UDC 621.039.78 DOI: 10.18698/1812-3368-2019-6-40-49

INVESTIGATION OF THE NONSTATIONARY ENERGY DISTRIBUTION OF AN ATOMIC COLLISION CASCADE

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Abstract

In this paper, we derive a nonstationary distribution function describing the energy distribution of the cascade of moving atoms taking into account their multiplication. The function was derived by solving the Boltzmann kinetic equation. The development of the cascade was considered for the materials consisting of atoms of the same type without taking into account the binding energy of atoms at the crystal lattice sites. The scattering of moving atoms is assumed to be elastic and spherically symmetrical in a center-of-inertia system, and the interaction cross-section is assumed to be constant. The use of these assumptions allows us to derive simple analytic formulas for the nonstationary energy distribution function for the cascade and analyze its main distinctive features. The results obtained allow evaluating the accuracy of various approximate solutions

Keywords

Kinetic equation, model, atomic cascade, nonstationary energy distribution, collision, deceleration of atoms, interaction section

Received 03.12.2018

Introduction. One of the critical processes in designing nuclear reactors and thermonuclear facilities is the choice of materials withstanding prolonged exposure to ionizing radiation. When fast particles, especially neutrons, irradiate solids, the atoms of the crystal lattice receive the energy of the impinging particle. If the energy is greater than a threshold value, the atoms are knocked out of their equilibrium positions. Then the exchange of energy between moving atoms and atoms in the crystal lattice sites initiates new generations of knocked-on atoms. As a result of this, a so-called atomic collision cascade takes place. The cascade causes the initiation and accumulation of radiation defects (vacancies and interstitial atoms) in structural materials, making them change their physicomechanical properties [1, 2].

There is a large body of research investigating the development of atomic collision cascades in solids [3–9]. In Ref. [7], a steady-state distribution function describing the energy distribution of a cascade of moving atoms was derived for the simplest partial case of elastic and spherically symmetrical scattering in the center-of-mass system without taking into account the binding energy of atoms in the lattice sites. In Ref. [9], based on solving the Boltzmann kinetic equation, an energy distribution function was derived. This function describes the steady-state deceleration of a cascade of moving for the exponential interaction potential $\left(U \sim 1/r^n\right)$ taking into account the binding energy of atoms in the lattice sites.

In this paper, the Boltzmann kinetic equation was solved to derive the nonstationary energy distribution function describing the development of a cascade of moving atoms taking into account their multiplication. The scattering of the moving atoms is elastic and spherically symmetrical in the center-of-inertia, and the interaction cross-section is constant.

One of the advantages of using these approximations is that they allow deriving simple analytic expressions for the nonstationary distribution function of a cascade of moving atoms and analyzing its main features. These results can be used to evaluate the accuracy of various approximate solutions.

Problem statement. We consider a solid body consisting of atoms of the same type and neglect their binding energy in the crystal lattice sites. The kinetic equation describing a nonstationary energy distribution of moving atoms from an instantaneous equally distributed in the space monoenergetic source without taking into account the collisions between the atoms is given by [10]:

$$\frac{1}{\upsilon\Sigma\left(E\right)}\frac{\partial\Psi\left(E,t\right)}{\partial t}+\Psi\left(E,t\right)=\int\limits_{E}^{E_0}dE'P\left(E'\to E\right)\Psi\left(E',t\right)+$$

$$+\int\limits_{E}^{E_0}dE'P\left(E'\to E'-E\right)\Psi\left(E',t\right)+N_0\delta\left(E-E_0\right)\delta\left(t\right), \qquad (1)$$

where υ is velocity of atoms; $\Psi(E,t)$ is collision density of moving atoms, $\Psi\left(E,t\right)=\upsilon\Sigma\left(E\right)f\left(E,t\right)$, $f\left(E,t\right)dE$ is number of atoms with energy E in the range dE at the moment of time t per unit volume; $P\left(E'\to E\right)$ is scattering indicatrix (the probability of a moving atom with energy E' to transition to a unit energy range near E during collision), where $P\left(E'\to E\right)=\dfrac{\Sigma\left(E'\to E\right)}{\Sigma\left(E'\right)}$, $\Sigma\left(E'\to E\right)$, $\Sigma\left(E'\right)$ is differential and total cross-sections of the atom scattering, respectively; $\delta\left(t\right)$ is Dirac delta function; N_0 is total number of moving atoms in a unit volume; E_0 is initial energy of the atoms.

