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STRUCTURE TRANSFORMATION AND SELF-ORGANIZATION PROCESSES IN DEFORMED CRYSTALS

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The work investigates the patterns of self-organization processes in deformed semiconductor crystals of $HgTe-CdTe$ solid solutions. It is claimed that crystal in the process of deformation should be considered as an open non-equilibrium thermodynamic system that evolves not only to preserve its integrity, but also to create new types of structures (defects) capable of more effectively dissipating the supplied energy. The formation of a synergistic structure in the crystal with minimal entropy is result. New types of dissipative structures were discovered. Mechanisms of effective dissipation of elastic energy are analyzed. The regularities of relaxation processes in deformed crystals at different stages of the deformation curve $\sigma-\varepsilon$. On the basis of electrophysical studies, the transformation of electroactive defects in the near-surface layers of micro- and macroplastically deformed $HgTe-CdTe$ single crystals is analyzed. Self-organization in the "dislocation - point defect" system is realized by stable impurity atmospheres around freshly introduced dislocations. Shown process significantly depends on the type of impurity and the process temperature.

Keywords: $HgTe-CdTe$ semiconductor crystals, structures defects under deformation, deformation elastic energy.

Introduction.

The long-term history of the study of elastic-plastic deformation of crystals testifies to the relaxation nature of internal processes due to the generation and propagation of dislocations under the action of effective mechanical stresses. The multiplicity of structural states that are inherent in deformed materials only emphasizes the general laws of strain hardening that connect the processes of structure formation with the behaviour of load curve. It is shown that strain hardening occurs as a result of a change in the density of dislocations with deformation. Considering dislocations as sources of long-range fields, Taylor wrote down the equation that relates the strengthening of the crystal to the density of dislocations in the form $\sigma=\sigma_0+\alpha Gb\rho^{1/2}$, where σ_0 is the contribution to the strengthening of structural elements that form the yield strength; α is a coefficient whose value determines the interaction between dislocations; G is the shear modulus; b is the Burgers vector; ρ is the density of dislocations. The relationship between the laws of dislocation motion and the growth of plastic deformation is expressed by the Orovan equation $e=b\rho L/2$, where L is the length of the dislocations free path. However, it was established that the newly introduced dislocations are thermodynamically unbalanced defects of the crystal lattice, which lead to a significant

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structural and dynamic transformation of the defective subsystem. In addition, non-dislocation mechanisms of crystals plastic deformation with new type defective structures were discovered [1, 2]. Multistage deformation curves and fragmentation of the macrostructure of a deformed crystal (as an example [3]) indicate not only the significant transformation of the defective structure, but also, the complex energy dissipation mechanisms. The evidence is unique macrodefects in deformed crystals, which arise as a result of self-organization processes in the defective subsystem during the dynamic loading of the crystal. In order to get the answer under the questions about these processes driving forces and mechanisms of their implementation. The deformed crystal should be considered as an open thermodynamic system that evolves dissipation effective energy of deformation process that creates structures. That energy continuously enters the object through open channels.

In such open highly unbalanced systems, energy dissipation may not occur according to the Boltzmann law with entropy growth (as in closed systems), but by its decrease due to certain quasi-stationary states [4]. The behaviour of such systems in conditions far from equilibrium is an irreversible process: a successive transition from one non-equilibrium state to another, which occurs with a decrease in entropy, that is, an increase in the organization of the system. Such processes are described by non-equilibrium thermodynamics. They are characterized by the spontaneous arrangement of structures and the presence of bifurcation points, branching points of evolution.

A certain sign of self-organization is the staged change in the process of evolution of the main parameters that reflect its structural state. Important factor in such processes are the mechanisms of energy dissipation, which can change during the evolution of the system. The self-organization of the deformed crystal is experimentally manifested in the gradual change of the macroscopic parameters. It has been established that in structures with existing interphase boundaries (heterogeneous systems), the efficiency of energy dissipation is determined by the parameters of interphase interaction [5,6]. Therefore, the goal of self-organization of deformation is not only the preservation of the integrity of the crystal at this stage, but also the generation of structures of a new type capable of effectively dissipating the added energy during the subsequent deformation process. That is, in the process of deformation of the crystal, a process of spontaneous self-organization occurs due to the emergence of new spatial structures. Therefore, the deformation process should be considered at the macro- and micro-levels from the standpoint of self-organization of the crystal with the aim of forming a synergistic structure with minimal entropy.

