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Chapter

Modeling Plastic Deformation in Irradiated Materials

Nicholas Kamyshanchenko, Vladimir Krasil'nikov,
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Abstract

The classification of physical models of plastic deformation localization phenomena in the temperature range including the low-temperature radiation embrittlement effect is done. The new approach for the dislocation channeling mechanism description considering the collective behavior of dislocations and their interaction with radiation defects is proposed. The dislocation collective behavior model in materials irradiated, for example, by reactor radiation including neutron and accompanying gamma radiation is proposed on the basis of the evolution equation for dislocation density taking into account Burgers type nonlinearity. It is shown that the localized structures such as Danilov-Zuev's relaxation waves can be described. The possibility of localization effects (embrittlement) decreasing by the plastic deformation microlevel switching-on is demonstrated in relation with the thermal activated processes. The model describing dose dependence of uniform elongation of irradiated materials is constructed. This model is in good agreement with the experimental data of low-activated alloy based on chromium under (e, γ)—beam radiation.

Keywords: radiation, gamma-quants, embrittlement, deformation wave

1. Introduction

Since Paul Ulrich Villard's discovery of gamma rays, there are manifold phenomena occurring under the influence of high intensive flows of particles, including gamma radiation, in solid state physics. Gamma radiation is shortwave electromagnetic radiation with wavelength of $\lambda < 1$ nm. If an atomic nucleus is in an excited state, then its transition from the excited state into the normal state causes gamma-quant emission. Also gamma radiation can appear, for example, as a result of decay and annihilation of elementary particles and bremsstrahlung. Gamma radiation can be considered as a gamma-quant (photon) beam that demonstrates characteristic corpuscular properties due to its high energy. For example, gamma-quants with energy of from 10 keV to 10 MeV are produced in nuclear reactors.

Note, intensity and spectrum of gamma radiation uniquely characterize radioisotopes. Since decay of many nuclides, for example, ^{137}Cs, ^{60}Co, ^{22}Na, ^{152}Eu, is accompanied by gamma radiation, then knowledge of gamma radiation spectrum allows to identify composition and a number of radioactive isotopes in materials and also to define the degree of burnout of nuclear fuel in the reactors.

A structure and properties of the substances exposed to radiation experience significant changes called radiation damages. The radiation damages created in solid crystalline bodies destroy the proper crystal structure due to a displacement of atom from the host crystal lattice and formation of radiation defect complexes (point defects, clusters, dislocation loops, pore lattices, and so on). Besides, nuclear reactions can originate under radiation; therefore transmutants (new elements) can arise.

There are basic physical phenomena in the solid bodies under radiation. This is radiation growth and radiation swelling, radiation-stimulated and radiation-induced processes, low-temperature and high-temperature radiation embrittlement, radiation creep, radiation doping and erosion of the surface, and others.

Radiation affects essentially on the operating ability of materials. For instance, the atomic defect excess created by radiation accelerates diffusion processes and produces selection centers of new phases in alloys that are easy getting old. If it accumulates significant amount of decay products, then they can segregate, for example, as gas bubbles.

Many of radiation phenomena appear directly in the conditions of operation of the nuclear reactors. It is considered that energy is directly realized by uranium fission in the reactor in the middle of the order of 195–200 MeV. Most of this energy (about 168 MeV) is realized as kinetic energy of fission fragments. A part of the energy (about 24 MeV) is realized as β-particles, γ-quants, and neutrino. The rest of the energy is carried away by fission neutrons. It is necessary to consider that gamma radiation accompanies a neutron flow at interaction of reactor radiation with radiation protection materials based by metal hydride compounds and affects radiation doze power behind protection.

In wide test temperature region, radiation embrittlement includes conditionally two temperature intervals:

LTRE: low-temperature radiation embrittlement—at the test temperatures up to $0.4 \, T_m$ (T_m is melting temperature).

HTRE: high-temperature radiation embrittlement—at the test temperatures higher than $0.5 \, T_m$.

In the LTRE region, embrittlement can be accompanied by radiation hardening, that is, increasing a yield point of materials. In the HTRE region, embrittlement can be accompanied by hardening relaxation. But there is a common feature of both phenomena; exactly, they are accompanied by the localization effects of plastic flow. In the HTRE, localization evolves mainly along grain borders, and it leads to speeded up formation of wedge-shaped cracks. In the LTRE one, localization goes in a grain body. Upon that, the factor that leads directly to destruction of a deformed irradiated material is formation of localized high density dislocation charges that contain, according to a theory, the beginning of a crack [1].

Manifold complexes of defects and nuclear reaction products are formed in the materials irradiated in reactors by neutrons and γ-quants that are the base of LTRE mechanism models to be constructed. The helium LTRE theory is widely known. Helium is generated by (n,α)- or (γ,α)-reactions in the construction materials under radiation. For instance, helium is formed by the two-stage reaction of the thermal neutron: $Ni^{58} + n \rightarrow Ni^{59} + \gamma$ and $Ni^{59} + n \rightarrow Fe^{56} + \alpha$.

Helium is practically insoluble in metals and at elevated temperatures migrates to grain boundaries and other defects where gas bubbles are formed that essentially influence embrittlement of the materials.

