Correlation properties of atomic-collision cascades and athermal annealing of defects

D. L. Maslov

Institute of Problems in Technology of Microelectronics and Ultrapure Materials, USSR Academy of Sciences

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The asymptotic behavior of the pair correlation function of defects produced in a three-dimensional atomic-collision cascade is obtained for r smaller than the characteristic size of the cascade. This asymptotic form of the correlation function is used to find the cascade efficiency, ξ_{eff}, i.e., the share of defects that survive athermal annealing.

INTRODUCTION

In the kinetic theory of linear atomic-collision cascades it is customary to consider single-particle quantities, such as the momentum distribution function of the moving atoms or the associated densities of the particle number, energy, and momentum, at one point of space.[1] In a number of cases, however, this information is insufficient. For example, to consider the first post-cascade stage, the athermal annealing of the defects, i.e., the spontaneous annihilation of close vacancies and interstices, we must know the pair correlation function $K_{iv}(r)$. This function describes the distribution of the defects generated by the cascade, for times in which the energy of the moving atoms becomes lower than the threshold energy $\varepsilon_d (\sim 10\ \text{eV})$ for Frenkel-pair formation, i.e., after the conclusion of the cascade. The form of this function should be obtained from the solution of the corresponding kinetic equations that describe the cascade stage.

A close asymptote of the correlation function of the vacancies was obtained in Ref. 2 for a model one-dimensional case. The purpose of the present paper is to calculate the asymptotic form of $K_{iv}(r)$ in the three-dimensional case for r smaller than the characteristic cascade size $l(\varepsilon_0)$ [$l(\varepsilon)$ is the mean free path of an atom of energy ε, and ε_0 is the energy of the atom initiating the cascade], and to obtain with the aid of this asymptotic form the cascade efficiency ξ_{eff}, i.e., the fraction of the defects that survive athermal annealing. A close asymptote $K_{iv}(r)$ suffices to find ξ_{eff}, since the size R of the spontaneous annihilation zone satisfies the relation $a_0 \lesssim R \ll l(\varepsilon_0)$, where a_0 is the interatomic distance.[3]

GENERAL EQUATIONS

Consider a collision cascade produced by a particle having a momentum $\mathbf{p}_0$ and appearing at a point $\mathbf{r} = 0$ at the instant of time $t = 0$. We assume the primary-particle mass to be equal to the target-atom mass, and neglect the loss to ionization and electron excitation when the atoms collide, and also the scattering-probability anisotropy relative to the crystallographic axes. The atom motion is assumed classical. The number of moving atoms per unit volume is small, and the collisions between them can be disregarded (linear cascade). Under these conditions, the averaged (over the fluctuations) single-particle distribution function $\langle f(\mathbf{p}_0|\mathbf{p}\mathbf{r}t)\rangle$ satisfies the kinetic equation[4,5]

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_{\mathbf{p}}\nabla_{\mathbf{r}}-\hat{\mathbf{L}}_{\mathbf{p}}\right)\langle f\rangle=\delta_{\mathbf{p},\mathbf{p}_0}\delta(\mathbf{r})\,\delta(t), \tag{1}$$

where

$$\hat{\mathbf{L}}_{\mathbf{p}}(\langle f\rangle)=\sum_{\mathbf{p}',\mathbf{p}''}\left(u_{\mathbf{p}'\to\mathbf{p},\mathbf{p}''}\langle f(\mathbf{p}_0|\mathbf{p}'\mathbf{r}t)\rangle-w_{\mathbf{p}\to\mathbf{p}',\mathbf{p}''}\langle f(\mathbf{p}_0|\mathbf{p}\mathbf{r}t)\rangle\right). \tag{2}$$

Here $w_{\mathbf{p}\to\mathbf{k},\mathbf{q}}$ is the probability (per unit time) that a moving atom with momentum $\mathbf{p}$ will be scattered by an immobile one, acquiring thereby a momentum $\mathbf{k}$, and that a new moving atom with momentum $\mathbf{q}$ will be produced;

$$u_{\mathbf{p}\to\mathbf{k},\mathbf{q}}=w_{\mathbf{p}\to\mathbf{k},\mathbf{q}}+w_{\mathbf{p}\to\mathbf{q},\mathbf{k}}. \tag{3}$$

We put

$$G(\mathbf{p}_0|\mathbf{p}_1\mathbf{r}_1\mathbf{p}_2\mathbf{r}_2t)=\langle f(\mathbf{p}_0|\mathbf{p}_1\mathbf{r}_1t)f(\mathbf{p}_0|\mathbf{p}_2\mathbf{r}_2t)\rangle,$$
$$\tilde{G}=G-\delta_{\mathbf{p}_1,\mathbf{p}_2}\delta(\mathbf{r}_1-\mathbf{r}_2)\langle f(\mathbf{p}_0|\mathbf{p}_1\mathbf{r}_1t)\rangle. \tag{4}$$