The **aim** of work was to establish regularities of self-organization processes and energy relaxation mechanisms at the macro- and micro-levels in elastic-plastically deformed $Cd_xHg_{1-x}Te$ crystals ($x = 0 - 0.18$) with different defect structures.

Deformation regularities of crystals of $HgTe - CdTe$ solid solutions were studied by uniaxial compression methods on Regel-Dubov relaxometer. The dimensions of the samples were $2 \times 2 \times 6\ mm^3$. Deformation was performed by uniaxial compression along the long rib at a constant speed. To study the kinetics of deformation, we used a synchronous recording during uniaxial deformation of the load curve "stress-strain" ($\sigma - \varepsilon$).

Fragmentation of the structure and interphase interaction of structural elements in the process of uniaxial deformation of $Cd_xHg_{1-x}Te$ crystals.

The traditional description of the plastic deformation of solids is not able to explain the deformation processes at the stages of easy sliding and strain hardening. The basis of this approach is the Taylor scheme, which allows the action of five sliding systems in the crystal to ensure its arbitrary shape change without breaking the integrity. However, in practice, Taylor's scheme has been proven to be unfeasible: as a rule, the number of active systems is less than five, and in many cases, sliding occurs mainly one at a time. This circumstance leads to the appearance of turning points in the deformed crystal [7]. As a result, rotational modes and, accordingly, higher structural levels of deformation are included in plastic flow along with translational slip. Along with microdeformation (moving dislocations), macroplastic fluidity takes place, in which three-dimensional structural elements take part. Therefore, when describing deformation, this problem can be solved only by taking into account the hierarchy of structural levels of deformation [7]. Thus, the carriers of plastic deformation in a crystalline material are defects of various natures, possessing an internal stress field that is inherent to the defect or induced by external stresses. The defect type and its own field are interconnected. Knowing the field, you can determine the type of defect and vice versa.

The rotational modes of the crystal lattice after uniaxial plastic deformation of $Cd_xHg_{1-x}Te$ crystals were detected X-ray by the authors [8]. However, at this time, this phenomenon has not been properly interpreted.

Therefore, the peculiarity of this type of deformation is not only the rotational plastic deformation of the lattice, but also the emergence of new structural elements of the deformation as a result. This is facilitated by any inhomogeneity that has stress fields, in particular, clusters of dislocations, grain boundaries in polycrystals, as well as local regions with a concentration of subboundaries in single crystals.

One of the sources of such deformation in $Cd_xHg_{1-x}Te$ single crystals is the clustering and crossing of subboundaries, which is characteristic of the studied crystals. In particular, they are characterized by the presence of blocks with an average size of $0.2-0.5\,mm$, which consisted, as a rule, of several sub-blocks an order of magnitude smaller, a developed substructure with the formation of a grid and a heterogeneous distribution of dislocations with a density of at least $10^5\ cm^{-2}$, as well as their local clusters in the area of stress concentrators. The average misorientation of the blocks along the axis of the ingot from which the samples were cut varied in 10 to 1 minutes. The density of etching dislocation pits along the boundaries of the blocks reached $10^8-10^9\ cm^{-2}$.

For example, a grain boundary of special orientation that does not contain grain boundary dislocations is a crystal structure defect that does not have a long-range intrinsic stress field. Therefore, the migration of such a boundary does not lead to plastic deformation [3]. At the same time, the movement of dislocations possessing their own field leads to plastic deformation. Therefore, the carriers of plastic shear can be arbitrary defects that have their own stress fields and are much larger than atomic ones.

The characteristic sizes of sources of internal stresses can have a different range - from atomic to values that make up tenths of the size of the deformed sample, and the sources themselves can exist before deformation or be created during it.

Therefore, an arbitrary area bounded by a closed surface, which has its own stress field, can be considered a structural element of deformation (SED). Since this area is macroscopic, its movement is generally characterized by two quantities: displacement and rotation. The reason for the formation of SED is the inhomogeneity of plastic deformation.

