Kinetics of dislocation ensembles in deformable irradiated materials

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The development of plastic instability in the initial deformation stages of irradiated materials is studied. The dependence of the fraction of dislocations which overcome obstacles in the dynamic regime (dislocation "channeling") on the degree of radiation hardening (irradiation dose) and the dislocation velocity is analyzed. It is shown that this effect plays a role in radiation embrittlement of reactor materials.

The investigation of radiation hardening and, as a rule, the associated embrittlement is one of the most practical issues in reactor materials science. Radiation hardening of materials appears not only as an increase in the yield stress and decrease of the rate of hardening of materials but also in the formation of a "creep tooth" and a creep plateau on the strain curves of the Chernov–Lüders type.[1,2] According to modern ideas, the existence of these effects indicates plastic instability in materials, which could be the cause of the sharp decrease in the plasticity.

Figure 1 shows typical strain curves for reactor steels at test temperatures below $0.3T_m$ (T_m — melting temperature). Our analysis[3] showed that strain curves of this type (curve *2*) are observed in many materials even at irradiation doses $\leqslant 10^{-2}-10^{-1}$ dpa (displacement per atom). The minimum or the plateau in the curve *2* is due to plastic instability effects — dislocation channeling: destruction of obstacles by moving dislocations and localization of glide in given volumes of the material followed by deformation.[1] For the subsequent analysis, it is especially important that the material leaves the plastic instability regime mainly as a result of the development of transverse glide of screw dislocations. At higher irradiation doses ($\geqslant 1-10$ dpa, curve *3*) the stage corresponding to the plateau in curve *2* passes directly into the fracture stage of the material.

The modern approach to plastic deformation, as a collective dislocation process, is to describe the localization and self-organization of dislocations based on a study of the evolution of dislocation ensembles in the deformed materials. In Refs. 4 –7 the kinetics of a dislocation ensemble were studied in detail theoretically in a synergetic approach and models making it possible to explain not only the evolution of the local density of dislocations in unirradiated materials but also the formation of defect-free channels and localization of deformation in irradiated materials.

There also exist models[8] that study the appearance of plastic instability and localization of plastic deformation based on a description of the behavior of single dislocations. Other models (see, for example, Ref. 9) proceed from a dislocation ensemble which is characterized by a dislocation distribution function that depends on the radius vector **r** and time t.

However, since the plastic deformation of a material is associated with mobile defects, it is natural to assume that the dislocation distribution function depends not only on the radius vector **r** and time t but also on the dislocation velocity **v** and its orientation in space. In the present paper we study the dislocation distribution functions averaged over orientations of dislocation lines in space. The dislocations in an ensemble themselves can be treated as a collection of segments of dislocation lines (see Ref. 10).

In the present work we investigated the development of plastic instability in an irradiated material taking account of the dependences of the velocity distribution function of dislocations in an ensemble.

1. MODEL

The subject of the description are mobile dislocations which interact with fixed obstacles of different nature but are not held back (do not "hang up") on them. For example, they move in a channeling regime.[2] This situation corresponds, for example, to the typical case of the initial stages of deformation of an irradiated material when the dislocation ensembles formed "intersect" obstacles, consisting of small clusters, loops, and micropores. It is obvious that such a situation can occur in the presence of both a wide spectrum of dislocation velocities (energies) and different mechanisms of interaction of dislocations with obstacles.

