoms, the energy of the primary knocked-out A atoms (and all the atoms in later generations or stages of the cascade) will almost always be small compared with U_0^{AB}. If $U_0^{AA}\gtrsim U_0^{AB}$, then all the conditions in a cascade occur in the energy range $\varepsilon\ll U_0^{AA}$ and the characteristic energy transfer is $\omega\sim\varepsilon$. In this range of energies the important feature is the behavior of the potential in the spatial region $r\gtrsim a$, where the potential can be approximated by a power-law dependence on r: $U(r)\propto r^{-n}$ (Ref. 13). The power exponent is $n>1$, which reflects the screening of the Coulomb interaction of the nuclei of atoms at large distances from one another.

If the problem is regarded as isotropic relative to the crystallographic axes, the probability $w_{\mathbf{p}\to\mathbf{p}',\mathbf{p}''}$ can be expressed in terms of the scattering cross section differentiated with respect to energy transfer $d\sigma(\varepsilon,\omega)/dw$. In the case of a power-law potential,[14] we find that

$$\frac{d\sigma(\varepsilon,\omega)}{d\omega}=\frac{C}{\varepsilon^{1+2m}}\Phi\left(\frac{\omega}{\varepsilon}\right),\quad m=\frac{1}{n},\quad 0<m<1,\tag{8}$$

whereas in the case of low-angle scattering if $x\ll1$, then

$$\Phi(x)\propto x^{-(1+m)}\tag{9}$$

[in the case of the Coulomb potential when $n=1$ the asymptote of Eq. (9) is identical with the exact form of $\Phi(x)$], whereas for any form of scattering if $x\to1$, then

$$\Phi(x)\to\text{const.}\tag{10}$$

The scattering of identical particles can be normalized using the condition

$$\int_0^1 dx\,x\Phi(x)=1.\tag{11}$$

The energy range $l(\varepsilon)$ and the energy relaxation time $\tau(\varepsilon)$ are described by

$$\frac{\varepsilon}{l(\varepsilon)}=-\frac{d\varepsilon}{dx}=N\int_0^{\varepsilon}d\omega\,\omega\frac{d\sigma(\varepsilon,\omega)}{d\omega},\tag{12}$$

$$\tau(\varepsilon)=l(\varepsilon)/v(\varepsilon).\tag{13}$$

Here, N is the number of target atoms per 1 cm^3 and $v(\varepsilon)=(2\varepsilon/M)^{1/2}$ is the velocity of an atom.

It is clear from Eqs. (9)–(12) that, as expected, the stopping power is dominated by the processes characterized by $\omega\sim\varepsilon$. Using Eqs. (8), (12), and (13), we find that

$$l(\varepsilon)=\frac{\varepsilon^{2m}}{NC},\quad\tau(\varepsilon)=\frac{\varepsilon^{2m-1/2}}{NC(2/M)^{1/2}}.\tag{14}$$

The value of $\tau(\varepsilon)$ increases with ε for soft (weakly screened) potentials ($1<n<4$, $\frac{1}{4}<m<1$), whereas for hard (strongly screened) potentials ($n>4$, $m<\frac{1}{4}$), we find that $\tau(\varepsilon)$ decreases with ε. It should be noted that $l(\varepsilon)$ always increases as a function of ε.

GENERATIONS OF KNOCKED-OUT ATOMS

In the high-energy range $\varepsilon\gg\varepsilon_b$, where ε_b is the binding energy of an atom at an equilibrium position, the probability w satisfies the laws of conservation of energy and momentum:

$$w_{\mathbf{p}\to\mathbf{p}',\mathbf{p}''}\propto\delta_{\mathbf{p},\mathbf{p}'+\mathbf{p}''}\delta(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}'}-\varepsilon_{\mathbf{p}''}).\tag{15}$$

Therefore, the knocking out of an atom from its equilibrium position is formally equivalent to "decay" of a moving atom with a momentum $\mathbf{p}$ into two atoms with momenta $\mathbf{p}'$ and $\mathbf{p}''$. Consequently, in the description of a cascade we can use the concept of generations or stages developed in Ref. 15 for phonon decay. As pointed out already, a typical energy transfer amounts to $\omega\sim\varepsilon$. Therefore, when a new moving atom appears the dominant processes are those characterized by $\varepsilon_{\mathbf{p}'}\sim\varepsilon_{\mathbf{p}''}\sim\varepsilon_{\mathbf{p}}$. It therefore follows that the energy $\varepsilon_{\mathbf{p}}$ is shared approximately equally between the scattering and knocked-out atoms. Therefore, a cascade can be regarded qualitatively as a sequence of generation of atoms, and the energy of atoms in each succeeding generation is half the energy of atoms in the preceding one. The lifetime of a generation characterized by an energy ε is $\tau(\varepsilon)$, so that the duration of a cascade initiated by an atom of energy ε_0 is given by