The equation for the diagonal part of the correlator $\tilde{G}$, an equation specially introduced in Ref. 6 for a linear cascade process by comparing the balance control equations, is

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_{\mathbf{p}_1}\nabla_{\mathbf{r}_1}+\mathbf{v}_{\mathbf{p}_2}\nabla_{\mathbf{r}_2}-\hat{\mathbf{L}}_{\mathbf{p}_1}-\hat{\mathbf{L}}_{\mathbf{p}_2}\right)\tilde{G}$$
$$=\delta(\mathbf{r}_1-\mathbf{r}_2)\sum_{\mathbf{k}}u_{\mathbf{k}\to\mathbf{p}_1,\mathbf{p}_2}\langle f(\mathbf{p}_0|\mathbf{k}\mathbf{r}_1t)\rangle. \tag{5}$$

Note that Eq. (5) can be obtained, by linearization over a small number of moving particles, from a more general equation for the correlator of the distribution function of a gas with paired interatomic collisions.[7]

We know[1,8,9] that the Green's function $\langle f\rangle$ of the kinetic equation satisfies, besides Eq. (1), also the equivalent "inverse" (adjoint) equation

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_{\mathbf{p}_0}\nabla_{\mathbf{r}}-\hat{\mathbf{L}}^{+}\right)\langle f\rangle=\delta_{\mathbf{p},\mathbf{p}_0}\delta(\mathbf{r})\,\delta(t), \tag{6}$$

where

$$\hat{\mathbf{L}}^{+}(\langle f\rangle)=\sum_{\mathbf{p}',\mathbf{p}''}\left(u_{\mathbf{p}_0\to\mathbf{p}',\mathbf{p}''}\langle f(\mathbf{p}'|\mathbf{p}\mathbf{r}t)\rangle-w_{\mathbf{p}_0\to\mathbf{p}',\mathbf{p}''}\langle f(\mathbf{p}_0|\mathbf{p}\mathbf{r}t)\rangle\right). \tag{7}$$

Using this fact, and recognizing also that the general solution of (5) is a convolution of three single-particle Green's functions, we can likewise rewrite (5) in an equivalent "inverse" form[6]

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_{\mathbf{p}_0}(\nabla_{\mathbf{r}_1}+\nabla_{\mathbf{r}_2})-\hat{\mathbf{L}}^{+}\right)G=\hat{\mathbf{Q}}(\langle f\rangle), \tag{8}$$

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where

$$\hat{\mathbf{Q}}(\langle f\rangle)=\sum_{\mathbf{k},\mathbf{k}'} u_{\mathbf{p}_0\to\mathbf{k},\mathbf{k}'}\langle f(\mathbf{k}|\mathbf{p}_1\mathbf{r}_1 t)\rangle\langle f(\mathbf{k}'|\mathbf{p}_2\mathbf{r}_2 t)\rangle \tag{9}$$

[we have changed in (8) from the diagonal part $\tilde{G}$ to the total correlator G]. The action of $\hat{\mathbf{L}}^+$ on G is defined in analogy with (7).

The "inverse" collision integral $\hat{\mathbf{L}}^+$ is not a collision integral in the usual sense, i.e., the divergence of the flux in momentum space. The operator $\hat{\mathbf{L}}^+$ therefore does not vanish upon summation with the additive collision invariants 1, $\mathbf{p}$ and ε_p. This circumstance makes it possible to obtain from (6) and (8) equations for the hydrodynamic quantities (particle-number density, energy, momentum) and their correlators in closed form, something impossible by using Eqs. (1) and (5), since upon summation over $\mathbf{p}$ with appropriate weight these equations reduce to unclosed conservation laws.[1)]

PAIR CORRELATION FUNCTION

To solve the athermal-annealing problem we must know the density correlator for times when the cascade proper has already terminated, i.e., no more atoms are knocked out. This value can be taken to mean as the limit, as $t\to\infty$, of the corresponding nonstationary correlator. When taking the limit with respect to t, however, we encounter a problem which we illustrate using as the example the correlator of the knocked-out atoms

$$\bar{N}_{ii}(\mathbf{p}_0|\mathbf{r}_1\mathbf{r}_2)=\lim_{t\to\infty}\sum_{\mathbf{p}_1,\mathbf{p}_2} G(\mathbf{p}_0|\mathbf{p}_1\mathbf{r}_1\mathbf{p}_2\mathbf{r}_2 t). \tag{10}$$