Two other important points should be noted concerning: a) interdislocation interaction and b) mechanisms by which dislocations leave the regime under study.

a) According to Ref. 11 , the contribution of interdislocation interaction must be estimated by comparing it with the external applied (and acting on a dislocation) stress f_{ext}. In an unirradiated material the interdislocation interaction should be taken into account by "starting from the end of the section of strain hardening" where the dislocation density

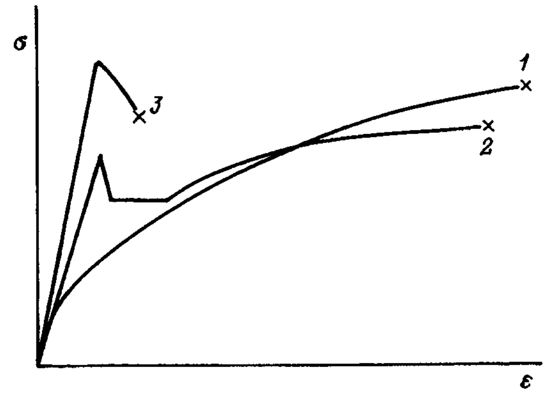

FIG. 1. Typical strain curves (σ — load, ε — deformation) for reactor steels at test temperatures below $0.3T_m$ (T_m — melting temperature). *1* — Initial (unirradiated) material, *2* — material irradiated to "low" doses ($10^{-2}-10^{-1}$ dpa), *3* — material irradiated to doses above 1 dpa.

$\rho(\varepsilon)$ in the material is large, the distances between dislocations ($r \approx \rho^{-1/2}$) are short, and the interdislocation interaction forces are comparable to the external applied stress.

In our case of an irradiated material conditions are realized such that the external stress acting on a dislocation is high (practically the maximum possible stress), provided that the sharp drop in the rate of strain hardening (Fig. 1) is taken into account, while the dislocation density in an ensemble (initial stages of the formation of a localized deformation) is still not so high that condition $f \geqslant f_{\text{ext}}(1/2\pi)Gb^2\rho(\varepsilon)^{1/2}$, where f is the interdislocation interaction force, G is the shear modulus, and b is Burgers vector, would be satisfied. This allows us to neglect the interdislocation interaction in the ensemble for the time being when studying the interaction with fixed obstacles — radiation defects — at the initial stages of deformation.

b) To describe the interaction of a dislocation ensemble with obstacles, we study the most likely case where some dislocations will pass through an obstacle without changing their direction of motion, while other dislocations will be "scattered," changing their direction of motion, as can happen, for example, in the case of screw dislocations. As already noted above, this corresponds to the case of the deformation of an irradiated material, when the system leaves the channeling regime as a result of the motion of screw dislocations and subsequent development of multiple glide.

To characterize the dislocation structure of a crystal quantitatively it is necessary to give the distribution function $n(\mathbf{r},\mathbf{v},t)$ of the dislocations over their coordinates $\mathbf{r}$ and velocities $\mathbf{v}$ and time t so that

$$\rho_{\text{total}} = \sum_i \int d\Omega n(\mathbf{r},\mathbf{v},t) \tag{1}$$

is the total density of all dislocations with arbitrary orientations and moving with velocity $\mathbf{v}$, and $d\Omega$ is an element of solid angle in coordinate space.

In the case that the dislocations interact with certain fixed obstacles, we shall investigate the development of plastic deformation on the basis of a general kinetic equation for $n(\mathbf{r},\mathbf{v},t)$ of the following form:

$$\frac{\partial n}{\partial t} + \mathbf{v}\cdot\frac{\partial n}{\partial \mathbf{r}} + \mathbf{a}\cdot\frac{\partial n}{\partial \mathbf{v}} = \left(\frac{\hat{1}}{\tau}\right) n, \tag{2}$$

where $\mathbf{a}$ is the acceleration of a dislocation under an external load F; $(\hat{1}/\tau)$ is an operator corresponding to the reciprocal of the relaxation time, which we assume to be determined by the expression

$$\left(\frac{\hat{1}}{\tau}\right) n = \frac{|\mathbf{v}|^m}{A}\left(\frac{1}{4\pi}\int d\Omega_{\mathbf{v}'} n(\mathbf{r},\mathbf{v}',t) - n(\mathbf{r},\mathbf{v},t)\right). \tag{2a}$$