It should be noted that the experimental fixation of such rotations is complicated by the fact that the technique of X-ray diffraction analysis allows to fix only the rotation of the crystallographic planes of the lattice, but not the material rotation of the substance. Coincidence of the crystallographic rotation with the material rotation is possible when the crystal as a whole (without plastic shifts) takes a new orientation (fig. 1).

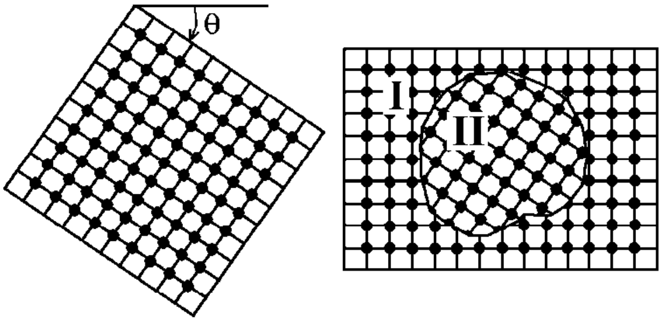

Fig. 1. Probable patterns of crystal lattice rotation.

It is also possible to form a twin formed under conditions of complete plastic accommodation of the shear type, for example, by changing the orientation of the crystallographic axes by non-invariant shifts in a certain plane, accommodated by dislocation slip. With the appropriate selection of invariant and non-invariant displacements, such an influence can preserve the material arrangement of matter, including the rotational mode.

The most likely mechanism of crystallographic rotation in the studied $Cd_xHg_{1-x}Te$ crystals is the accumulation of dislocations of the same sign as a result of simple sliding. In particular, two vertical walls of dislocations of different signs cause crystallographic unfolding in the region between the dislocation boundaries. In general, rotational processes would not be necessary if plastic flow were carried out with the participation of five slip systems. However, in real conditions, this requirement is not fulfilled in most cases. As a result, a reversal is necessary to unlock the landslides.

So, in addition to shears, a deformed crystal undergoes powerful plastic twists. That is, the single initial orientation of the single crystal is replaced by regions of misorientation angles, i.e., the crystal is broken into separate fragments turned relative to each other. This phenomenon is known as asterism [7] and was observed by many researchers, and the amount of crystallographic rotation at large deformations reached 10–20°.

An important factor in the analysis of plastic deformation processes is the dissipation of elastic energy. It was established that the movement of a planar cluster of dislocations in the stress concentrator field is not accompanied by significant dissipation of elastic energy [9], but only redistributes the stress concentrator field in the crystal without significantly reducing the total energy of the loaded crystal.

Effective dissipation of the elastic energy of a loaded crystal without breaking its integrity is possible in several ways: by the action of multiple sliding on five systems; sliding along a limited number of systems (in the limit of one) with the corresponding rotation of the structural elements of the deformation; due to the formation of twins or martensite deformation. Therefore, it is obviously advisable to analyze the degree of relaxation of elastic stresses during the plastic flow of the crystal and, accordingly, the dissipation of the energy injected into the loaded crystal. Depending on the type of lattice, the structure of the material and the load conditions, the system will choose the path that provides the maximum degree of dissipation of elastic energy.

Studies show [9] that if in a deformed system rotations of the structural elements of the deformation as a whole are possible, then the system chooses a deformation mechanism associated not with multiple sliding, but with a limited number of its systems plus rotation. The latter path more effectively dissipates the energy of the deformed material than multiple slip. This is consistent with the general statement [4] about the most effective energy dissipation channel – the turbulent (eddy) nature of motion. Therefore, in the general case, the presence in a plastically deformed crystal of rotating modes and the vortex character of fluidity is always predominant. The ratio between translational and rotational modes of deformation depends on the type of crystal and the conditions of its deformation.

A deformed crystal is a typical non-equilibrium system that moves further away from equilibrium as plastic deformation progresses. The theory of behaviour of such systems is considered in [4], where it is shown that outside the region of stability of the thermodynamic branch (corresponding to equilibrium conditions) in the system, a new type of organization can arise with the formation of radically new structures, fundamentally different from the equilibrium ones predicted by classical thermodynamics. Such structures are known as *dissipative* structures. Their appearance reflects the efforts of an unbalanced system to order, but not according to the Boltzmann principle, but due to fluctuations that are stabilized due to the exchange of energy with the external environment.