Summation over $\mathbf{p}_1$ and $\mathbf{p}_2$ produces in the right-hand side of Eq. (8) for G—in the source $\hat{\mathbf{Q}}$—a product of the mean values $\langle n_i\rangle$:

$$\langle n_i\rangle=\sum_{\mathbf{p}}\langle f(\mathbf{p}_0|\mathbf{p}rt)\rangle. \tag{11}$$

The summation in (11) should be carried out from values $\varepsilon_{\mathbf{p}}=\varepsilon_d$. Introduction of a threshold energy in the equations, however, would greatly complicate the problem and prevent derivation of the self-similar solutions which we intend to find. On the other hand, if we let $\varepsilon_d\to 0$, then $\langle n_i\rangle$ will have no finite limit as $t\to\infty$, for in the absence of a threshold the number of knocked-out atoms would increase without limit. In the classical problem with a total cross section that diverges at small momentum transfers this unpleasant situation sets in even earlier: the value of $\langle n_i\rangle$ at $\varepsilon_d=0$ turns out to be indeterminate at any instant $t>0$, since the sum in (11) diverges for small $\mathbf{p}$ [this can be verified by summing Eq. (1) over $\mathbf{p}$]. It is readily seen that a similar problem arises also in the calculation of the cross correlators of the interstice and vacancy densities.

To get around the foregoing difficulty, it is necessary to consider, in lieu of the density, a quantity, firstly, having a finite limit as $t\to\infty$ and at $\varepsilon_d=0$, and secondly, representing correctly the spatial distribution of the defects. Such a quantity is the energy density

$$\langle E(\mathbf{p}_0|\mathbf{r}t)\rangle=\sum_{\mathbf{p}}\varepsilon_{\mathbf{p}}\langle f(\mathbf{p}_0|\mathbf{p}rt)\rangle. \tag{12}$$

That $\langle E\rangle$ has the necessary properties is attested to by the following considerations. As a rule the atom mean free path $l(\varepsilon)$ decreases with decrease of ε. Therefore the energy concentrated in a volume dV at an instant t such that $\varepsilon\ll\varepsilon_0$, and hence $l(\varepsilon)\ll l(\varepsilon_0)$, will not "spread" out of dV, but will be consumed in knocking out atoms inside dV. On the basis of these considerations it is proposed in Ref. 1 that there exists a finite limit

$$\langle\bar{E}(\mathbf{p}_0|\mathbf{r})\rangle=\lim_{t\to\infty}\langle E(\mathbf{p}_0|\mathbf{r}t)\rangle \tag{13}$$

and the limiting value of the vacancy density as $t\to\infty$ is

$$\langle\bar{n}_v(\mathbf{p}_0|\mathbf{r})\rangle=c_0\langle\bar{E}(\mathbf{p}_0|\mathbf{r})\rangle/\varepsilon_d, \tag{14}$$

where $c_0=\text{const}\sim 1$ is chosen such as to ensure the correct known value of the total number N_0 of the vacancies:

$$N_0=\int d^3r\langle\bar{n}_v\rangle=c_0\frac{\varepsilon_0}{\varepsilon_d}. \tag{15}$$

It follows from the same considerations that the knocked-out atom cannot move away far from the vacancy it leaves behind. It can therefore be assumed that

$$\langle\bar{n}_i(\mathbf{p}_0|\mathbf{r})\rangle=\langle\bar{n}_v(\mathbf{p}_0|\mathbf{r})\rangle, \tag{16}$$

where $\langle\bar{n}_i\rangle$ is the limiting value of the interstice density. The assumptions (13) and (14) can be proved by using the asymptotic forms obtained in Ref. 5 for the Green's functions of the kinetic equation (see the Appendix).

Relation (16) means that we neglect the existence of depleted and enriched bands, i.e., regions with predominant content of vacancies at the center and of interstices on the periphery of the cascade, respectively.[10] Disregarding the crowdion mechanism that forms these bands[10] (i.e., exit of interstices to the periphery along chains of the substituting collisions), which we are not in a position to take correctly into account within the framework of the isotropic-medium model, we note that spatial separation of vacancies and interstices takes place also for a cascade in an isotropic medium.[11] It follows from the results of Ref. 11, however, that the degree of this separation decreases as ε_0 is increased, i.e., as the number of atoms present in the cascade increases. We can therefore regard (16) as the limiting high-energy case.