$$t_c=\tau(\varepsilon_0)+\tau\left(\frac{\varepsilon_0}{2}\right)+\tau\left(\frac{\varepsilon_0}{2^2}\right)+\ldots\sim\int_0^{\varepsilon_0}\frac{d\varepsilon}{\varepsilon}\tau(\varepsilon).\tag{16}$$

It is clear from Eq. (16) that in the case of soft potentials the main contribution to the sum comes from the first generation or the lifetime of this generation, i.e., $t_c\sim\tau(\varepsilon_0)$; in the case of hard potentials the sum diverges, i.e., a cascade is "infinitely long." In fact, the concept of generations ceases to be valid when the energy of the atoms becomes comparable with the binding energy ε_b. Therefore, in the case of hard potentials the integral of Eq. (16) should be truncated at the lower limit $\varepsilon\approx\varepsilon_b$, which gives $t_c\sim\tau(\varepsilon_b)$. This means that in the case of hard potentials the duration of a cascade is determined by the lifetime of the last generation and is independent of the energy ε_0 of the primary atom.

During its lifetime a generation with an energy ε travels in space a distance $l(\varepsilon)$ and the whole cascade traverses a distance

$$l_c=l(\varepsilon_0)+l\left(\frac{\varepsilon_0}{2}\right)+l\left(\frac{\varepsilon_0}{2^2}\right)+\ldots\sim\int_0^{\varepsilon_0}\frac{d\varepsilon}{\varepsilon}l(\varepsilon)\sim l(\varepsilon_0).\tag{17}$$

In other words, the spatial extent of a cascade is always governed by the first generation.

The range of atoms in later generations characterized by energies $\varepsilon\ll\varepsilon_0$ is short: $l(\varepsilon)\ll l(\varepsilon_0)$. This means that evolution of a cascade near its end occurs under conditions of a weak spatial inhomogeneity, i.e., it occurs in a quasihydrodynamic regime. We shall therefore initially study a cascade in the spatially homogeneous case and then deduce quasihydrodynamic equations.

SPATIALLY HOMOGENEOUS CASE

The development of a cascade in the spatially homogeneous case corresponds to the situation when n_0 atoms with a momentum $\mathbf{p}_0$ and an energy $\varepsilon_0\equiv\varepsilon_{\mathbf{p}_0}$ are created at $t=0$ per 1 cm^3. The Green's function $g_{\mathbf{p}}(t)$ then satisfies the equation

$$\partial g_{\mathbf{p}}/\partial t=\hat{S}\{g_{\mathbf{p}}\}+\delta_{\mathbf{p}_0,\mathbf{p}}\delta(t)n_0L^3.\tag{18}$$

In view of the isotropy of the model, the function g_p depends only on $\varepsilon \equiv \varepsilon_p$ and on the angle θ between $\mathbf{p}$ and the z axis selected along $\mathbf{p}_0$. We shall introduce

$$\rho(\varepsilon) g_p(t) = \sum_{l=0}^{\infty} (2l+1) F_l(\varepsilon, t) \mathscr{P}_l(\cos\theta), \tag{19}$$

where $\rho(\varepsilon)$ is the density of states per 1 cm^3 and $\mathscr{P}_l(x)$ is a Legendre polynomial. Then, the equations for $F_l(\varepsilon,t)$ with different values of l can be separated and for $t > 0$ they become

$$\frac{\partial F_l(\varepsilon, t)}{\partial t} = N \int_{\varepsilon}^{\varepsilon_0} d\varepsilon' v(\varepsilon') \mathscr{P}_l[(\varepsilon/\varepsilon')^{1/2}] F_l(\varepsilon', t) \times \{\hat{\sigma}(\varepsilon', \varepsilon) + \hat{\sigma}(\varepsilon', \varepsilon' - \varepsilon)\} - N v(\varepsilon) F_l(\varepsilon, t) \int_0^{\varepsilon} d\varepsilon' \, \hat{\sigma}(\varepsilon, \varepsilon - \varepsilon'), \tag{20}$$

where

$$d\sigma(\varepsilon, \omega)/d\omega \equiv \hat{\sigma}(\varepsilon, \omega). \tag{21}$$

It should be pointed out that, on the basis of Eq. (9), in the case of power-law potentials the integral with respect to ε' in the last ("outgoing") term diverges for $\varepsilon' \gtrsim \varepsilon$. However, we can see that this divergence is cancelled by exactly the same divergence in the second term. The physical reason for this cancellation is the circumstance that the transport processes are in fact governed by the energy transfer cross section, whereas the usual total cross section occurring in the "outgoing" term has no specific meaning.