The first integral on the right-hand side of the kinetic equation (1) describes a transition of a moving atoms with energy E' to the state with the energy E. A knocked-on atom receives a kinetic energy $(E'-E)$. The second integral takes into account the formation of a knocked-on atom with the energy E, when the moving atom transitions to a state with the energy $(E'-E)$. If we omit the second integral in the right-hand side of the equation (1) we get a regular particle deceleration equation [10].

In case of the elastic spherically symmetrical scattering in the center-of-inertia system, the scattering indicatrix is given by [10]:

$$P(E' \to E) = \frac{1}{E'}. \tag{2}$$

Using Eq. (2), Eq. (1) can be transformed as follows:

$$\frac{1}{\upsilon\Sigma(E)}\frac{\partial\Psi(E,t)}{\partial t} + \Psi(E,t) = 2\int_E^{E_0}\frac{dE'}{E'}\Psi(E',t) + N_0\delta(E-E_0)\delta(t). \tag{3}$$

Solution of the kinetic equation. We apply a direct Laplace transformation to both sides of Eq. (3) [11]

$$\tilde{\Psi}(E,p) = \int_0^{\infty} dt\exp(-pt)\Psi(E,t), \tag{4}$$

and get the following expression:

$$\left(\frac{p}{\upsilon\Sigma(E)}+1\right)\tilde{\Psi}(E,p) = 2\int_E^{E_0}\frac{dE'}{E'}\tilde{\Psi}(E',p) + N_0\delta(E-E_0). \tag{5}$$

We separate the nonscattered radiation from the solution of the kinetic equation

$$\tilde{\Psi}(E,p) = \tilde{\Psi}_0(E,p) + \frac{N_0\delta(E-E_0)}{\left(\frac{p}{\upsilon_0\Sigma(E_0)}+1\right)}. \tag{6}$$

By substituting Eq. (6) in Eq. (5), we get the following expression

$$\left(\frac{p}{\upsilon\Sigma(E)}+1\right)\tilde{\Psi}_0(E,p) = 2\int_E^{E_0}\frac{dE'}{E'}\tilde{\Psi}_0(E',p) + \frac{2N_0}{E_0\left(\frac{p}{\upsilon_0\Sigma(E_0)}+1\right)}. \tag{7}$$

We take into account the fact that the scattering cross-section is constant $(\Sigma(E)=\text{const})$ and differentiate Eq. (7) with respect to the energy to get the differential equation for the function $\tilde{\Psi}_0(E,p)$:

$$\frac{\partial\tilde{\Psi}_0(E,p)}{\partial E}=-\frac{1}{E}\frac{\left(2-\dfrac{p}{2\upsilon\Sigma}\right)}{\left(1+\dfrac{p}{\upsilon\Sigma}\right)}\tilde{\Psi}_0(E,p). \tag{8}$$

The solution of Eq. (8) must satisfy the initial condition (see Eq. (7)):

$$\tilde{\Psi}_0(E_0,p)=\frac{2N_0}{E_0\left(\dfrac{p}{\upsilon_0\Sigma}+1\right)^2}. \tag{9}$$

The solution of Eq. (8) taking into account the initial condition (9) has the following form

$$\tilde{\Psi}_0(E,p)=\frac{2N_0}{E_0}\Sigma^2\upsilon_0\upsilon\frac{(p+\upsilon_0\Sigma)^3}{(p+\upsilon\Sigma)^5}. \tag{10}$$