We define $K_{iv}(r)$ so that $4\pi r^2K_{iv}(r)$ is the number of interstices with pair-component separation in the interval $(r, r+dr)$. Assuming next that (14) and (16) are valid for both the averaged and exact (fluctuating) quantities, we have

$$K_{iv}(r)=\int\frac{d\Omega_{\mathbf{r}}}{4\pi}\int d^3r'\langle\bar{n}_i(\mathbf{p}_0|\mathbf{r}')\bar{n}_v(\mathbf{p}_0|\mathbf{r}'+\mathbf{r})\rangle=\frac{c_0^2}{\varepsilon_d^2}\mathscr{E}(\varepsilon_{\mathbf{p}_0}|r), \tag{17}$$

where

$$\mathscr{E}(\varepsilon_{\mathbf{p}_0}|r)=\lim_{t\to\infty}\int\frac{d\Omega_{\mathbf{r}}}{4\pi}\int d^3r'\sum_{\mathbf{p},\mathbf{p}'}\varepsilon_{\mathbf{p}}\varepsilon_{\mathbf{p}'}G(\mathbf{p}_0|\mathbf{p}\mathbf{r}\mathbf{p}'\mathbf{r}'+\mathbf{r}t), \tag{18}$$

and $\boldsymbol{\Omega}_{\mathbf{r}}\equiv\mathbf{r}/r$. Note that the threshold energy ε_d enters in (17) only in the form of a scale factor that is not contained in $\mathscr{E}$.

The problem has thus been reduced to finding the radial correlation function of the energy density $\mathscr{E}(\varepsilon_{p_0}|r)$ at $\varepsilon_d=0$. The determination of its asymptote for $r\ll l(\varepsilon_0)$ in

the three-dimensional case does not differ in principle from the one-dimensional case.[2]

Carrying out in Eq. (8) for G all the transformations indicated in (18), we obtain an equation for $\mathscr{E}$:

$$\sum_{\mathbf{p}',\mathbf{p}''} w_{\mathbf{p}_0\to\mathbf{p}',\mathbf{p}''}[\mathscr{E}(\varepsilon_{\mathbf{p}'}|r)+\mathscr{E}(\varepsilon_{\mathbf{p}''}|r)-\mathscr{E}(\varepsilon_{\mathbf{p}_0}|r)]$$
$$+\int\frac{d\Omega_{\mathbf{r}}}{4\pi}\int d^3r'\sum_{\mathbf{k}',\mathbf{k}''}u_{\mathbf{p}_0\to\mathbf{k}',\mathbf{k}''}\langle\bar{E}(\mathbf{k}'|\mathbf{r}')\rangle\langle\bar{E}(\mathbf{k}''|\mathbf{r}'+\mathbf{r})\rangle=0. \tag{19}$$

We turn now to the case of a power-law interaction potential $V(r)\propto r^{-n}$, $n>1$. The differential (with respect to the energy transfer ω) scattering cross section takes then the form[12]

$$\frac{d\sigma(\varepsilon,\omega)}{d\omega}=\frac{C}{\varepsilon^{1+2m}}\Phi_m\left(\frac{\omega}{\varepsilon}\right),$$
$$m=\frac{1}{n},\quad 0<m<1,\quad C=\text{const}, \tag{20}$$

where $\Phi_m(x)$ is a function with known asymptotes.[12,5] The energy path $l(\varepsilon)$ takes for the cross section (20) the form

$$l(\varepsilon)=\varepsilon^{2m}/NC, \tag{21}$$

where N is the number of atoms of the medium per cm^3.

We seek $\mathscr{E}(\varepsilon_p|r)$ in the self-similar form

$$\mathscr{E}(\varepsilon_p|r)=\frac{\varepsilon^2}{l^3(\varepsilon)}g(\zeta),\quad \zeta=\frac{r}{l(\varepsilon)},\quad \varepsilon\equiv\varepsilon_p, \tag{22}$$

where, by virtue of the energy conservation law,

$$4\pi\int_0^\infty d\zeta\,\zeta^2 g(\zeta)=1. \tag{23}$$

We expand the mean value $\langle\bar{E}(\mathbf{p}|\mathbf{r})$ in a Fourier integral:

$$\langle\bar{E}(\mathbf{p}|\mathbf{r})\rangle=(2\pi)^{-3}\int d^3k\,e^{i\mathbf{kr}}\langle\bar{E}(\mathbf{p})\rangle_{\mathbf{k}}. \tag{24}$$

We express the Fourier transform $\langle\bar{E}(\mathbf{p})\rangle_{\mathbf{k}}$ likewise in the self-similar form:

$$\langle\bar{E}(\mathbf{p})\rangle_{\mathbf{k}}=\varepsilon h(kl(\varepsilon),\,\Omega_{\mathbf{p}}\Omega_{\mathbf{k}}) \tag{25}$$

where, by virtue of the energy-conservation law,

$$h|_{k=0}=1. \tag{26}$$

The dependence of $\langle\bar{E}(\mathbf{p}|\mathbf{r})\rangle$ on $\mathbf{r}$ in the three-dimensional case, in contrast to the one-dimensional, is not known even asymptotically. To find a close asymptote for the correlator, however, the properties (26) alone are sufficient. The reason is that both the correlator of $\mathscr{E}$ and $\langle\bar{E}\rangle$ contain the same inhomogeneity scale $l(\varepsilon)$, so that when r is much less than the inhomogeneity scale the actual form of $\langle\bar{E}\rangle$ is of no importance.

