



MODERN STATE OF PHYSICS IN THE RESEARCH OF MICROPLASMA BREAKDOWN IN SILICON P-N JUNCTIONS AND DIODES AND SCHOTTKY

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ANNOTATION

The reliability of semiconductor devices is primarily determined by the degree of perfection of the source material at the same time and very much depends on the technological processing methods used. Dislocations in the crystal structure are generated due to the occurrence of internal stresses, leading to plastic deformation of the material. Numerous studies have shown that one of the main causes of degradation and failure of semiconductor devices is the presence of internal mechanical stresses in them, the relaxation of which is accompanied by the appearance of structural defects.

KEY WORDS: *silicon, germanium, internal stresses, misfit dislocations.*

The reliability of semiconductor devices is primarily determined by the degree of perfection of the source material at the same time and very much depends on the technological processing methods used. Obtaining films on a single-crystalline substrate or epitaxial growth makes it possible to introduce a dopant with an arbitrary required concentration and obtain a p-n junction, avoiding the process of solid-phase diffusion. This is due to the fact that the degradation of almost all devices is based on the phenomena of diffusion, defect formation and decomposition of supersaturated solid solutions [1].

In devices containing p-n junctions with high impurity concentration gradients, degradation of parameters will be observed over time, associated, for example, with the spreading of concentration profiles due to diffusion. [2]. Taking into account all the factors that appear during the operation of devices, knowing the diffusion coefficients of impurities, it is possible to determine the amount of deformation of the concentration profile and predict the degree of degradation of electrical characteristics associated with changes in the profile. [3]. Analyzing these processes, the process of avalanche breakdown of real large-area p-n junctions, which has a microplasma character, remains poorly studied. Indeed, already in the very first studies of avalanche breakdown of pn junctions and Schottky diodes, it was shown that the breakdown in them is highly localized. [4]

The local breakdown region has small geometric dimensions and a significantly lower breakdown voltage compared to homogeneous regions. The region of such localized breakdown was called microplasma. However, [5-6] it was shown that dislocations do not always cause the appearance of microplasmas. In addition, in [7] it was theoretically proven that the phenomenon of microplasma breakdown can be interpreted as a special type of instability that occurs even in the case of an ideal p-n junction. In addition, analysis of experimental data shows that it is most likely not single dislocations that contribute to a local decrease in breakdown voltage, but their clusters.

Taking into account the above, it can be argued that the role of dislocations in the occurrence of microplasma breakdown is not fully understood. Most likely, the influence of dislocations manifests itself in conjunction with other factors. Let us consider separately the reasons leading to the appearance of dislocations. Dislocations in the crystal structure are generated due to the occurrence of internal stresses, leading to plastic deformation of the material

In epitaxial heterostructures, there are a number of reasons that cause internal stress. The main ones are thermal stresses; voltage mismatch; structural defects. Numerous studies have shown that one of the main causes of degradation and failure of semiconductor devices is the presence of internal mechanical stresses in them, the relaxation of which is accompanied by the appearance of structural defects [8-11].

Initial structural defects can contribute to the annihilation of radiation defects, both during and after irradiation. In particular, dislocations can be sinks of simple radiation defects (vacancies and interstitial atoms) - the main structural defects that arise during the relaxation of internal stresses, the density of which is especially high at the interface - the transition layer between two phases



or the contact surface of two grains in polycrystalline materials. Atoms and molecules at interfaces exhibit different properties than atoms and molecules in the bulk of a phase or material, since they are in a different environment. In this regard, the study of the properties of matter at interfaces and the phenomena that arise there constitutes a special field of physics and chemistry. Surface effects become important in nano-sized materials, where the surface fraction is very large and can begin to determine the properties of the material as a whole.

The increased defectiveness of the GR in devices with heterojunctions and a Schottky barrier allows us to hope that the parameters of such devices will change little when irradiated up to very high doses. In addition, the interaction of radiation defects with the original structural defects (both in the volume and in the GR region) in a certain range of irradiation doses can lead to a decrease in the generation-recombination component of the current and change the characteristics in the pre-breakdown region in a favorable direction. [12-13].