From all that was said before, it follows the mechanisms of plastic flow of irradiated deformed materials are the LTRE mechanisms in fact. It is possible to propose the following classification of plastic flow localization phenomena in irradiated materials:

i. Stationary dissipative structures (dislocation channeling)

ii. Moving fronts of deformation localization (the Chernov-Luders band type)

iii. Macroscopic bands (the Danilov-Zuev relaxation wave type).

In the works [1–3], it was shown these effects were observed in the materials with any crystal lattice type. We consider briefly these phenomena with the synergetic point of view [4].

2. Stationary dissipative structures (dislocation channeling)

Electron microscope investigations of deformed irradiated materials showed that its structure has some features as long channels in order of several parts of micron width, without any radiation defects (see, for instance, [2]). In the work [5], it was proposed a new approach to describing mechanisms of dislocation channel formation on the basis of considering collective processes of interaction between dislocation ensembles and radiation defects. Upon that, it is supposed by the experimental facts that in the irradiated deformed material, ensemble dislocations move with velocities closed to 0.1 of the sound velocity, that is, in dynamic regime. On the basis of the general kinetic approach to evolving the ensemble of dislocations interacting with obstacles, the expression for part of dislocations q overcoming obstacles in dislocation channel regime is obtained:

$$q = \exp\left(-|\mathbf{v}|^{m+1}/(2A|a(m+1)|)\right), \tag{1}$$

where $\mathbf{v}$ is an initial velocity of the dislocations running across obstacles, a is dislocation acceleration, $m < -1$, and constant A is proportional to a radiation hardening power $A \sim \sigma_{irr}/\sigma_{init}$ (σ_{irr} is stress after radiation; σ_{init} is stress before radiation). At $|\mathbf{v}| \to \infty$ (or increasing a), this fraction goes to unity, that is, at the high velocities (energies), the dislocations bypass obstacles without stopping. Thus, in irradiated deformed materials, the effect of sharp increasing the part of dislocations overcoming obstacles in a dynamic regime can be observed. Upon that this effect can be gotten in lower deformation velocities in increasing a hardening power (concentration of the defects arising from radiation).

3. Moving fronts of deformation localization (the Chernov-Luders band type)

Recently, the synergetic approach is employed more and more to describe the evolution of plastic deformation in materials. As known, the balance equation for a local dislocation density $\rho(x,t)$ underlies the synergetic models. In the work [6], one of these is considered. There, the balance equation was written as

$$\frac{\partial \rho(\mathbf{x},t)}{\partial t} + div(\mathbf{v}\rho(\mathbf{x},t) - D\nabla\rho(\mathbf{x},t)) = J(\rho(\mathbf{x},t)) \tag{2}$$

where $\mathbf{v}$ is velocity vector of dislocation sliding, D is dislocation diffusion coefficient, and $J(\rho(\mathbf{x},t))$ is the dislocation density functional determined by interaction of dislocation with each other. The velocity of sliding dislocations $\mathbf{v}$ can be represented from three parts: $\mathbf{v} = \mathbf{v}_{ext} + m(f_{int} + f_{cor})$, where $\mathbf{v}_{ext}$ is velocity from

external stress, m is dislocation mobility, and f_{int} origins from internal stress— $f_{int} = b\sigma_{int}$ supposing internal stress $\sigma = \alpha b G \sqrt{\rho}$, where b is Burgers vector quantity, α is a numerical coefficient, and G is shear modulus. f_{cor} is correlation force arising from mutual disposition of dislocations. We used the expression for it from [7]

$$f_{cor} = A_1 \frac{\partial \rho}{\partial x} \tag{3}$$

where $A_1 = \frac{Gb^2}{4\pi\rho_0}$ and ρ_0 is an average stationary dislocation density. Inserting expressions for forces in Eq. (2) and neglecting its right side ($J(\rho) \cong 0$ (argumentation in [6])), we obtain the basic equation of our model:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(V_{ext}\rho + mb^2 G\rho\sqrt{\rho} + \left(m\frac{Gb^2}{4\pi\rho_0} - D\right)\frac{\partial \rho}{\partial x}\right) = 0 \tag{4}$$

The solution of Eq. (4) is looked for as

$$\rho = \rho_0 + \rho_1(x,t) \tag{5}$$

where $\rho_1(x,t)$ is a dislocation density fluctuation near the average stationary dislocation density ρ_0. For the dislocation density fluctuation $\rho_1(x,t)$, we get the widely known Burgers equation:

$$\frac{\partial \rho_1}{\partial t} + \rho_1 \frac{\partial \rho_1}{\partial x} = \frac{1}{2Kb}\left(\frac{D}{m} - \frac{Gb^2}{4\pi}\right)\frac{\partial^2 \rho_1}{\partial x^2} \tag{6}$$

where K is determined by material constants. As well knowing the solution of Eq. (6) is a step, and $\rho(x,t)$ takes the form

$$\rho(x,t) = a\delta\left(1 + \tanh\frac{1}{2}\left(ax - a^2t\delta\right)\right) \tag{7}$$