Using (22), (24), and (20) we obtain an equation for the self-similar function $g(\zeta)$:

$$\int_0^1 dx\,\Phi_m(x)[x^{2-6m}g(\zeta x^{-2m})+(1-x)^{2-6m}g(\zeta(1-x)^{-2m})$$
$$-g(\zeta)]+P(\zeta)=0, \tag{27}$$

where $P(\zeta)$ is the self-similar representation of the source $\hat{\mathbf{Q}}$ in (8):

$$P(\zeta)=(2\pi)^{-4}\zeta^{-1}\int_0^\infty dk\sin(k\zeta)R(k), \tag{28}$$

$$R(k)=k\int_0^1 dx\,x(1-x)[\Phi_m(x)+\Phi_m(1-x)]$$
$$\times\int_0^{2\pi}d\varphi'\int_0^{2\pi}d\varphi\int_{-1}^{+1}d(\cos\theta)\,h(kx^{2m},\Omega'\Omega_{\mathbf{k}})\,h(k(1-x)^{2m},\Omega''\Omega_{-\mathbf{k}}), \tag{29}$$

where

$$\Omega'\Omega_{\mathbf{k}}\equiv\cos(\widehat{\mathbf{p}',\mathbf{k}}),\qquad \Omega''\Omega_{-\mathbf{k}}\equiv\cos(\widehat{\mathbf{p}'',-\mathbf{k}}),$$

$\mathbf{p}'$ and $\mathbf{p}''$ are the momenta of the scattered and knocked-out particles, respectively, where $\mathbf{p}_0=\mathbf{p}'+\mathbf{p}''$ and $\mathbf{p}'\mathbf{p}''=0$; (θ,φ), (θ',φ'), and (θ'',φ'') are the angular coordinates of the vectors $\mathbf{k}$, $\mathbf{p}'$, and $\mathbf{p}''$, respectively, with $\varphi''-\varphi'=\pi$.

Proceeding as in Ref. 2, we apply to (27) the Mellin transformation. For the Mellin transform of $g(\zeta)$:

$$\tilde{g}(s)=\int_0^\infty\frac{d\zeta}{\zeta}\zeta^s g(\zeta), \tag{30}$$

we obtain

$$\tilde{g}(s)=-\tilde{P}(s)/T(s), \tag{31}$$

where $\tilde{P}(s)$ is the Mellin transform of $P(\zeta)$, and

$$T(s)=\int_0^1 dx\,\Phi_m(x)[x^{2-6m+2ms}+(1-x)^{2-6m+2ms}-1]. \tag{32}$$

The poles of $\tilde{g}(s)$ coincide with the poles of $\tilde{P}(s)$ and with the zeroes of $T(s)$. A zero of $T(s)$ is located at the point $s_1=-1/2m+3$ (it is easy to verify that this zero is of first order). It follows from (26), (28), and (29) that $P(\zeta)\to\text{const}$ as $\zeta\to 0$. Therefore $\tilde{P}(s)$ has a first-order pole at the zero $s_2=0$. For $m>1/6$ the asymptote of $g(\zeta)$ at $\zeta\ll 1$ is determined by the residue of the function $\zeta^{-s}\tilde{g}(s)$ at the pole s_1. For $m=1/6$ the points s_1 and s_2 coalesce into one second-order pole with residue $\ln(1/\zeta)$. If $m<1/6$, the pole s_2 predominates. Thus, for $\zeta\ll 1$,

$$g(\zeta)=\begin{cases} c_1\zeta^{-(3-1/2m)}, & m>1/6, \quad (33a)\\ c_2\ln(1/\zeta), & m=1/6, \quad (33b)\\ c_3, & m<1/6, \quad (33c)\end{cases}$$

where $c_{1,2,3}=\text{const}\sim 1$, the determination of which calls already for knowledge of the actual form of $\langle\bar{E}(\mathbf{p}|\mathbf{r})\rangle$.

It is seen from (33a) that at $m>1/6$ the function $K_{iv}(r)$ increases as r decreases. In our approximation, the interstice–interstice and vacancy–vacancy correlators behave similarly. This indicates that the defects tend to cluster at short distance from one another, i.e., form nonoverlapping subcascades. At $m<1/6$ the atoms are uniformly distributed over the volume of the cascade. Relation (33) confirms thus the subcascade-formation criterion previously obtained from the treatment of the cascade as a sequence of succeeding generations of knocked-out atoms.[13] At the same time,

the criterion proposed in Ref. 14, according to which the critical exponent for subcascade formation is $m = 1/3$, is not confirmed, since the value $m = 1/3$ is not critical in Eq. (33).