We should note the result of (10) coincides with the solution of the corresponding steady-state problem [7] if $p=0$. Using Eq. (10), we find a Laplace image of the function $f(E,p)$ (see Eq. (6)):

$$\tilde{f}(E,p)=\frac{2N_0}{E_0}\Sigma\upsilon_0\frac{(p+\upsilon_0\Sigma)^3}{(p+\upsilon\Sigma)^5}+\frac{N_0\delta(E-E_0)}{(p+\upsilon_0\Sigma)}. \tag{11}$$

By applying the inverse Laplace transformation [11] to Eq. (11), we finally derive the nonstationary energy distribution of an atomic collision cascade

$$f(E,t)=\frac{2N_0}{E_0}\tau\left\{1+\frac{3}{2}\left[\left(1-\sqrt{\varepsilon}\right)\tau\right]+\frac{1}{2}\left[\left(1-\sqrt{\varepsilon}\right)\tau\right]^2+\frac{1}{24}\left[\left(1-\sqrt{\varepsilon}\right)\tau\right]^3\right\}\times$$
$$\times\exp\left(-\tau\sqrt{\varepsilon}\right)+N_0\exp(-\tau)\delta(E-E_0), \tag{12}$$

where $\tau=\upsilon_0\Sigma t$ is dimensionless time; $\varepsilon=E/E_0$ is dimensionless energy.

Analysis of the results. Let us investigate how the number of particles and the total energy change in a cascade of moving atoms.

We find a change over time of the total number of particles in the cascade:

$$N(t)=\int_0^{E_0}dEf(E,t). \tag{13}$$

To calculate the integral (13), we use the Laplace image (11):

$$\tilde{N}(p)=\int_0^{E_0}dE\tilde{f}(E,p)=N_0\left(\frac{1}{p}+\frac{\upsilon_0\Sigma}{p^2}+\frac{\upsilon_0^2\Sigma^2}{3p^3}\right). \tag{14}$$

By applying the inverse Laplace transform [11], we get

$$N(t) = N_0\left(1+\tau+\frac{1}{6}\tau^2\right). \tag{15}$$

According to Eq. (15), the number of moving atoms in the cascade is growing. Besides, this growth is not limited, as the binding energy of atoms in the lattice sites is not taken into account.

Let us determine a change over time of the total energy of the particles in the cascade:

$$E(t) = \int_0^{E_0} dEEf(E,t). \tag{16}$$

Using the Laplace image (11), we get

$$\tilde{E}(p) = \int_0^{E_0} dEE\tilde{f}(E,p) = \frac{1}{p}N_0E_0 \tag{17}$$

or

$$N(t) = N_0E_0. \tag{18}$$

Despite the growth of the number of moving atoms, their total energy remains constant. This can be explained by the fact that the binding energy of atoms in the lattice sites is not taken into account. Because of this, the energy a stationary atom has when it starts moving is equal to the energy given to it by a moving atom.

Relations (15), (18) can be used to evaluate the time period for which the result from Eq. (12) is valid without taking into account the binding energy of atoms. As the creation of knocked-on atom takes the energy ε_d, the amount of energy E_d spent on knocking out atoms will grow with time (see Eq. (15)):

$$E_d \approx \frac{1}{6}N_0\tau^2\varepsilon_d. \tag{19}$$

In this case, the result (12) taking into account the binding energy will also be valid as long as the quantity (19) is much less than the quantity (18), i.e., for the time

$$\tau \ll \sqrt{\frac{6E_0}{\varepsilon_d}}. \tag{20}$$

Let us make an evaluation using Eq. (20). Assume the neutron initiating the cascade has the energy of $\varepsilon_n =$ 14 MeV. These neutrons given a nucleus with the mass number of M the average energy of $2\varepsilon_n / M$ [10]. In this case, the initial energy of the knocked out atom is $E_0 =$ 0.5 MeV for iron ($M = 56$).

Assuming that $\varepsilon_d \approx$ 10 eV and using Eq. (20), we get that the result from Eq. (12) will also be valid for taking into account the binding energy of atoms in the lattice sites for iron for the time $\tau \ll 5,5 \cdot 10^2$.