where $\delta = \frac{1}{2Kb}\left(\frac{Gb^2}{4\pi} - \frac{D}{m}\right)$ and a is constant determined by the bound condition, $\rho_1(x,t) \sim \tanh\frac{1}{2}(ax - a^2t\delta) \to 0$, at $x - at\delta \to 0$. It corresponds to the edge of Chernov-Luders band or the area of a sharp stepwise transition from a certain value of dislocation density to another value. Irradiation increases the step height. This is shown qualitatively in **Figures 1** and **2**. There are three plots corresponding to Eq. (7) for three irradiation dose values: $p_1 < p_2 < p_3$.
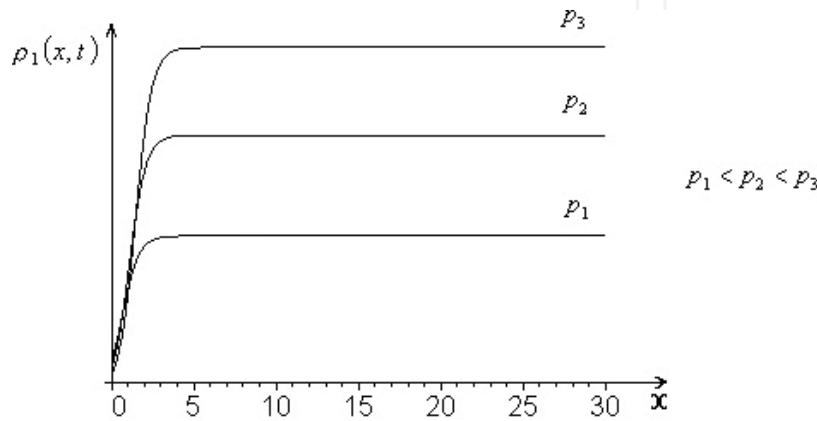

Figure 1.
The dependence of step height on irradiation dose: $p_1 < p_2 < p_3$. It corresponds to the edge of Chernov-Luders band.
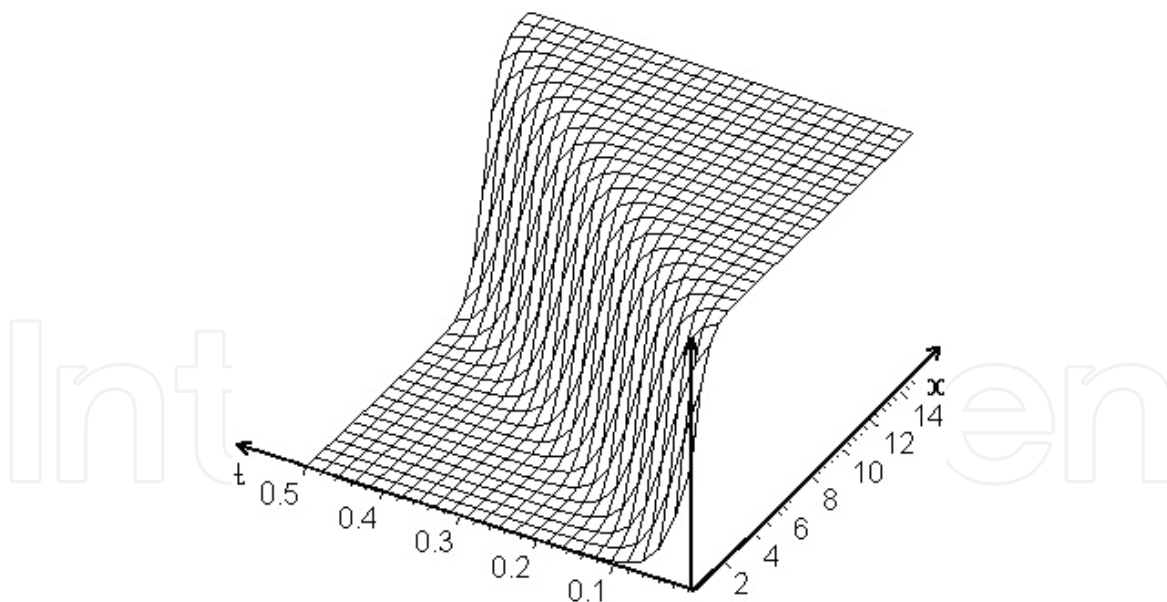
Figure 2.
Three-dimensional plot of step propagation of plastic deformation in sliding plane.

4. Macroscopic bands (the Danilov-Zuev relaxation wave type)

Now, in the dislocation density balance Eq. (2), we take into account correlation forces [7] originating from redistribution of energy between the interaction dislocations more exactly:

$$f_{cor} = A_1 \frac{\partial \rho}{\partial x} + A_2 \frac{\partial^3 \rho}{\partial x^3} \qquad (8)$$

where $A_1 = \frac{Gb^2}{4\pi\rho_0}$, $A_2 = \frac{b\sigma_{ext}L}{8\pi\rho_0^2}$, and L is an average relaxation length of a dislocation ensemble [7]. The right side of Eq. (2) can be represented as $J(\rho) = k_1 - k_2\rho^2$ (see [6]) where k_1 characterizes a dislocation source and k_2 is responsible for interaction of the dislocations which can annihilate in particular.