The functions F_l with $l = 0$ or 1 should satisfy the laws of conservation of atomic energy per cm^3

$$E(t) = \int_0^{\varepsilon_0} d\varepsilon \, \varepsilon F_0(\varepsilon, t) = n_0 \varepsilon_0 = E_0 \tag{22}$$

and of the projection along the z axis of the atomic momentum per cm^3

$$P(t) = \int_0^{\varepsilon_0} d\varepsilon \, M v(\varepsilon) F_1(\varepsilon, t) = n_0 p_0 = P_0. \tag{23}$$

In the case of power-law potentials a solution of the system (20) in the $\varepsilon < \varepsilon_0$ case can be found in the self-similar form:

$$F_l(\varepsilon, t) = A_l \varepsilon^{\alpha_l} \varphi_l(\xi), \quad \xi = (t_0 \pm t)/\tau(\varepsilon), \tag{24}$$

where A_l, α_l, and t_0 are certain constants. Substituting Eq. (24) into Eq. (20), and using Eq. (8), we obtain the following equations for φ_l:

$$\pm \frac{d\varphi_l(\xi)}{d\xi} = \int_{\varepsilon/\varepsilon_0}^{1} \frac{dx}{x} x^{2m - 1/2 - \alpha_l} \varphi_l(\xi x^{2m-1/2}) \mathscr{P}_l(x^{1/2}) \times [\Phi(x) + \Phi(1-x)] - \varphi_l(\xi) \int_0^1 dx \, \Phi(x). \tag{25}$$

Hence, we can see that the self-similar solution is obtained only for $\varepsilon \ll \varepsilon_0$, when the lower limit of the integral can be replaced with 0.

We shall now consider the energy $E(t)$. Substituting F_0 from Eq. (24) into Eq. (22) and going over from integration with respect to ε to that with respect to ξ, we obtain

$$E(t) \propto \operatorname{sign}\left(\frac{1}{4} - m\right)(t_0 \pm t)^{-\beta} \int_{0,\infty}^{\xi_0(t)} \frac{d\xi}{\xi} \varphi_0(\xi) \xi^{\beta},$$
$$\xi_0(t) = \frac{t_0 \pm t}{\tau(\varepsilon)}, \quad \beta = \frac{2}{1-4m}(\alpha_0 + 2). \tag{26}$$

The lower limit in the integral is 0 for $m < \frac{1}{4}$ and ∞ for $m > \frac{1}{4}$. The energy $E(t)$ is independent of t and, firstly, we have $\beta = 0$, i.e., $\alpha_0 = -2$. Secondly, it should be possible to replace the integration limit $\xi_0(t)$ with infinity if $m < \frac{1}{4}$ and with 0 if $m > \frac{1}{4}$. A similar analysis of $P(t)$ gives $\alpha_1 = -\frac{3}{2}$.

The normalization constants A_0 and A_1 are defined, in accordance with Eqs. (22) and (23), using the energy E_0 and momentum P_0 per cm^3. The sign in front of t in the self-similar variable ξ is found by considering the number of atoms in 1 cm^3:

$$n(t) = \int_0^{\varepsilon_0} d\varepsilon \, F_0(\varepsilon, t), \tag{27}$$

which in the case of the self-similar solution subject to $\alpha_0 = -2$ behaves as follows:

$$n(t) \propto (t_0 \mp t)^{2/(1-4m)}. \tag{28}$$

The number of atoms should increase. This condition can be satisfied if we select the plus sign for $m < \frac{1}{4}$ and the minus sign for $m > \frac{1}{4}$.