For an interface of arbitrary orientation (hkl), an expression has been obtained for the first time that establishes the relationship between the misfit parameter f of the epitaxial heterosystem, the number of dislocation families involved in the process of misfit stress relief, the linear densities of misfit dislocations of each family, as well as the values of the projections of the edge components of the Burgers vectors of misfit dislocations on interface boundaries. To obtain the expression, long-range fields of normal and shear stresses arising in the near-surface layer of the epitaxial film are considered. Criteria for the optimal and non-optimal course of the relaxation process of relieving tensions of inconsistency have been formulated [14]. Relaxation of internal mechanical stresses in heterogeneous device structures can lead to their degradation [15]. The main reasons for the occurrence of internal stresses in heterogeneous device structures are thermal expansion of contacting materials $\Delta\alpha$, which leads, when the system temperature (ΔT) changes, to the appearance of thermal stresses (TS) mismatch of crystalline film and substrate lattices Δa , as a result of which misfit stresses (MS) arise, each of which is associated with microdeformations, and therefore local stresses. At a high concentration of defects, the microstrain fields of individual defects overlap, resulting in inhomogeneous or homogeneous macrostrain. Let two materials, characterized by thermal expansion coefficients $\alpha_1(T)$ and $\alpha_2(T)$, be brought into contact at T_0 . This can be done in various ways: thermal compression, fusion, deposition of a film of material 2 on a substrate of material 1.

After cooling the resulting geostructure to room temperature T_k , both materials will be in a stressed state. If the structure of the geostructure is a layered structure, then the elastic deformation in the substrate and film is described by the diagonal tensors $\varepsilon(1)$ and $\varepsilon(2)$ with components

$$\varepsilon_{xx}(1) = \varepsilon_{yy}(2) \quad \varepsilon_{zz}(1) = -2\nu_i \varepsilon_{zz}(1)/(1 - \nu_i)$$

Here the z axis coincides with the direction of the normal to the phase boundary, ν_i - Poisson's ratios of mating materials ($i = 1, 2$) The stress tensors $\sigma^{\wedge(1)}$ and $\sigma^{\wedge(2)}$ can be obtained from $\varepsilon_{xx}(1) = \varepsilon_{yy}(2) \quad \varepsilon_{zz}(1) = -2\nu_i \varepsilon_{zz}(1)/(1 - \nu_i)$, using the equilibrium conditions of the system, Hooke's law.

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$$\sigma_{xx}^{(t)} = \sigma_{yy}^{(t)} = E_1^* \varepsilon_{xx}^{(t)}, \quad \sigma_{zz}^{(t)} = 0 \quad \text{with attitude } |\varepsilon_{xx}^{(t)}|_{z=0} - \varepsilon_{xx}^{(l)}|_{z=0} = |\gamma_{lt}|,$$

$$\text{где } \gamma_{lt} = \int_{T_k}^{T_0} (\alpha_2 - \alpha_1) dT$$

$E_1 = E_1 / (1 - \nu_i)$, E_1 - Young modules, $i = j = 1, 2$. The deformation of both parts of the heterostructure is inhomogeneous in z . If the thickness of the substrate in d_1 is much greater than the thickness of the film d_2 , then the inhomogeneity of deformations in the film can be neglected and considered $\varepsilon_{xx}^{\wedge(2)} \approx \varepsilon_{xx}^{\wedge(2)}|_{z=0} = \text{const}$

Under the influence of moments of force applied to the film and substrate, the heterostructure bends. For the radius of curvature of the system for $d_1 \ll d_2$

$$\text{we get the expression } R = \frac{E_1^* d_1^2}{6E_2^* d_2 \nu_{12}}$$

The sign of the curvature of the system in the presence of only thermal stresses is determined by the sign of the value ν_{12} . Thermal stresses were experimentally discovered in various semiconductor heterostructures, as well as in semiconductor-insulator and



semiconductor-metal systems [16]. They are practically present in any device structures, since the latter are necessarily formed when elevated temperatures $T \neq T_k$. Thermal stresses can arise in heterosystems not only during the cooling process, but also during the manufacture of the system due to the presence of temperature gradients.

In contrast to thermal stresses that arise in any heterosystems regardless of the crystal structure of the mating materials, mismatch stresses arise only during the epitaxial growth of one material onto another.