Let us analyze the final result for the distribution function (12). Figure 1 shows the change over time of this function $\left(f' = f\left(E_0 / N_0 \right) \right)$ for different values of the energy. If the energy decreases the peak of the time history shifts to the right and its height increases. The first fact is straightforward. The less energy, the more time is required to reach it during deceleration. The second fact (the increase of the function's peak) is due to the multiplication of atoms in the cascade.

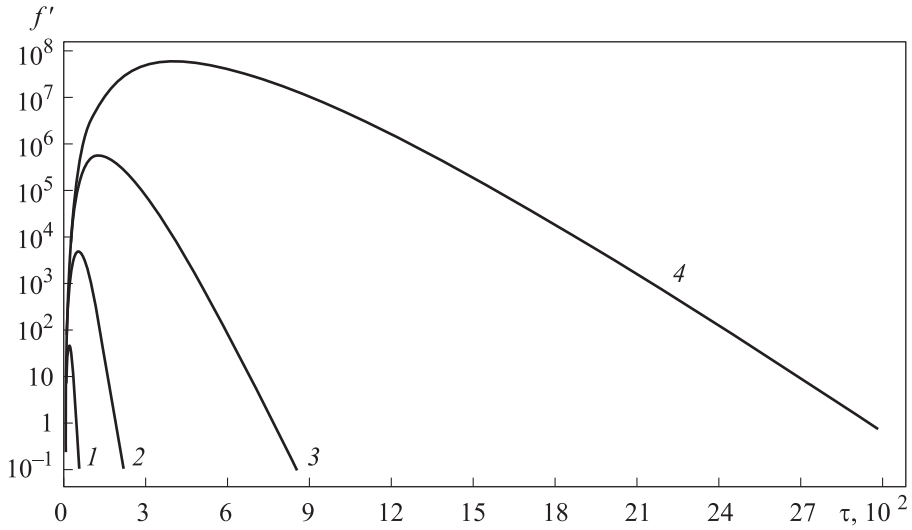

Fig. 1. Time histories of the distribution function for the energy $\varepsilon = E / E_0$ 10^{-1} (*1*), 10^{-2} (*2*), 10^{-3} (*3*) 10^{-4} (*4*)

Figure 2 shows the plot of the distribution function (12) $(f'(\varepsilon))$ vs. energy at different time points. As time progresses, the atoms shift to the lower energy region due to deceleration. We should also take into account that the area under each curve for a given time point is equal to the number of atoms at this time point. The area increases with time according to the law determined by Eq. (15).

Comparing the results with the distribution function of decelerating atoms without taking into account atom multiplication. The distribution function for the decelerating atoms without taking into account their multiplication is described by Eq. (1), where the second integral in the right-hand side is omitted. We use the procedure similar to the one used before and determine

$$\tilde{f}_{dec}\left(E, p \right) = \frac{N_0}{E_0} \Sigma \upsilon_0 \frac{\left(p + \upsilon\Sigma \right)}{\left(p + \upsilon\Sigma \right)^3} + \frac{N_0 \delta\left(E - E_0 \right)}{p + \upsilon_0 \Sigma}. \qquad (21)$$