Supposing $\rho_1 = \rho_0 u(x,t)$, one obtains the dimensionless equation for the relative density $u(x,t)$ of dislocations from Eq. (2):

$$\frac{\partial u}{\partial t} + \theta \frac{\partial u}{\partial x} + u \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} + \frac{\partial^4 u}{\partial x^4} = -\chi_1 u - \chi_2 u^2, \qquad (9)$$

where θ is the numerical coefficient and χ_1, χ_2 are responsible for the velocity of dislocation formation and their annihilation, respectively. In the work [8], it is shown that χ_1, χ_2 are extremely small for the parameter numerical values of a real standard metal. Due to this, the right side of Eq. (9) is considered to be equal to zero. Then Eq. (9) goes to Kuramoto-Sivashinsky's equation type:

$$\frac{\partial u}{\partial t} + \theta \frac{\partial u}{\partial x} + u \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} + \frac{\partial^4 u}{\partial x^4} = 0, \qquad (10)$$

solution [9] of which describes spatial quasi-periodical structures. For Eq. (10), the Cauchy problem was solved at the different initial conditions for the dimensionless function $u(x,t)$. The same level values of $u(x,0)$ were set at the initial time moment under a random distribution in x on the segment [0, 30]. In **Figure 3**, the plot I corresponds to the level $u(x,0) = 0.2$; the plots II and III do $u(x,0) = 0.5$ and
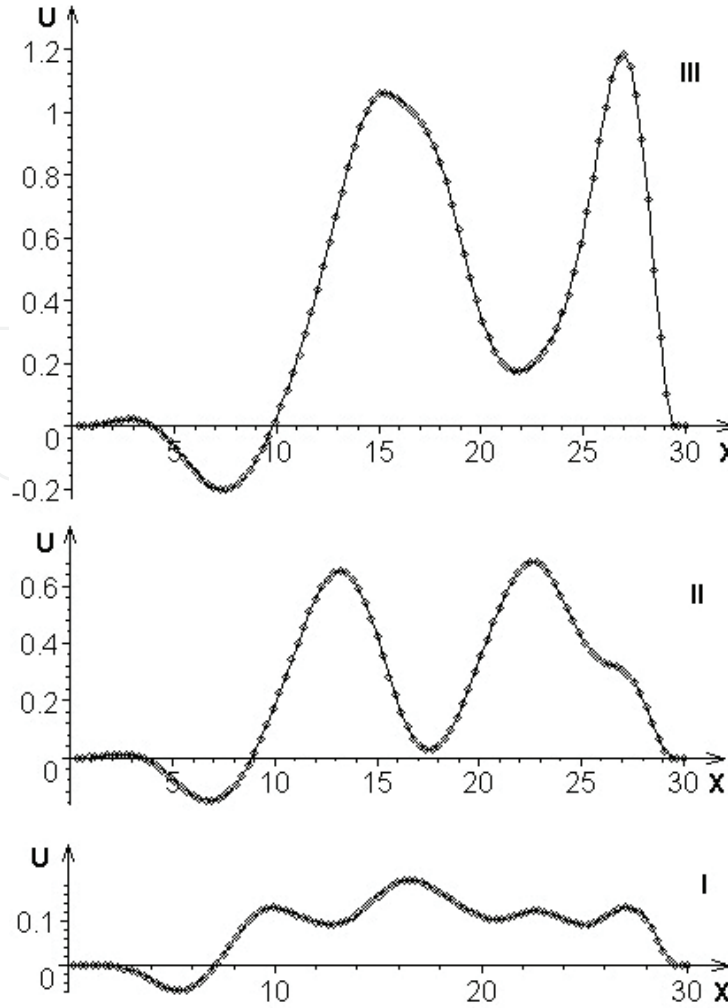
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Figure 3.
*The plots of the Eq. (10) solution constructed for the time interval $\Delta t = 7.3$. The plot **I** corresponds to $u(x, 0) = 0.2$; the plots **II** and **III** do $u(x, 0) = 0.5$ и $u(x, 0) = 1$, respectively.*

$u(x, 0) = 1$, respectively. These plots show that the spatially inhomogeneous quasi-periodical dislocation structures are formed in a sample in a certain time interval Δt (here $\Delta t = 7.3$). The level of the $u(x, 0)$ initial density corresponds qualitatively to the certain irradiation dose level of the material. From **Figure 3**, one can see that the localized dislocation structures are formed faster and become more striking in increasing the irradiation dose. The similar wavy deformation distribution is experimentally got in a material sample [10] (**Figure 4** [11] shows the pattern of the deformation distribution along a sample during the initial straining stages).

The appreciable effect of the right side of Eq. (2) on a solution form $u(x, t)$ begins from the χ_1, χ_2 values of 10^{-3}. **Figure 5** shows relaxation of the random dislocation distribution $u(x, 0)$ during time on the x-interval equal to 45 of relative units.

The right side of Eq. (10) not equal to zero determines so-called "point" kinetics of dislocation interactions involving microlevels of plastic deformation. It may say the structures are formed when the point kinetics is absent.