If the materials are dissimilar (hetero-epitaxy), then each of them is characterized by its own crystal lattice parameter, a (i). On the surface of the substrate there is a potential relief with a period a , due to the periodic arrangement of atoms at lattice sites. During epitaxial deposition of a film, it is energetically more favorable for the atoms of the deposited substance to be located in potential wells, i.e. complete the substrate grid. In this case, the interatomic distances in the film in planes parallel to the interface turn out to be equal to the lattice parameter of the substrate.

Since in the general case $a_1 \neq a_2$, the film turns out to be deformed (tetragonal distortion). An idea of the magnitude of the mismatch stresses arising in this case can be obtained by comparing them with the theoretical ultimate strength of the crystal, which, according to various estimates, lies between $G/2\pi$ and $G/30$, where G is the shear modulus. Because the

$$\sigma_{\Pi} = \frac{2 \cdot (1 + \nu) \cdot G \cdot \varepsilon}{1 - \nu}$$

then in the case when the lattice mismatch $f = 2 \frac{a_2 - a_1}{a_2 + a_1}$

on the order of one percent, mismatch stresses can exceed the tensile strength of the crystal.

In autoepitaxy, also $a_1 \neq a_2$ due to different doping of the film and substrate. Therefore, auto-epitaxial systems in the sense of the occurrence of internal mechanical stresses are completely similar to geosystems. In this case, the mismatch stresses are called concentration stresses, since the difference in the lattice parameters of the film and the substrate is determined by the composition and concentration of dopant impurities.

Concentration stresses also arise in systems with a composition gradient or a concentration gradient of impurities (p-n junctions).

The nature and sign of deformations associated with DS depend on the nature of the defects. Thus, the sign of the deformation caused by point defects is determined by the difference between the radii of the defect and the matrix atom. Regions of tension and compression are associated with edge dislocations (the latter on the side of the extra half-plane in the crystal).

Depending on the nature of the defects (point, linear, three-dimensional), the corresponding stress fields attenuate with distance from the defect at different rates. Deformations caused by point defects decrease in proportion to the cube of the distance.

Assuming a uniform distribution of point defects (vacancies, between site impurity atoms), the average relative strain associated with their presence

$$\varepsilon = \sum_k \beta_k N_k$$

where N_k are the defect concentrations and β_k are the corresponding deformation constants.

In the case of dislocation according to the hyperbolic law. The presence of a dislocation wall (disclination) leads to the appearance of a field of alternating stresses, and accumulations of dislocations of the same sign lead to the appearance of long-range tensile stresses on one side of the accumulation and compression stresses on the other side. Three-dimensional defects (clusters, micropores, inclusions) lead to extended strain fields.

Another reason for the occurrence of deformations associated with internal stresses is surface tension (ST), which plays a noticeable role in very thin continuous or island layers. Depending on the sign of the surface energy of the tensile force. Such stresses are inversely proportional to the thickness of the film and become negligible at $d \sim 100 \text{ \AA}$.

When creating integrated circuits, internal stresses caused by shrinkage of polycrystalline or amorphous films associated with aging processes, in particular oxygen diffusion, become of great importance.

Significant stresses can be associated with surface topography, scratches, and the edges of a non-continuous film.

In the general case, internal stresses of various origins are simultaneously present in heterosystems. However, essentially their occurrence is due to the same reason: the presence of intrinsic deformations at the phase boundaries associated with the difference in the equilibrium distances between atoms in the contacting layers.

The presence of internal stresses increases the energy of the system, and at certain stresses increases the energy of the system, and under certain conditions the system relaxes and transitions to a state with lower energy. In semiconductor heterosystems, internal stresses are usually relaxed through plastic deformation, but other methods of relaxation are also possible (elastic bending, continuity, swelling, peeling, cracking, destruction). Classification of relaxation mechanisms, with the exception of elastic bending, are phase transitions.

Plastic deformation, as well as twinning and cracking, are dislocation mechanisms: they are associated with the generation and movement of dislocations. We will not dwell on twinning here, since this type of relaxation is plastic deformation of the system associated with the generation of specific dislocations, called misfit dislocations. [32]

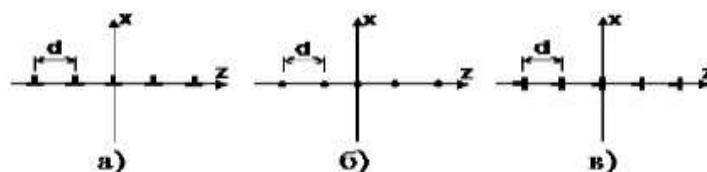


Fig. 1. Representation of a family of misfit dislocations in the form of three dislocation systems: edge misfit dislocations (a); screw misfit dislocations (b); edge dislocations creating a low-angle boundary(c).[17]