Here $d\Omega_{\mathbf{v}'}$ is an element of solid angle in velocity space. The proposed structure of the operator (2a) of the reciprocal relaxation time signifies that the frequency of collisions with obstacles for a dislocation moving with velocity $\mathbf{v}$ equals $|\mathbf{v}|^m/A$ (we assume below that $m < -1$), where A is a constant which takes account of the presence of stops of different nature and the concentration (we note that, evidently, depending on the parameter m, the dimension of A in different cases will be different). The expression (2a) presupposes, by analogy with classical mechanics, that a dislocation, treated as a quasiparticle, is scattered elastically in the potential field of an obstacle $|\mathbf{r}|^{-k}$ ($k>0$). It is known that in this case the effective differential cross section for elastic scattering (and therefore the collision frequency also) is proportional to $|\mathbf{v}|^m$ with $m=-4/k$ (see Ref. 12). On the other hand, it is also know that moving dislocations can interact with obstacles according to the law $\sim 1/r$, where r is the distance from an obstacle to the dislocation axis,[13] as happens, for example, for an edge dislocation in the case of a Cottrell impurity atmosphere.[14] In this case, $m=-4 < -1$. In what follows we shall develop this model for the general case $m < -1$.

We note that the spatiotemporal distribution function $f(\mathbf{r},t)$ of dislocations can be expressed in terms of $n(\mathbf{r},\mathbf{v},t)$ by means of the formula

$$f(\mathbf{r},t) = \frac{1}{4\pi}\int d\mathbf{v} n(\mathbf{r},\mathbf{v},t).$$

The condition of balance for $f(\mathbf{r},t)$ follows from the kinetic equation (2). In the present model (no interactions between dislocations) it has the form

$$\frac{\partial f(\mathbf{r},t)}{\partial t} + \operatorname{div}\mathbf{j} = 0,$$

where $\mathbf{j} = \frac{1}{4\pi}\int d\mathbf{v}\, \mathbf{v} n(\mathbf{r},\mathbf{v},t)$.

We shall study the spatially uniform case

$$\frac{\partial n(\mathbf{r},\mathbf{v},t)}{\partial \mathbf{r}} = 0. \tag{3}$$

The latter relation means that $\Delta = n_1 - n_2 \ll \alpha d$ (d — average distance between stops, α — coefficient of order 1 with dimension of length), i.e. the distribution function of a dislocation ensemble remains practically unchanged over a distance of the order of the distance between stops. Then the kinetic equation (2) will have the form

$$\frac{\partial n(\mathbf{v},t)}{\partial t}+\mathbf{a}\cdot\frac{\partial n(\mathbf{v},t)}{\partial \mathbf{v}}=\left(\frac{\hat{1}}{\tau}\right)n(\mathbf{v},t). \tag{4}$$

To Eq. (4) we add the initial condition

$$n(\mathbf{v},0;\mathbf{v}_0)=\delta(\mathbf{v}-\mathbf{v}_0), \tag{5}$$

signifying that at time $t=0$ the dislocation velocity is close to $\mathbf{v}_0$.

We now introduce the parameter $\rho^*(\mathbf{v}_0,t;m)=\rho_{\mathrm{act}}/\rho_{\mathrm{total}}$, where ρ_{act} is the density of dislocations which have passed "through" an obstacle. The parameter $\rho^*(\mathbf{v}_0,t;m)$ denotes the relative fraction of dislocations in an ensemble which have passed "through" an obstacle. From the physical meaning of the distribution function $n(\mathbf{v},t;\mathbf{v}_0)$ as the probability density of dislocations moving with velocity $\mathbf{v}_0$, we can establish the integral equation