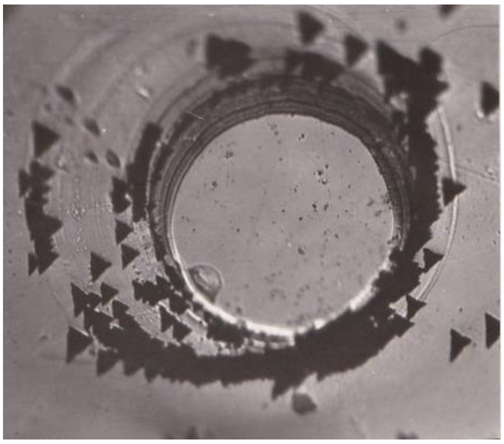

Fig. 2. Local deformation regions of the crystal by torsion with concentric slip lines of dislocations revealed by selective etching.

In a deformed crystal, the accumulation of deformation defects causes "Benard instability" (analogous to the Benard cell in a heated liquid), the formation of new dissipative structures and the transition from deformation by the movement of individual elementary defects to the macroscopic movement of new structural elements.

New types of dissipative structures were observed in deformed $Cd_xHg_{1-x}Te$ crystals after their selective dislocation etching. In particular, after a small residual deformation (at the "tooth" of yield strength $\varepsilon \approx 2-2.5\,\%$), macrodefects of a spherical type with concentric slip lines of dislocations and etching pits were detected (fig. 2). Observation of selective set of paintings with such defects shows that they are placed randomly and do not overlap with each other.

The general appearance of such formations indicates that plastic deformation of the lattice takes place around a certain spherical region of the crystal by "twisting" it around an axis perpendicular to the crystal plane, with circular generation of dislocations. Systematic studies of patterns of selective etching show that in the case of existing microuniformities of the type of inclusion of another phase, which generates local stresses, or after the creation of local stresses by the method of microidentification, dislocation patterns are created around such stress concentrators, which correspond to lattice (plane) symmetry, but are far from spherical forms Therefore, the identified structural complexes should be interpreted as system of local stress relaxers, which under conditions of external load through rotational components ensure effective dissipation of elastic energy in the deformed crystal.

Starting from the debris layer and at the stages of deformation ($\varepsilon \approx 0.45-1.5\%$), along with traditional dislocation slip lines, there is also fragmentation of the dislocation structure in the form of cells of a regular geometric shape bordering each other by dislocation boundaries (fig. 3). Similar cellular dislocation structure was observed in uniaxially deformed Si crystals and locally deformed $NaCl$ crystals [1], as means of relaxation of mechanical stresses near their concentrators. It is obvious that the formation of specific dislocation structure is the result of the evolution of synergistic structure with the aim of minimizing the energy of interacting structural-deformation elements and effective elastic energy dissipation.

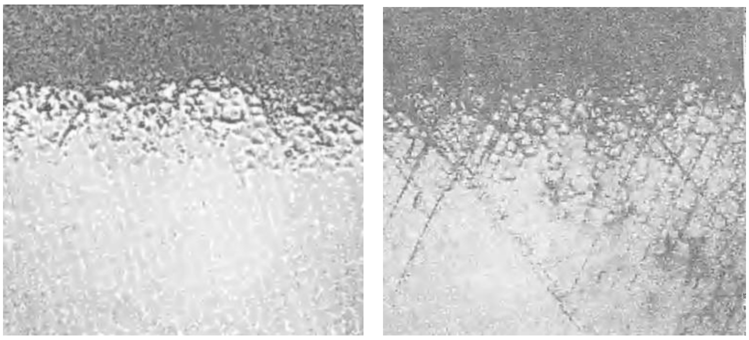
a) b)

Fig. 3. An example of the cellular structure of the $Cd_{0.2}Hg_{0.8}Te$ crystal after its plastic deformation at: a - $\varepsilon \sim 0.45\,\%$, b - $\varepsilon \sim 4.5\,\%$ ($\times 800$).