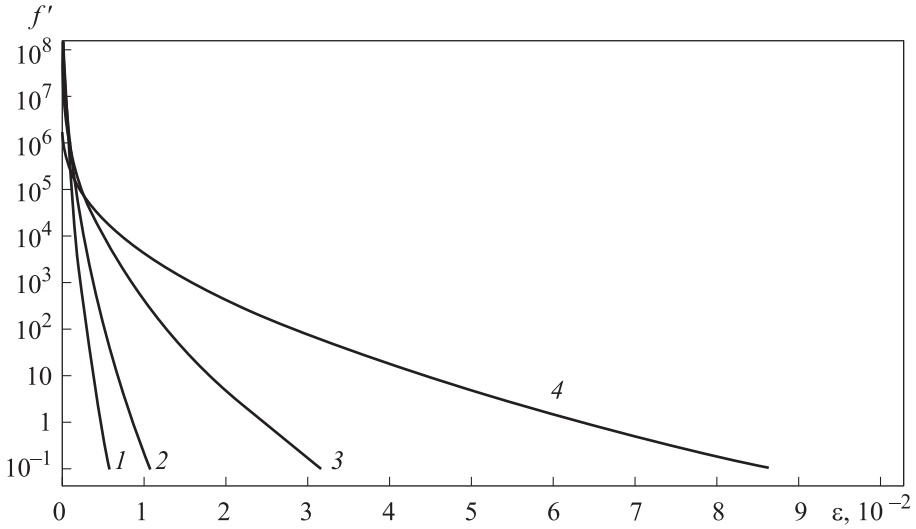

Fig. 2. Distribution function vs. energy $(\varepsilon = E / E_0)$ at time τ = 300 (*1*), 200 (*2*), 100 (*3*) and 50 (*4*)

After applying the inverse Laplace transformation, we get the following result (also see [10]):

$$f_{dec}\left(E,t\right)=\frac{N_0}{E_0}\tau\left[1+\frac{1}{2}\left(1-\sqrt{\varepsilon}\right)\tau\right]\exp\left(-\tau\sqrt{\varepsilon}\right)+N_0\exp\left(-\tau\right)\delta\left(E-E_0\right). \quad (22)$$

The atom multiplication is not taken into account here. Therefore, we can easily conclude that the total number of atoms does not change with time:

$$N_{dec}\left(t\right)=\int\limits_0^{E_0} dEf_{dec}\left(E,t\right)=N_0. \quad (23)$$

Let us analyze the result from Eq. (22) and compare it with the one from Eq. (12). Figure 3 shows the change over time of the function (22) $\left(f'_{dec}=f_{dec}E_0/N_0\right)$ for the same energy values as for Eq. (12) in Fig. 1.

For the latter case, the peaks of the distribution shift to the right with decreasing energy, whereas the peak height increases. The first fact can also be explained that the smaller the energy, the more time it takes to reach it during deceleration. The peak height increases because the rate of increase of the number of atoms for a given energy does not depend on it (see Eq. (22)), while the fall time significantly decreases with decreasing energy (the exponent in Eq. (22) is $\tau\sqrt{\varepsilon}$). The factor is also present during the cascade development, but the peak height growth is much more significant due to the multiplication of atoms (see the curves in Fig. 1 and Fig. 3). Figure 4 shows the plot of the distribution function (22) $\left(f'_{dec}(\varepsilon)\right)$ vs. energy at different time points. As time