CASCADE EFFICIENCY

We consider the simplest athermic-annealing model,[15] according to which a vacancy and an interstice recombine with unity probabilty under the influence of elastic attraction forces if the distance between them is less than the size R of the spontaneous-annihilation zone. The duration of the recombination act is of the order of the atom oscillation period (10^{-13}–10^{-12} s), while the time of cascade evolution is usually much shorter, $\sim 10^{-14}$ s (Ref. 16). It can therefore be assumed that all the defects in the cascade are generated instantaneously and enter the recombination stage simultaneously. The recombination during the time of the cascade can be neglected, inasmuch as for $\varepsilon \gg \varepsilon_d$ the probability of capture of a moving atom by vacancy is low. The temperature is assumed to be so low that the defects do not diffuse.

Let $q(r)dr$ be the probability of finding the nearest accessible vacancy at a distance $(r, r+dr)$ from a given interstice. By "nearest accessible" is meant that at distances $0 < r' < r$ from the given interstice there are no other vacancies, and at a distance $0 < r' < r$ from the chosen vacancy there are no other interstices.[2)] The quantity $q(r)$ is used in the theory of tunneling electron–hole recombination in disordered semiconductors,[17–19] from which we borrowed its definition. The number of annihilated interstices (vacancies) is

$$N^* = N_0 \int_0^R dr\, q(r), \tag{34}$$

and the cascade efficiency is

$$\xi_{eff} = \frac{N_0 - N^*}{N_0} = \int_R^\infty dr\, q(r). \tag{35}$$

Strictly speaking, $q(r)$ can be calculated only if one knows at least the four-particle correlator for two interstices and two vacancies. It can, however, be stated that when the number of vacancies landing in the instability zone of a given interstice is small, viz.,

$$N_R = \int_0^R dr \bar{K}_{iv}(r) \ll 1, \tag{36}$$

where

$$\bar{K}_{iv}(r) = 4\pi r^2 K_{iv}(r)/N_0, \tag{37}$$

we have

$$q(r) = \bar{K}_{iv}(r), \tag{38}$$

i.e., any vacancy landing in the instability zone of the given interstice is automatically also the nearest accessible one. We obtain then for ξ_{eff}

$$\xi_{eff} = 1 - N_R$$

$$= \begin{cases} 1 - c_1' \dfrac{\varepsilon_0}{\varepsilon_d} \left[\dfrac{R}{l(\varepsilon_0)} \right]^{1/2m}, & m > 1/6, \quad (39a) \\ 1 - c_2' \dfrac{\varepsilon_0}{\varepsilon_d} \left[\dfrac{R}{l(\varepsilon_0)} \right]^3 \left[3 \ln \dfrac{l(\varepsilon_0)}{R} + 1 \right], & m = 1/6, \quad (39b) \\ 1 - c_3' \dfrac{\varepsilon_0}{\varepsilon_d} \left[\dfrac{R}{l(\varepsilon_0)} \right]^3, & m < 1/6, \quad (39c) \end{cases}$$

$$c_{1,2,3} = \text{const} \sim 1.$$

Expression (39) can be generalized for N_R values that are not small compared with unity, by calculating $q(r)$ by the following equation proposed in Ref. 17:

$$q(r) = \bar{K}_{iv}(r) \left[1 - \int_0^r dr' q(r') \right]^2. \tag{40}$$

The right-hand side in (40) is a product of two probabilities: that of encountering some vacancy at a distance $(r, r+dr)$ from a given interstice, and the probability that this vacancy is the nearest accessible in accordance with the definition above. From (35) and (40) we get

$$\xi_{eff} = (1 + N_R)^{-1}, \tag{41}$$

which agrees with (39) for $N_R \ll 1$ [we have neglected in (41) small terms of type N_0^{-1}, which are small compared with unity]. Although (40) is not rigorous (the probabilities in it are not independent[18,19]), it agrees splendidly in the case of a uniform particle distribution with the results of computer simulation, all the way to $N_R \approx 1$, and remains of the correct order of magnitude for $N_R \gtrsim 1$ (Ref. 18).

Let us compare our results with the expression for ξ_{eff} obtained in Ref. 15 for uniform distribution of the effects over the cascade volume:

$$\xi_{eff} = \exp(-4/3 \pi \tilde{n} R^3), \tag{42}$$

where $\tilde{n}$ is the defect density averaged over the cascade volume. For $\tilde{n}R^3 \ll 1$, Eq. (42) is of the same order as (39c). For larger $\tilde{n}R^3$, on the other hand, expression (42) predicts an exponential decrease of ξ_{eff} with increase of R, while (41) predicts a power-law decrease. The cause of this difference is that (42) is derived by assuming the fact that the given interstice can recombine with a vacancy "occupied" by an even closer interstice, i.e., (42) describes the recombination of all the neighbors, not only the nearest accessible ones. This assumption corresponds to replacing the exponent of the expression in square brackets in (40) by unity,[18] and it is this which leads to the exponential result (42). Clearly, this approach decreases ξ_{eff} substantially.