$$\begin{aligned}n(\mathbf{v},t-t';\mathbf{v}_0)&=\rho^*(\mathbf{v}_0,t;m)\,\delta(\mathbf{a}t+\mathbf{v}_0-\mathbf{v})\\&\quad-\int_0^t dt'\frac{\partial}{\partial t'}\rho^*(\mathbf{v}_0,t';m)\frac{1}{4\pi}\\&\quad\times\int d\Omega_{\mathbf{w}}n(\mathbf{v},t-t';\mathbf{w}|\mathbf{a}t'+\mathbf{v}_0|),\end{aligned} \tag{6}$$

where $\mathbf{w}$ is a unit vector ($|\mathbf{w}|=1$) in an arbitrary direction. In Eq. (6) the first term is the fraction of dislocations which have passed through an obstacle and acquired in time t a velocity $\mathbf{a}t+\mathbf{v}_0$. The second term takes account of the fraction of dislocations whose velocity changed direction as a result of the first collisions with obstacles and acquired an arbitrary direction $\mathbf{w}$. Obviously, these directions are knocked out of the probability density $n(\mathbf{v},t;\mathbf{v}_0)$, as is indicated by the minus sign in front of the second term.

2. DISLOCATION GLIDE

Substituting the integral equation (6) into the kinetic equation (2), we obtain an equation for ρ^*

$$\frac{\partial}{\partial t}\rho^*(\mathbf{v}_0,t;m)+\frac{|\mathbf{a}t+\mathbf{v}_0|^m}{2A}\rho^*(\mathbf{v}_0,t;m)=0. \tag{7}$$

The function ρ^* must satisfy the relations

$$0\leqslant\rho^*(\mathbf{v}_0,t;m)\leqslant 1,\quad \rho^*(\mathbf{v}_0;m)=1.$$

We shall assume that the direction of the initial velocity $\mathbf{v}_0$ is the same as the vector of the applied load σ. The solution of Eq. (7) has the form

$$\rho^*(\mathbf{v}_0,t;m)=\exp\left(\frac{|\mathbf{v}_0|^{m+1}-(|\mathbf{a}|t+|\mathbf{v}_0|)^{m+1}}{2|\mathbf{a}|A(m+1)}\right), \tag{8}$$

with $m\neq-1$. For $m<-1$ the asymptotic representation of the solution (8) is expressed by the formula

$$q=\lim_{t\to\infty}\rho^*(\mathbf{v}_0,t;m+1)=\exp\left(-\frac{|\mathbf{v}_0|^{m+1}}{2|\mathbf{a}|A|m+1|}\right). \tag{9}$$

This is the fraction of dislocations which have the initial velocity and pass through an obstacle. As $|\mathbf{v}_0|\to 0$ this fraction becomes infinitesimal. As $|\mathbf{v}_0|\to\infty$ (or as $|\mathbf{a}|$ increases) this fraction tends to 1, i.e., as their velocity (energy) increases, dislocations start to "slip past" obstacles without stopping.

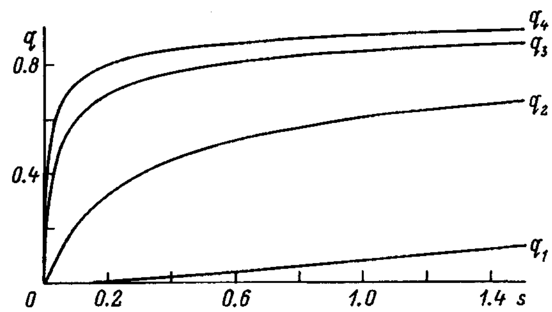

FIG. 2. Fraction of dislocations overcoming obstacles in the dynamic regime versus the initial dislocation velocity. q_1, q_2, q_3, and q_4 correspond to the following values of the density of obstacles: $p_1=10^{-4}\%$, $p_2=10^{-3}\%$, $p_3=10^{-2}\%$, and $p_4=10^{-1}\%$, increasing as a result of irradiation.

The dependence of the fraction of dislocations which overcome an obstacle in the dynamic regime on the dislocation velocity is illustrated qualitatively in Fig. 2.