Generalizing and following a concept of structure levels, it is possible to expect that switching-on micro- and meso-levels affects positively plastic deformation of irradiated and nonirradiated materials. So in materials deformed in the conditions of superplasticity, the effect of "running cell" is observed. When even extension exhausts its supply (it is small in these materials), the first neck stage must evolve, that is, deformation of a sample as a whole occurs (macro level N), the mechanism of grain border sliding (macro level N-1) is switched on and does not allow for long
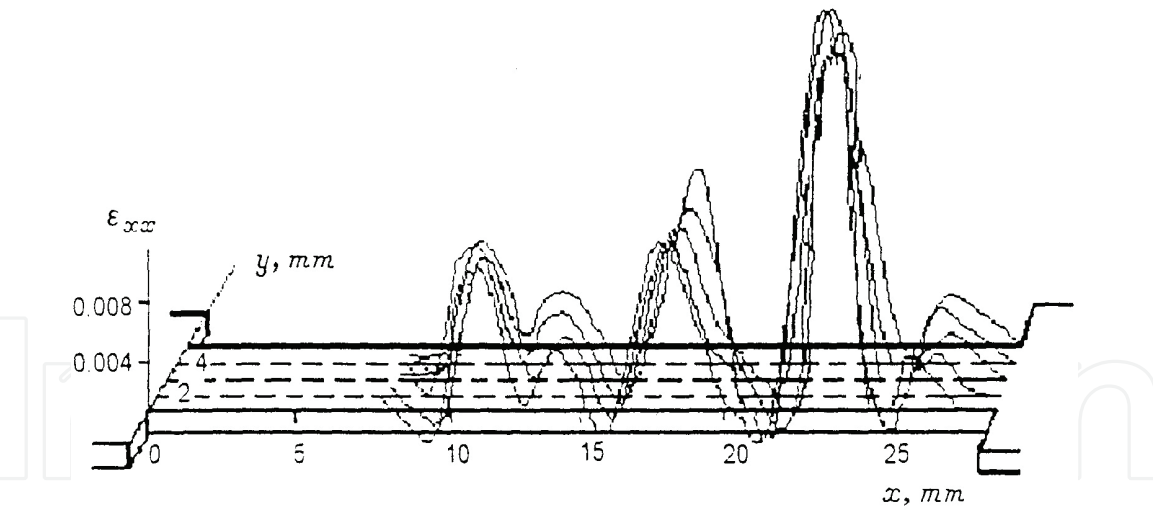
Figure 4.
*The pattern of the deformation distribution along a sample during the initial straining stages (**Figure 1** of the work [11]).*
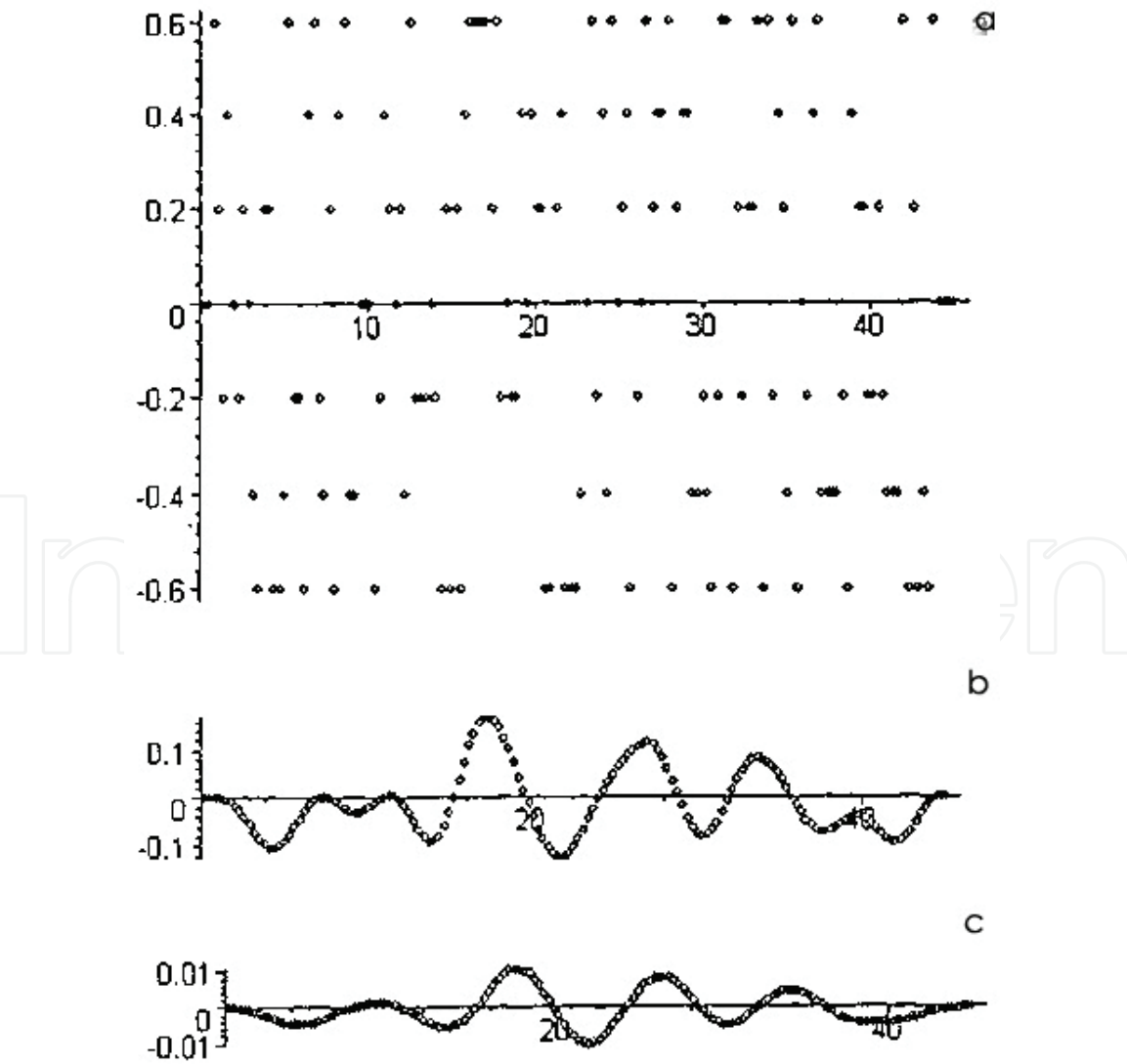