We shall now go back to the equations for φ_0 and φ_1 using the values $\alpha_0 = -2$ and $\alpha_1 = -\frac{3}{2}$ found above. Noting that $\mathscr{P}_0(x^{1/2}) = 1$ and $\mathscr{P}_1(x^{1/2}) = x^{1/2}$, we find that φ_0 and φ_1 are described by the same equations:

$$\pm \frac{d\varphi_{0,1}(\xi)}{d\xi} = \int_0^1 \frac{dx}{x} x^b \varphi_{0,1}(\xi x^{\pm a}) [\Phi(x) + \Phi(1-x)] - \varphi_{0,1}(\xi) \int_0^1 dx \, \Phi(x), \tag{29}$$

where the upper sign applies if $m > \frac{1}{4}$ and the lower if $m < \frac{1}{4}$, and we also have

$$a = |2m - 1/2|, \quad b = 2m + 3/2. \tag{30}$$

We shall assume that $\varphi_0 = \varphi_1 = \varphi$ and select the normalization condition in the form

$$\frac{1}{a} \int_0^{\infty} \frac{d\xi}{\xi} \varphi(\xi) = 1. \tag{31}$$

We can then calculate A_0 and A_1, and find finally that

$$F_0(\varepsilon, t) = \frac{E_0}{\varepsilon^2} \varphi(\xi),$$
$$F_1(\varepsilon, t) = \frac{P_0}{\varepsilon p(\varepsilon)} \varphi(\xi), \quad p(\varepsilon) = M v(\varepsilon). \tag{32}$$

Hence, we can determine the constant t_0. This can be done by calculating again $n(t)$ using F_0 from Eq. (32). This gives[1]

$$n(t) = c n_0 \left[\frac{t_0 \mp t}{\tau(\varepsilon_0)}\right]^{2/(1-4m)} \sim n_0 [\xi_0(t)]^{2/(1-4m)}, \quad m \gtreqless 1/4, \tag{33}$$

where

$$c=\frac{1}{a}\int_0^\infty \frac{d\xi}{\xi}\,\xi^{\pm 1/a}\varphi(\xi)\sim 1. \tag{34}$$

Recalling the conditions which are imposed on $\xi_0(t)$ as the upper limit of the integral (26), we can see that the self-similar solution is valid for times t such that $n(t)\gg n_0$, i.e., when the cascade heated by each initial atom consists of a large number of particles. It is also clear that at $t=0$ the value of $n(t)$ found in this way cannot be exact, but we can expect a correct order of magnitude of this number. Assuming that $n(0)\sim n_0$ in Eq. (33), we find that

$$t_0\sim\tau(\varepsilon_0). \tag{35}$$

We shall now summarize the results. The self-similar solution for the first two angular moments of the Green's function is given by Eq. (32); the function φ is then normalized by the condition (31). The self-similar variable ξ and the conditions under which the self-similar solution is valid are different for soft and hard potentials.

In the case of soft potentials ($m>\frac{1}{4}$), we have

$$\xi=(t_0-t)/\tau(\varepsilon). \tag{36}$$

The time $t_0\sim\tau(\varepsilon_0)$ is the "duration" of a cascade. The self-similar solution is valid if

$$\varepsilon\ll\varepsilon_0,\quad t_0-t\ll\tau(\varepsilon_0), \tag{37}$$

i.e., near the end of a cascade. In the case of hard potentials ($m<\frac{1}{4}$) the condition for validity of the self-similar solution can be reduced to

$$\varepsilon\ll\varepsilon_0,\quad t\gg\tau(\varepsilon_0), \tag{38}$$

so that the self-similar variable is

$$\xi=t/\tau(\varepsilon_0) \tag{39}$$

and the time t_0 drops out from the equations. The full development of a cascade then requires an "infinite" time.

We now have to consider also the role of the higher angular momenta of F_l characterized by $l\geqslant 2$. It is clear from Eq. (32) that

$$F_1/F_0\sim(\varepsilon/\varepsilon_0)^{1/2}, \tag{40}$$

i.e., under the conditions when the self-similar solution is valid, we have $F_1\ll F_0$. This means that the process by which the self-similar solution is established is accompanied by simultaneous isotropization of the distribution. Therefore, it is natural to assume that in the self-similar solution the moments F_l with $l\geqslant 2$ can be ignored, especially as their vanishing is not in conflict with any conservation laws.

It therefore follows that the self-similar Green's function for the spatially homogeneous problem is

$$\rho(\varepsilon)g_{\mathbf p}(t)=\varphi(\xi)\left\{\frac{E_0}{\varepsilon^2}+3\frac{P_0}{p(\varepsilon)\varepsilon}\cos\theta\right\}, \tag{41}$$

where E_0 and P_0 are the total energy and momentum of particles in 1 cm^3 and θ is the angle between $\mathbf p$ and $\mathbf P_0$. This form of the Green's function is obtained when each cascade initiated by a single initial atom already contains many atoms.