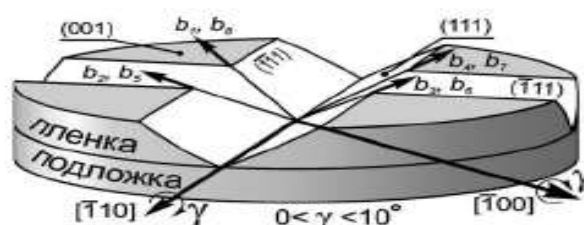


Fig. 2. Schematic representation of the Burgers slip vectors b1-b2 in the case of a vicinal interface (001) deviating by an angle γ as a result of rotation around the [-110] or [-100] axis.

The numbers of the Burgers vectors and the Miller indices of the slip planes and Burgers vectors are given in accordance with the data in Table 1.1. The table shows the structural characteristics of 600-misfit dislocations located in the singular interface (001) of the semiconductor heterosystem [28]. The crystal lattice parameter of the film exceeds the substrate parameter.

Family number	Sliding plane	Burgers vector direction, b	Direction of dislocation lines, E	Type of helical dislocation component
1	(-1-11)	[101]	[-110]	левая
2	(-1-11)	[011]	[-110]	правая
3	(111)	[-101]	[1-10]	левая
4	(111)	[0-11]	[1-10]	правая
5	(1-11)	[011]	[-1-10]	левая
6	(1-11)	[-101]	[-1-10]	правая
7	(-111)	[0-11]	[110]	левая
8	(-111)	[101]	[110]	правая

The technology strives to perform epitaxial growth at lower growth temperatures since this allows the creation of sharp heterointerfaces between layers and reduces the number of structural defects. Therefore, the main mechanism for the formation of misfit dislocations is sliding - it occurs at lower temperatures compared to dislocation creep [18.22.23.24.].

Let us consider a separate misfit dislocation, which consists of the following parts [21.25.26].



- firstly, this is a straight dislocation section located at the interface or near it, and is directly the misfit dislocation itself. This part of the dislocation removes the misfit between the two mating materials and reduces the energy of the heterosystem;

-secondly, these are one or two dislocation sites that connect the ends of the misfit dislocation with the surface of the film feathers. These regions pass through the entire thickness of the film feathers; in the literature they are called threading [20,27,28] or threading [21] dislocations. The term “penetrating dislocations” is also used [29].

In foreign literature, starting from the first works of Matthews, these dislocations are called “threading dislocations”. The most accurate translation to the English version is “piercing dislocations.”

The operation of Heigen-Schrank sources and modified Frank-Reed sources leads to the accumulation of misfits with the same Burgers vector at the interface of 600-dislocations. From [19.29] it follows that the accumulation of identical misfit dislocations having a screw component can lead to the appearance of long-range shear stresses in the epitaxial film. An example of the experimental observation of L-shaped misfit dislocations is shown in (Fig. 1.7). This figure shows an image of an electronic microscopy (Fig. 1.7.a)

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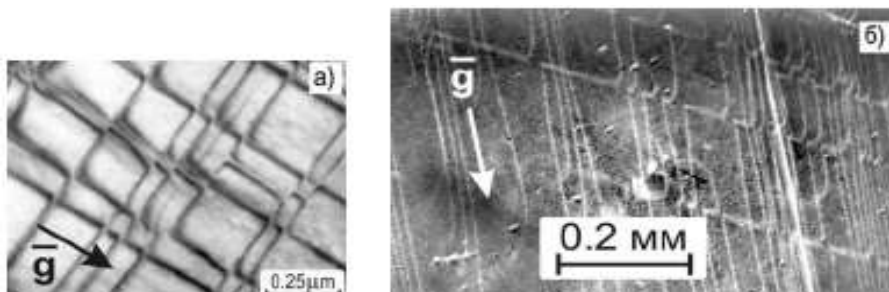


Fig3 Experimental images of Γ -base misfit dislocations [28].

Electron microscopic image (a) in the heterosystem (001). X-ray topogram (b), which shows two families of L-shaped dislocations rotated by 120° in the neutral plane of the stressed crystal (111).