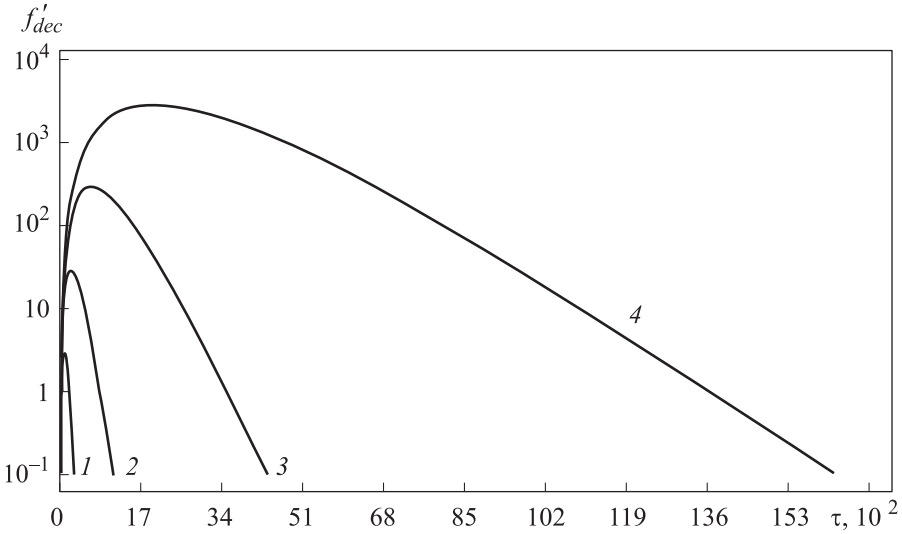

Fig. 3. Time histories of the distribution function without taking into account atom multiplication for the energy values $\varepsilon = 10^{-1}$ (*1*), 10^{-2} (*2*), 10^{-3} (*3*) and 10^{-4} (*4*)

progresses, atoms shift to the lower energy area due to deceleration. We should also note that the area under each curve corresponding to a certain point in time is equal to the total number of atoms at this point, and this number remains constant (see Eq. (23)). Compared to the curves in Fig. 2, the curves in Fig. 4 are much narrower as the multiplication of atoms was not taken into account here.

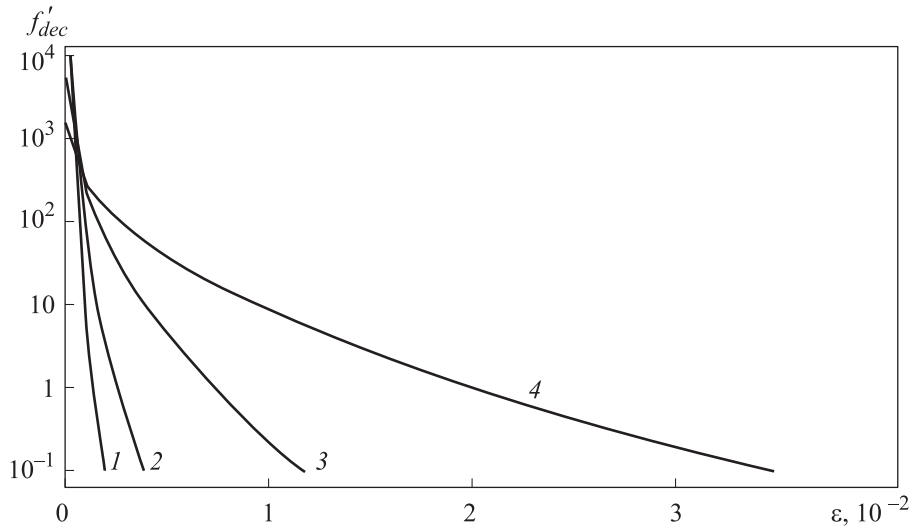

Fig. 4. Energy distribution function vs. energy ε without takin into account the binding energy at points in time τ = 300 (*1*), 200 (*2*), 100 (*3*) and 50 (*4*)

Conclusion. Based on the solution of the Boltzmann kinetic equation, we derived a distribution function (12) describing the nonstationary energy distribution of a cascade of moving decelerating atoms taking into account their multiplication. To solve the equation, it was assumed that the scattering of moving atoms is elastic and spherically symmetrical in the center-of-inertia system, the interaction cross-section is constant, a solid irradiated consists of atoms of the same type, and the binding energy of the atoms was not taken into account. Based on the laws of conservation, we formulated the criterion (20) indicating for which points in time the result from Eq. (12) will also be valid if the binding energy is taken into account.

We analyzed the special features of the distribution function caused by the increased number of atoms of in the cascade and having a generic character. Besides, we compared this distribution against the similar result, which does not take into account the multiplication of atoms in the cascade (22), and identified the principal differences between these functions. It should be noted that the results obtained can be used to evaluate the accuracy of various approximate solutions.

Translated by K. Zykova

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Please cite this article as:

Aleksandrov A.A., Akatev V.A., Metelkin E.V., et al. Investigation of the nonstationary energy distribution of an atomic collision cascade. *Herald of the Bauman Moscow State Technical University, Series Natural Sciences*, 2019, no. 6, pp. 40–49.
DOI: 10.18698/1812-3368-2019-6-40-49