Two conclusions follow from (39) and (41). First, for a non-uniform defect distribution in the cascade volume ($m > 1/6$) the athermal annealing is more intensive than for a uniform distribution ($m < 1/6$), a manifestation of the "cumulative" singularity of the correlator. Second, ξ_{eff} is independent of energy if $m > 1/6$, since $l(\varepsilon_0) \propto \varepsilon_0^{2m}$. The effective value of m depends on ε_0 and on the atomic number Z of the colliding particles (in the case of equal masses), with m increasing as ε_0 increases and as Z decreases.[1,20] Following the known[20] method of estimating m, we can verify that the case $m < 1/6$ can be realized only in heavy targets with $Z \gtrsim 70$; in lighter ones, however, it is preferable to use $m > 1/$

6 for practically all values of ε_0. Starting from the foregoing, the independence of ξ_{eff} of ε_0 explains qualitatively the results of some actual computer experiments.

When Cu and Ag are bombarded by ions[21] and Mo by neutrons (see Ref. 22 and the citations therein), the efficiency saturates, as manifested by an initial decrease ξ_{eff} from values close to unity when ε_0 increases, followed by a tendency to a constant value for larger ε_0. In Refs. 21 and 22 is discussed only the initial ξ_{eff} decrease, which is ascribed to the recombination-stimulating action of the thermal peak. This action, however, is effective only at high energy per atom in the region captured by the cascade, corresponding $\varepsilon_0 \lesssim 10$ keV (Ref. 23). The constancy of ξ_{eff} at $\varepsilon_0 > 10$ keV can therefore be attributed to the above singularity of the athermal annealing.

Let us mention also the results of a computer simulation of the cascade and athermal stages in α-Fe and Cu (Ref. 24), which show that the fractions ξ_{dv} and ξ_{di} of vacancies and interstices coalescing into divacancies and di-interstices remain practically constant as ε_0 ranges over the entire interval in question, from 0.5 to 20 keV. By divacancy (di-interstice) is meant in Ref. 24 two vacancies (interstices) separated by a distance shorter than the lattice constant. An estimate for ξ_{dv} and ξ_{di} can be obtained in our approximation by proceeding just as in the calculation of ξ_{eff}, and therefore, just as ξ_{eff}, the values of ξ_{dv} and ξ_{di} are independent of ε_0 for $m > 1/6$.

Equation (41) leads to

$$\ln \eta \equiv \ln (\xi^{-1}-1) = \alpha \ln R + \text{const}, \tag{43}$$

where $\alpha = (2m)^{-1}$ for $m > 1/6$ and $\alpha = 3$ for $m < 1/6$. Equation (43) with $\alpha \approx 2/3$ describes satisfactorily the $\xi_{\text{eff}}(R)$ dependence deduced from the computer simulation of cascades in Cu for $\varepsilon_0 \lesssim 8$ keV and $U(r)$ in the form of the Moliere approximation of the Thomas–Fermi–Firsov potential.[3] This attests to a non-uniform distribution of the defects in the cascade, with an effective value $m^* \approx 3/4$. As expected, the dependence of ξ_{eff} on ε_0 in Ref. 25 is quite weak.

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APPENDIX

Let us prove relations (13) and (14). It is shown in Ref. 5 that over long times, when the number of atoms participating in the cascade is large, the solution of Eq. (1) takes the following asymptotic form:

$$\rho(\varepsilon)\langle f(\mathbf{p}_0|\mathbf{p}\mathbf{r}t)\rangle = \varphi(\xi)\left\{\frac{\langle E(\mathbf{p}_0|\mathbf{r}t)\rangle}{\varepsilon^2} + 3\frac{\langle \mathbf{P}(\mathbf{p}_0|\mathbf{r}t)\rangle \mathbf{p}}{\varepsilon[\mathbf{p}(\varepsilon)]^2}\right\}. \tag{A1}$$