Nagai was the first to observe the rotation between the crystal lattices of the film and the substrate in the InGa/GaAs heterosystem with a vicinal (001) orientation of the interface [30.31]. He proposed a model in which the reversal is a consequence of the presence of steps on the surface of the substrate and the mismatch between the cells of the film and the substrate.[17]



Fig. 4. RHEED pattern from a 25 nm Ga/Si(001)60 film around <001>, nucleation of the first monolayer by deposition. The surface cell (2*4) is oriented parallel to the edges of the terraces.[17]

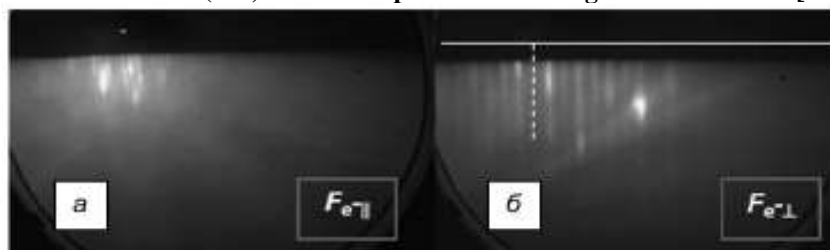


Fig. 5. RHEED pattern from a 25 nm Ga/Si(001)60 film around <011>, nucleation of the first monolayer by mixing. The surface cell (2*4) is oriented perpendicular to the edges of the terraces.[17].

The commonality of the reasons for the occurrence of internal stresses in heterosystems allows us to develop a general approach to considering the mechanisms of their relaxation. Most clearly, one can study the mechanisms of relaxation in single-crystal epitaxial systems. Relaxation processes proceed similarly in systems with diffusion layers that play (substrates) with the lattice parameter. Therefore, let us consider the relaxation of internal stresses, for example, in epitaxial systems.

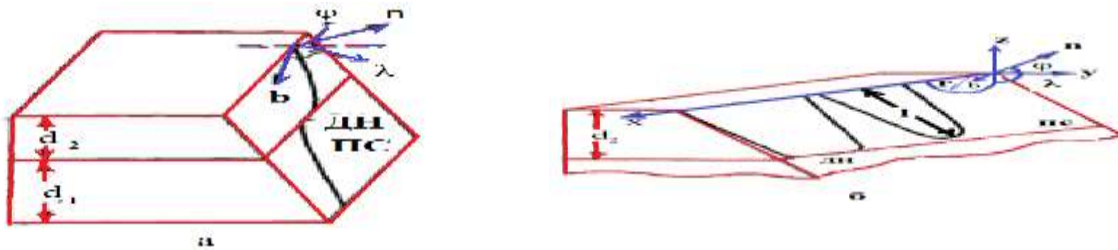


Figure 6. Various mechanisms of DN occurrence:

a-due to the bending of growth dislocations; b- by generating and expanding dislocation half-loops. [32]

During plastic deformation, the total length of dislocation lines per unit volume of the deformed material increases due to:

- 1) increasing the length of dislocations existing in the material
- 2) regenerative propagation of existing dislocations
- 3) the nucleation of new dislocations in the form of dislocation loops or half-loops.

All theoretical works that consider the relaxation of internal stresses in heterosystems are based on the concept of DN, introduced in [33-38], the authors of which proceed from the idea that the electron beam can be in one of two equilibrium states with a uniform elastic deformation and with a mesh straight edge dislocations at the interface. This network can be rectangular or hexagonal depending on the crystallographic orientation of the interface.

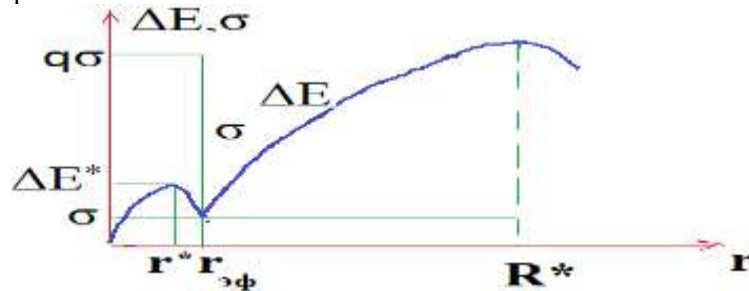


Fig-7. Dependences of stress σ on the distance to the concentrator and changes in the thermodynamic potential on the radius of the dislocation loop.