Figure 5.
The spatially temporary evolution of the dislocation density, according to Eq. (10) with the right side being equal to 10^{-3} in relative units. The account time is 0.3 (a), 1 (b), and 5 s (c).
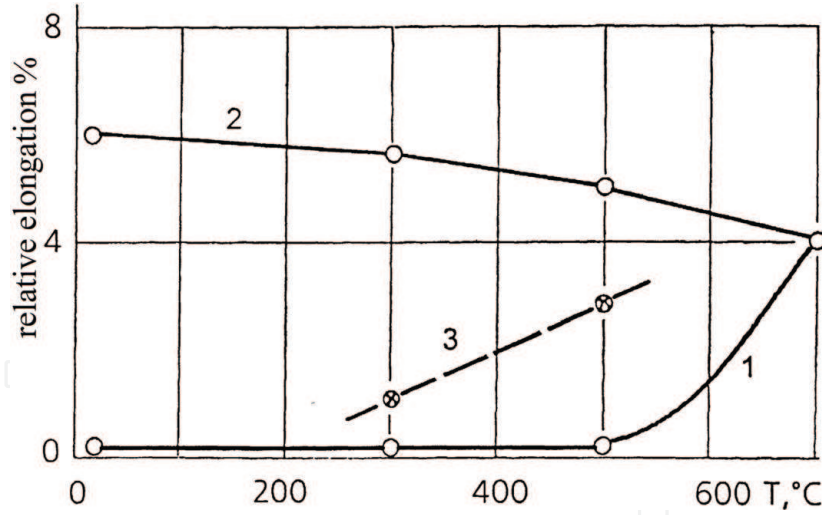
Figure 6.
The temperature dependence of relative extension of a low alloyed chromium irradiated with a fluence of approximately 0.1 displacements per atom (dpa) (1), the initial material (2), and the material irradiated and deformed by bends (3).

wave modes to be established. The neck only starting to arise relaxes due to the mechanism of grain border sliding.

The next example of the effect of switching-on (N-1) level is based on the investigation results of low alloyed chromium [12]. **Figure 6** shows this material when irradiated is absolutely brittle in the rather wide temperature range up to 500°C (plot 1). A part of amount of samples after irradiation was deformed by bend in 30–40°. As a result, new dislocations were created there, and plasticity became not equal to zero after radiation tests (plot 3). So in this case too, switching on the lower structure level (here microlevel) of plastic deformation leads to essential lowering material embrittlement. Thus, the synergetic law conception and applying the structure level conceptual design to study processes of material radiation embrittlement give us not only the investigation direction but the pointing of the ways to solve the specific problems for the material radiation embrittlement to be reduced.

5. Modeling dose dependence of uniform elongation of materials

Experiment shows it is possible for both the monotonous decrease [13] and non-monotonic behavior [14] of uniform elongation dependence ε_p to take place on radiation dose Φt as result of radiation. It does not take into consideration possible deformation hardening in traditional approaches to description of this phenomenon.

Here a new approach is represented allowing to explain peculiar properties of the $\varepsilon_p(\Phi t)$ dependence of irradiated materials considering deformation hardening [15].

The approach is based on the following equation system:

$$\frac{d\sigma}{d\varepsilon} = \sigma \tag{11}$$

$$\sigma = \alpha G b \sqrt{\rho(\varepsilon) + N(\Phi t)d} \tag{12}$$

$$\rho(\varepsilon) = \rho_\infty - (\rho_\infty - \rho_0)e^{-\beta\varepsilon} \tag{13}$$

$$\frac{d\sigma}{d\varepsilon} = A + Be^{-\gamma\varepsilon} \tag{14}$$

$$N = N(\Phi t) \tag{15}$$

where Eq. (11) is a known criterion of plastic stability loss of samples stretched by uniaxial stress with constant speed when a plastic flow localization occurs and a neck is formed. This equation defines a limit value of uniform elongation ε_p. $\frac{d\sigma}{d\varepsilon}$ is the coefficient of deformation hardening, σ plastic flow stress, and ε relative deformation. Eq. (12) determines the plastic flow stress dependence on dislocation density ρ as a function of deformation ε and the dislocation loop density $N(\Phi t)$ on dose (d—a size of a dislocation loop). Coefficient α is of the order of unity. Eq. (13) is an empiric formula of dislocation density dependence on relative deformation ε (see, e.g., [16]). Here ρ_0 is the value of dislocation density of undeformed material, and ρ_∞ is the saturation value of dislocation density at large values of ε. The values of ρ_0 and ρ_∞ are taken from the experimental data [16, 17].