In the case of a steady-state source, Eq. (41) is identical with the distribution functions of the stationary problem, obtained in Ref. 8. The energy spectrum of atoms then has the familiar form $F(\varepsilon)\sim E_0/\varepsilon^2$ (Ref. 6).

It should also be noted that the difference between the soft and hard potentials in the case of the self-similar solution is in full agreement with the qualitative concept of generations. The Maxwellian potential ($m=\frac{1}{4}$) does not admit the self-similar solution when $\tau(\varepsilon)=\text{const}$, since in this case $n(t)$ in Eq. (33) is meaningless.

It was shown in Ref. 7 that in the case of the Maxwellian potential the number of atoms in a cascade rises exponentially: $n(t)\propto\exp[t/\tau(\varepsilon_0)]$. The exponential rise is intermediate between the $t^{1/a}$ law (hard potentials) and the $(t_0-t)^{-1/a}$ law (soft potentials).

The existence of the self-similar solutions of the system (20) in the case when $l=0$ or 1 is influenced only by the general form of the cross section (8) and not by the specific properties of the function $\Phi(x)$ [subject to the condition for the existence of the normalization integral of Eq. (31), whose convergence in the final analysis depends on the limiting form of Φ for $x\ll 1$ and $x\to 1$]. Therefore, the selection of the potential of the interaction between atoms in the form of a power law is not essential. Another example of potentials admitting the existence of self-similar solutions is the hard-sphere potential when the scattering cross section can be deduced from Eq. (8) by the formal substitution $m=0$ and $\Phi(x)\equiv\text{const}$. Then, $N(t)$ becomes[2]

$$N(t)=n(t)/n_0\sim[t/\tau(\varepsilon_0)]^2. \tag{42}$$

The exact expression for $N(t)$ was obtained in Ref. 7 for the hard-sphere potential:

$$N(t)=1+t/\tau(\varepsilon_0)+{}^1/_6(t/\tau(\varepsilon_0))^2. \tag{43}$$

A comparison of Eqs. (42) and (43) shows that the exact solution reduces asymptotically to the self-similar solution for $t\gg\tau(\varepsilon_0)$.

QUASIHYDRODYNAMIC EQUATIONS

We shall now investigate the spatial evolution of a cascade initiated by an atom created at time $t=0$ at a point $\mathbf r=\mathbf r_0$ with a momentum $\mathbf p_0$. The Green's function then satisfies Eq. (7). It follows from the above that if we are interested in time intervals such that the number of atoms in a cascade is large, the atomic mean free paths are much less than the dimensions of a cascade. Therefore, following the usual approach to a hydrodynamic description, we shall obtain a Green's function of a cascade in the form[3]

$$\rho(\varepsilon)G_{\mathbf p}(\mathbf r,t)=\varphi(\xi)\left\{\frac{E(\mathbf r,t)}{\varepsilon^2}+3\frac{\mathbf P(\mathbf r,t)\mathbf p}{\varepsilon[p(\varepsilon)]^2}\right\}, \tag{44}$$

i.e., we shall replace the constants E_0 and $\mathbf P_0$ in Eq. (41) with the values of E and $\mathbf P$ that vary slowly with $\mathbf r$ and t and represent, respectively, the density of the energy and momentum of particles in this cascade. A characteristic scale of these quantities along $\mathbf r$ is the size of the cascade l_c. The equations for E and $\mathbf P$ are obtained as usual from the balance of energy and momentum. Substituting Eq. (44) into Eq. (7), multiplying the equation by $\varepsilon_{\mathbf p}$, and summing over $\mathbf p$, we find that

$$\partial E/\partial t+s^2(t)\operatorname{div}\mathbf P=0. \tag{45}$$

Here,

$$s^2(t)=\begin{cases} c'v_0^2[(t_0-t)/\tau(\varepsilon_0)]^{1/a}, & m>{}^1/_4, \\ c'v_0^2[t/\tau(\varepsilon_0)]^{-1/a}, & m<{}^1/_4, \end{cases} \tag{46}$$

where $v_0=p_0/M$ is the velocity of an atom initiating the cascade and

$$c'=\frac{1}{a}\int_0^\infty \frac{d\xi}{\xi}\,\xi^{\mp 1/a}\varphi(\xi)\sim 1. \tag{47}$$