In the case of heterogeneous nucleation of dislocations, the dependence $\Delta E(r)$ takes on the form shown in Fig. 2. The additional left maximum corresponds to the region of action of stress concentrators. Its height ΔE^* is significantly lower than that of the main one, and at real temperatures only loops of radius r^* corresponding to this maximum are generated.

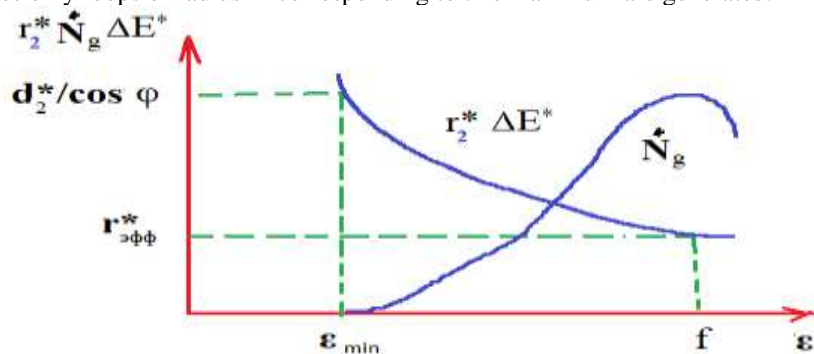


Fig.8. Dependence of the critical radius of nucleation and the generation rate of dislocation loops, as well as the change in the thermodynamic potential of the system when a half-loop occurs on elastic deformation of the film.

[32]



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[32]

$$\varepsilon = -b \cdot \cos^{\lambda} \int_{t'}^{\frac{t-t_0}{\varepsilon+t'}} v(t, t_1) N_D(t_1) dt_1 = \frac{2(1+\nu)Gb^3 \cos^3 \lambda \cos^3 \varphi}{1-\nu} \cdot \frac{D}{k \cdot T} \cdot \int_{t'}^{\frac{t-t_0}{\varepsilon+t'}} \left(\varepsilon - \frac{t_0}{t-t_0-t'} \right) N_D(t_1) dt_1$$

$t_0 \equiv \frac{W_0(1-\nu)}{2Gb\nu(1+\nu)\cos\lambda\cos\varphi}$ ε decreases, ΔE^* and r^* according to [5] increase and, accordingly, R^* increases so that later formed dipoles remain unexpanded. The straight sections of the MD lying at the interface are short, and in the volume of the film there is a larger number of dislocation dipoles and reaction products between them.

If the deposition rate is high, then the change in film thickness from $d_2 = R^* \cos \varphi$ to $d_2 = R^* \cos \varphi$ occurs in a short time. Then we can assume that almost all semi-loops nucleated on the surface, the density of which is relatively low, expand, as a result of which $\Delta E(r^*)$ increases and N_d sharply decreases. Thus, relaxation mainly occurs due to the expansion of a small number of half-loops, creating straight sections of DN at the interface.

The theory of relaxation of misfit stresses through the heterogeneous nucleation of dislocation half-loops on the surface of a growing film [35-38] is semi-quantitative in nature, which is due to ignorance of the nature of stress concentrators. It does not take into account the direct interaction of dislocations, the presence of many slip planes and the non-conservative movement of dislocations.

Dislocations in an unrelaxed heterosystem are in the stress field of the heterointerface. Depending on the direction of the Burgers vector, these stresses tend to either bring the dislocations closer to the interface or move them away from it. As a result, stress-induced selective absorption of point defects by dislocations occurs, namely: those from dislocation movement which requires the completion of the extraplane, will absorb interstitial atoms and emit vacancies, the same creep of which requires its shortening, will be sources of interstitial atoms and sinks of vacancies. As a result, under the influence of irradiation, dislocation mismatches that are ineffective for accommodation are dissolved and due to this, extraplanes associated with the MD are completed. [32]

Thus, from one mechanism of plastic deformation associated with dislocation sliding. In fact, this corresponds to a mechanical dislocation model without thermal fluctuations ($T=0$), where temperature is taken into account only by coefficients in the relations between ε and N_d . In fact, at a sufficiently high temperature, the role of the latter is also manifested in diffusion processes associated with the non-conservative movement of dislocations.

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