Further, there are the experimental dependences of deformation hardening coefficient $d\sigma/d\varepsilon$ (hardening speed) on deformation ε at different dose values of material radiation in the proposed model (see **Figure 7**).

Computer processing of the curves depicted in **Figure 7** leads to Eq. (14) for the dependence of deformation hardening coefficient on relative plastic deformation ε: the values of parameters A, B, γ of Eq. (14) for corresponding doses are given in **Table 1**.

Eq. (15) is the dose dependence of radiation defect density N. In this model, N is considered as volume density of dislocation loops. Consider the options of the dose dependence Eq. (15) of dislocation loop density $N(\Phi t)$:

1. The monotonic dependence obtained in [18]

$$N(\Phi t) = N_0 \left(1 - e^{-\xi\frac{\Phi t}{2}}\right)^{\frac{1}{2}},\tag{16}$$
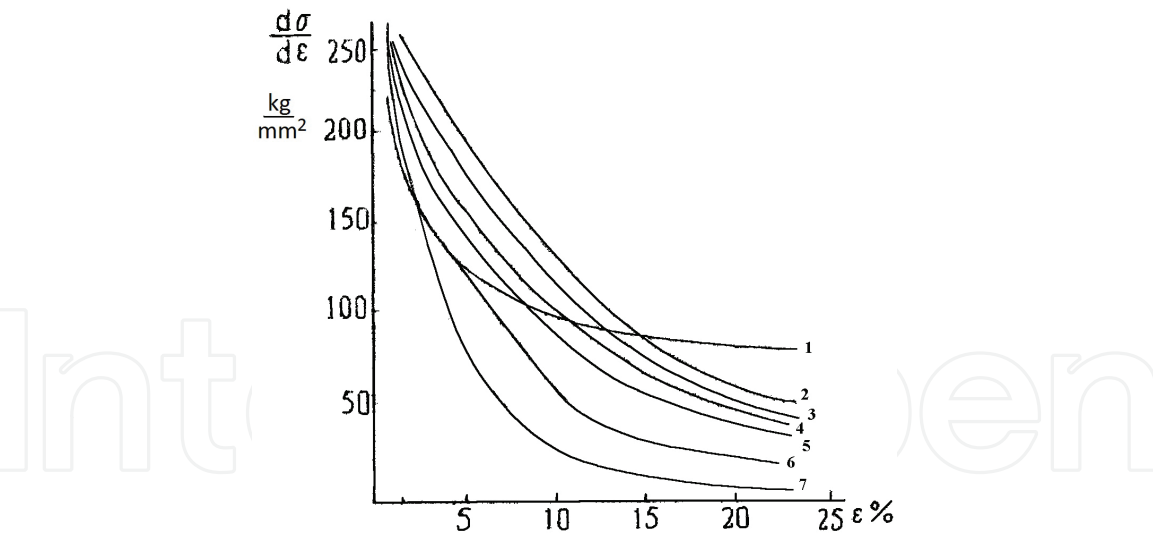

Figure 7.
The dependence of deformation hardening coefficient on relative plastic deformation ε: The curve 1 corresponds to unirradiated nickel; the curves 2, 3, 4, 5, 6, and 7 correspond to nickel irradiated by electrons with energy of 225 MeV (dose of radiation is 10^{-3}, 10^{-2}, 10^{-1}, 2×10^{-1}, 5×10^{-1}, and 5×10^0 (dpa), respectively).

Dose dpa	0	10^{-3}	10^{-2}	10^{-1}	2×10^{-1}	5×10^{-1}
A (kg/mm²)	816.59	222.84	59.33	257.88	171.96	430.47
B (kg/mm²)	1454.48	1731.54	2653.8	2268.2	2399.68	2684.6
γ	0.24	0.09	0.09	0.11	0.13	0.27

Table 1.
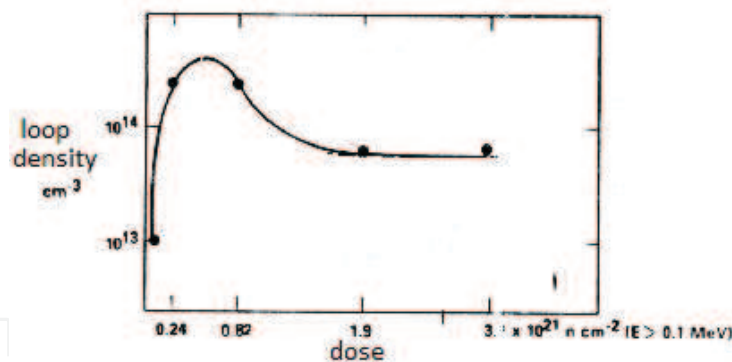*Parameters of Eq. (4) for different doses.*

Figure 8.
The nonmonotonic dependence of dislocation loop density on radiation dose.

where ξ is a numerical coefficient and N_0 is the saturation value of loop density

2. The nonmonotonic dependence of a type presented in **Figure 8** [19].

The dependence of dislocation loop density on radiation dose can be described by the following analytic formula:

$$N(\Phi t) = N_0 e^{-(\Phi t - \Phi t_0)^2} \tag{17}$$

in the area of maximum. The nonmonotonic dependence of dislocation loop density on radiation dose is associated with the processes of growing a loop size. At the beginning of its evolution, the loops increase. Their density increases too. Upon reaching a certain radiation dose as a function of temperature and the speed of a displacement, the loops begin to interact with each other. As a result, the process of decreasing its density and loss of its defectiveness begins what is observed by [19].