Similarly, multiplying Eq. (7) by **p** and summing over **p**, we find that

$$\partial\mathbf{P}/\partial t+{}^1/_3\nabla E=0. \tag{48}$$

Equations (45) and (48) resemble the system of equations describing second sound, which is to be expected because the total energy and momentum of the whole system of particles are conserved both in an atomic cascade and in phonon hydrodynamics. The important difference is that the velocity $s(t)$ of second sound depends on time. It is of the order of the average random velocity of atoms in a cascade at time t: $s(t)\sim v(\langle\varepsilon\rangle_t)$. It follows from Eqs. (45) and (48) that

$$\partial^2\mathbf{P}/\partial t^2+{}^1/_3 s^2(t)\nabla(\operatorname{div}\mathbf{P})=0, \tag{49}$$

i.e., the equation is of the wave type in which the propagation velocity is a given decreasing function of time.

We shall now go back to the distribution (44). The quantities E and $\mathbf{P}$ vary at a rate characterized by a time constant $l_c/s(t)$. On the other hand, the factor $\varphi(\xi)$ changes in a time $\tau(\varepsilon)$, where ε is the average energy at a moment t. We can easily see that

$$\frac{l_c/s(t)}{\tau(\langle\varepsilon\rangle_t)}\sim\frac{l_c}{l(\langle\varepsilon\rangle_t)}\gg 1. \tag{50}$$

Therefore, the main fast process of the change in G is a change in the energy distribution of the atoms which does not alter the spatial dependence of the energy and momentum densities. These densities vary much more slowly in space. As pointed out above, the anisotropy of the distribution (44) is weak. However, the smallness of the anisotropy is not related to the relaxation of the momentum of the system. Therefore, both E and $\mathbf{P}$ are described by wave-type rather than diffusion-type equations.

It is also illuminating to compare the problems of atomic and phonon cascades. For both cascades the spatially homogeneous case can be described by a self-similar solution. However, in the spatially inhomogeneous case there is a fundamental difference: a phonon cascade again evolves in a self-similar manner, whereas an atomic cascade evolves quasihydrodynamically. This is due to the fact that the range in a phonon cascade increases as the new generations appear and the size of the region occupied by the particles is governed by the last generation, whereas in an atomic cascade the range decreases and the size of this region is determined by the first generation.

Equations (45) and (48) are suitable for describing the sputtering of atoms, provided we allow for the influence of the surface on the development of a cascade. In the most widely used variant of sputtering theory,[17] the problem of a cascade is solved as in the case of an unbounded medium and the surface simply acts as a virtual plane crossed by a flux of sputtered particles. In fact, the influence of the surface must be allowed for more correctly. In our case we would have to solve again the transport equation in the surface region and derive quasihydrodynamic equations using a new distribution function. However, this is a fairly major task. Therefore, we shall allow for the influence of the surface by an approximate boundary condition applicable to hydrodynamic quantities $E(\mathbf{r},t)$ and $\mathbf{P}(\mathbf{r},t)$, as in the case of the Milne problem.[18] We shall assume that the surface is totally absorbing. This means that the distribution function on the surface should vanish for particles with a nonzero component of the velocity directed away from the surface. However, this condition cannot be satisfied by the quasihydrodynamic distribution function (44) for any value of E or $\mathbf{P}$. Therefore, we can simply require that the boundary condition should be satisfied on the average:

$$j_{\mathbf{vn}>0}|_{\mathbf{r}\in S}=0, \tag{51}$$

where $j_{\mathbf{vn}>0}$ is the flux of particles moving from a surface S and the direction of the inner normal to S is taken to be positive. The condition (51) together with the distribution function (44) yields

$$\{E(\mathbf{r},\ t)+\tilde{c}s(t)P(\mathbf{r},\ t)\}|_{\mathbf{r}\in S}=0, \tag{52}$$

where $\tilde{c}\sim 1$. The exact value of $\tilde{c}$ can be found only by solving the transport equation for the surface layer, so that in our approximation the quantity $\tilde{c}$ is an unknown parameter of the theory.

[1] An analysis of the equation for the self-similar function $\varphi(\xi)$ of Eq. (29) shows that if $\Phi(x)$ has a small-angle asymptote (9), then the integral (34) diverges. However, this is not so important, because an analysis leading to the selection of the sign of the self-similar variable and an estimate of t_0 should be carried out not for $n(t)$, but for the average energy per particle at a time t.

[2] In this case the integral of Eq. (34) converges.

[3] It should be noted that this form of the distribution function (in the steady-state problem) was postulated in Ref. 16.

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