Here $\rho(\varepsilon)$ is the density of states per cm^3, $\varphi(\xi)$ is a self-similar function,

$$\xi = (t_0 \mp t)/\tau(\varepsilon) \quad (m \gtrless 1/4), \quad \tau(\varepsilon) = l(\varepsilon)/v(\varepsilon),$$

$$t_0 \sim \tau(\varepsilon_0), \quad v(\varepsilon) = (2\varepsilon/M)^{1/2},$$

M is the particle mass, $p(\varepsilon) = Mv(\varepsilon)$, and $\langle \mathbf{P} \rangle$ is the momentum density. The quantities $\langle E \rangle$ and $\langle \mathbf{P} \rangle$ satisfy the system of quasihydrodynamic equations[5]

$$\frac{\partial \langle E \rangle}{\partial t} + s^2(t)\,\mathrm{div}\langle \mathbf{P} \rangle = 0, \tag{A2}$$

$$\frac{\partial \langle \mathbf{P} \rangle}{\partial t} + \frac{1}{3}\nabla \langle E \rangle = 0 \tag{A3}$$

where $s(t)$ has the meaning of speed of sound in the cascade:

$$s^2(t) \propto \begin{cases} (t_0-t)^a, & m > 1/4, \\ t^{-a}, & m < 1/4, \end{cases} \qquad a = |2m-1/2|^{-1}. \tag{A4}$$

Let us consider the case $m < 1/4$. Assuming that as $t \to \infty$ the derivative $\partial \langle E \rangle / dt \to 0$, it follows from (A3) that $\langle \mathbf{P} \rangle \propto t$. We get then from (A2)

$$\partial \langle E \rangle / dt \propto s^2(t)\, t \to 0, \qquad t \to \infty$$

and our assumption is justified. The case $m > 1/4$ is similarly considered. Thus,

$$\frac{\partial \langle E \rangle}{\partial t} \propto \begin{cases} (t_0-t)^b, & t \to t_0, \quad m > 1/4, \\ t^{-b}, & t \to \infty, \quad m < 1/4, \end{cases} \tag{A5}$$

where $b = (2m + 1/2)a$. This proves (13). [For $m > 1/4$ the cascade evolves within a finite time t_0 which replaces in this case the ∞ in Eq. (13)].

To prove (14) we define a quantity $F(\mathbf{p}_0|\varepsilon\mathbf{r})$ such that d^3rF is the average number of atoms knocked out of a volume element d^3r near r, with energies in the interval $(\varepsilon, \varepsilon + d\varepsilon)$, during the entire lifetime of the cascade (F is called "recoil density" in Ref. 1):

$$F(\mathbf{p}_0|\varepsilon\mathbf{r}) = \lim_{t \to t_0, \infty} \sum_{\Omega_{\mathbf{p}}} \int_0^t dt' \sum_{\mathbf{p}', \mathbf{p}''} w_{\mathbf{p}' \to \mathbf{p}'', \mathbf{p}} \langle f(\mathbf{p}_0|\mathbf{p}'\mathbf{r}'t') \rangle, \tag{A6}$$

and $m \gtrless 1/4$. Then

$$\langle \bar{n}_v(\mathbf{p}_0|\mathbf{r}) \rangle = \int d\varepsilon F(\mathbf{p}_0|\varepsilon\mathbf{r}). \tag{A7}$$

Substituting (A1) and (20) in (A6) and recognizing that $\langle E \rangle$ varies slowly with time compared with $\varphi(\xi)$ (Ref. 5) and can be taken outside the integral, we get

$$F(\mathbf{p}_0|\varepsilon\mathbf{r}) = \langle \bar{E}(\mathbf{p}_0|\mathbf{r}) \rangle \int_0^{t_0, \infty} dt' \int_{\varepsilon}^{\varepsilon_0} \frac{d\varepsilon'}{\varepsilon'^3} \frac{\varphi(\xi')}{\tau(\varepsilon')} \Phi_m\left(\frac{\varepsilon}{\varepsilon'}\right), \quad m \gtrless 1/4, \tag{A8}$$

where $\xi' = (t_0 \mp t)/\tau(\varepsilon')$. Interchanging the integration with respect to t' and ε' for $\varepsilon \ll \varepsilon_0$ we get

$$F(\mathbf{p}_0|\varepsilon\mathbf{r}) = \frac{\langle \bar{E}(\mathbf{p}_0|\mathbf{r}) \rangle}{\varepsilon^2} \int_0^{\infty} d\xi' \varphi(\xi'), \tag{A9}$$

where it is taken into account that[5]

$$\int_0^1 dx x \Phi_m(x) = 1. \tag{A10}$$

From (A9) and (A7) we obtain relation (14) with c_0 evaluated:

$$c_0 = \int_0^{\infty} d\xi' \varphi(\xi'). \tag{A11}$$

[The constant c_0 in (A11) differs from that used in Ref. 1

since, in contrast to Ref. 1, we did not replace $\Phi_m(x)$ by its small-angle asymptote.]

[1)]Note that $\hat{L}^+$ acts only on the initial momentum; the running momenta enter in (7) only via the conservation laws.
[2)]The definition of $q(r)$ is, of course, symmetric with respect to interstice–vacancy permutation.

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