Eq. (11) considering Eqs. (12)–(14) takes the form

$$\left(\frac{A + Be^{-\gamma \varepsilon}}{\alpha Gb}\right)^2 = \rho_0 + N(\Phi t) - (\rho_\infty - \rho_0)e^{-\beta \varepsilon} \tag{18}$$

Eq. (18) admits a numerical solution only. The numerical solution of Eq. (18) leads to the dependence of uniform elongation ε_p on dose for Eqs. (16) and (17) to be used. The respective curves are represented by **Figure 9**.
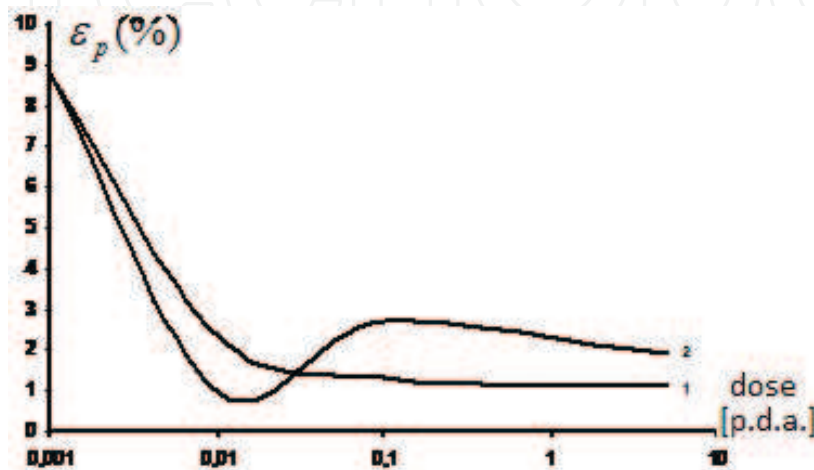

Figure 9.
The dependences of uniform elongation on radiation dose. The curve 1 corresponds to the monotonic dependence of the loop density (16) on dose. The curve 2 corresponds to the nonmonotonic dependence (17).
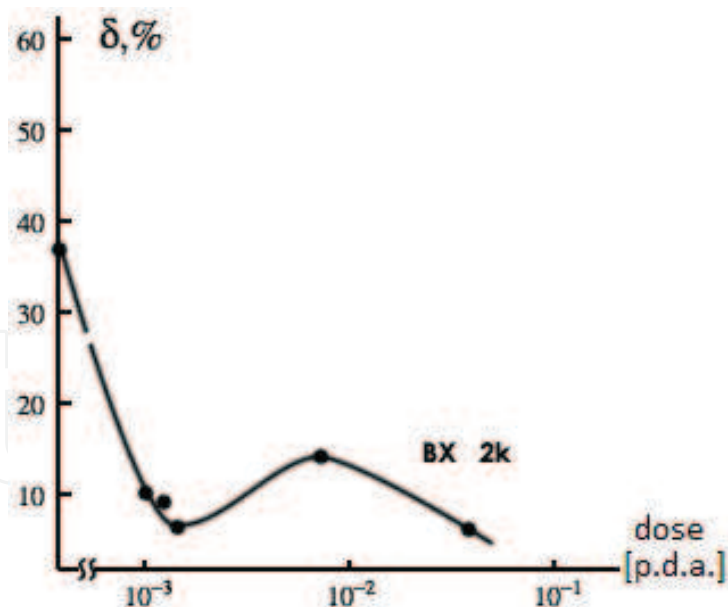
Figure 10.
The experimental dose dependence of elongation of low-activated alloy based on chromium VCh-2 K under
(e, γ)—Beam radiation.

The experimental nonmonotonic dependence $\varepsilon_p(\Phi t)$ of low-activated alloy based on chromium VCh-2 K irradiated by (e, γ)—beams in a dose interval of $10^{-3} \div 10^{-1}$ (dpa)—is represented in **Figure 10**.

Comparison graphs of $\varepsilon_p(\Phi t)$ in **Figures 9** and **10** show alignment of modeling and experimental results.

6. Conclusions

1. Evolution of the ensemble of dislocations interacting with obstacles in irradiated materials is analyzes, and the expression for part of dislocations overcoming obstacles is obtained on the basis of the general kinetic approach.

2. Formation of the front Chernov-Luders band is due to the presence of a nonlinear term called the Burgers nonlinearity in the evolution equation for dislocation density.

3. The description of the process of formation of space–time self-organizing dislocation structures is offered. The qualitative agreement of a dislocation density distribution is shown along sample length with the experimentally detected deformation distribution called the Danilov-Zuev relaxation waves in irradiated materials.

4. The description of the dependences of radiation embrittlement of reactor materials on radiation dose is suggested. It is found out that monotonic and nonmonotonic dependences of uniform elongation of irradiated materials are determined by the form of the dislocation loop density dependence on radiation dose.

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