For this, for example, we set $m=-3/2$, which corresponds to a dislocation–obstacle interaction law $\sim r^{-8/3}$. In order for a dislocation to acquire acceleration $a=|\mathbf{a}|$, according to Newton's second law $a=F/m^*$, a force $F>F_0/l$ (per unit length of the dislocation) must be applied, where F_0 is the maximum dislocation restraining force developed by one defect and l is the distance between defects,[15] $m^*=(db^2/4\pi)\ln(R/r_0)$ is a known expression[16] for the effective mass per unit length of a dislocation, d is the mass density of the metal, b is the magnitude of Burgers vector. Setting $l=n_i^{-1/3}$ and $|\mathbf{v}_0|=us$, where n_i is the number of defects per unit volume (specifically, irradiation produced defects) and u is the velocity of sound, we transform Eq. (9) to a form convenient for plotting

$$\begin{aligned}&q=\exp(-1/Q),\\&Q=2A|m+1|(F_0 4\pi n^{1/3})/(db^2\ln(R/r_0))\\&\qquad\times u^{|m+1|}p^{1/3}s^{|m+1|},\end{aligned}$$

where p is the defect density and n is the density of atoms of the main material. To obtain a clear picture, we choose the following values of the parameters: $F_0=1.6\times10^{-4}$ dynes, $u=3.3\times10^4$ cm/s, $d=8$ g/cm^3, $\ln(R/r_0)=8, n=8\times10^{22}$ cm^{-3}, $b=3\times10^{-8}$ cm, and $A=10^{-16}$ s$^{5/2}\cdot$cm$^{-3/2}$. For these values the function $q(s)$ has the form shown in Fig. 2. The quantity s is plotted along the abscissa. According to our data and the data of other authors,[17] a relative increase in the yield stress of a material by a factor of 4–20 is observed in most model and reactor materials even at doses $10^{-2}-10^{-1}$ dpa. Moreover, one can see that under otherwise equal conditions, the fraction of dislocations in irradiated materials which have overcome obstacles in the dynamic regime now becomes substantial (according to Ref. 8 , the criterion of the dynamic or "pseudorelativistic" regime is that dislocations reach velocities ~ 0.1 of the velocity of the sound).

Figure 2 also shows that the dynamic (pseudorelativistic) deformation regime is reached in irradiated materials at lower dislocation velocities.

As investigations by Popov showed,[8] for dislocation densities $\approx 10^{10}$ cm^{-2} pseudorelativistic effects must be taken into account to describe the evolution of dislocation structures, i.e., the dislocation velocities can approach the sound velocity ($\geqslant 0.1u$). In the case of, for example, irradiated nickel and vessel steel, such a dislocation density corresponds to stresses $\geqslant 100$ MPa, and hence such effects can appear even at the initial stages of deformation, which correspond to the Chernov–Lüders strain interval. As numerous experiments have shown, high dislocation densities are observed in deformation channels formed in irradiated materials even near the yield stress. This results in the appearance of the Chernov–Lüders plastic instability.[1,2]

The model presented in this work, in our opinion, may be directly related to, for example, the problem of the brittleness of irradiated materials in reactor vessels. The latest investigations[18] show that deformation and fracture processes in vessel steels are accompanied by dynamic dislocation channeling and ''destruction'' by dislocations of very small defects in the form of micropores, loops, and precipitates in vessel steels. Localized-deformation channels, encountering interfaces, could be responsible for the sharp stress concentration, proportional to the total dislocation ''charge,'' and give rise to microcracks.

In summary, in the model presented above, the development of plastic instability in an irradiated deformable material was studied taking account of the velocity dependence of the distribution function of dislocations in an ensemble. It was shown that a sharp increase in the fraction of dislocations which overcome obstacles in the dynamic regime can be observed in these materials. As the degree of hardening (concentration of defects arising under irradiation) increases, this effect can be reached at lower deformation velocities.

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