Dislocation fragments are strongly disoriented in the process of plastic deformation of microregions with transverse dimensions of $0.2-0.3\,\mu m$. Fragments are deformed homogeneously, there are no dislocation formations such as clusters or inhibited shear bands inside them. There are no microprotrusions and other morphological features on the borders of the fragments, which indicate a non-uniform flow of plastic deformation in them. Since the characteristic disorientation between the fragments is a few degrees, the interfragment boundaries are intergranular type boundaries. Therefore, significant uncompensated densities of dislocations are distributed in these areas, and joint disclinations are located in the joints, so they are a source of significant stresses. When stresses equal to $(1/70-1/90)G$ (shear modulus - G) are reached, the appearance of cracks that can reach characteristic sizes of $100\,\dot{A}$ is likely.

The study of the phenomenon of fragmentation made it possible to establish that its root cause is powerful elastic stresses, the sources of which arise at intergrain boundaries and their joints. In fact, fragmentation is the result of plastic accommodation, the inhomogeneity of which is in the volume of the grain and manifests itself in the form of a fragmented substructure. It is near the junctions of subboundaries or morphological features of the original ones (ribbons, protrusions, folds) that the nucleation of new boundaries is observed, which grow inside the grains and divide them into disoriented crystalline elements. The driving force of this process is internal stresses, and their sources (plastic incompatibilities) accumulate at the boundaries due to the difference in their own plastic deformations of adjacent grains. Their appearance is inevitable, since crystalline grains are differently oriented relative to macroscopic deformation stresses and therefore exhibit different plastic ductility. However, as the misorientations between the resulting fragments grow, the process described above is reproduced already at their borders and junctions, forming a new generation of fragments, etc.

The uniform orientation of the lattice inside the structural elements is unstable in relation to plastic deformation, and the fragmentation process is infinite (continuous). An important role in the fragmentation process of the crystal lattice during the submicrocrystalline structure formation of is played by the dislocation-disclination mechanism of reorientation of the crystal lattice, which involves the formation of the above-mentioned substructures with a high excess density of dislocations of the same sign and their subsequent rearrangements into localized misorientation boundaries. Thus, a fragmented substructure is a structure of mutually disorientated regions (subgrains), separated by small-angle and medium-angle subboundaries (fragment walls).

In general, in the process of deformation during the evolution of the dislocation substructure, the main chain of structural transformations in the dislocation ensemble is as follows: disordering, structural meshes of the cell, anisotropic fragments, isotropic fragments. An increase in the total degree of deformation is accompanied by the development of the fragmentation process, and the volume fraction of the fragmented substructure increases in proportion to the true deformation. This process is caused by relaxation of long-range stress fields and self-organization of the dislocation substructure.

Therefore, a uniaxially deformed crystal at this stage (3) can be modelled as a complex structure, which includes: 1) a “debris” layer formed at the previous pseudo-elastic stage of deformation in the near-surface regions of the crystal (1) and interfacially interacting with the volume crystal; 2) locally fragmented cells within the volume of the crystal (2), disoriented relative to each other at certain angles and having different Young's moduli $E_1 ... E_n$ (fig. 4).

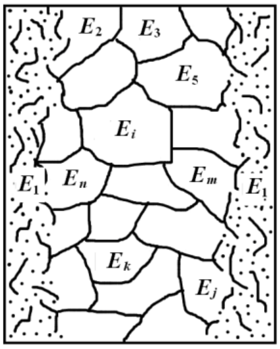

Fig. 4. Volume-local fragmentation scheme of deformed crystal with regions possessing distinct Young's module.

Therefore, the behaviour of the load diagram will be determined by the interphase interaction of two types: 1) between the "debris" layer, which has the highest Young's modulus, and the volume of the deformed crystal; 2) directly between the local cells of the fragmented structure in the volume of the crystal. Quantitative assessment of energy parameters of such interaction, which determine the degree of elastic interaction at the boundaries of such fragments, was carried out in [5].

The analysis of the plastic deformation of crystals based on ideas about dissipative structures allows us to understand some features of the macrofluidity of solid bodies that do not find justification in the mechanics of a deformed solid body and exclusively in the dislocation concept of deformation.

In this regard, we will discuss the mechanism of self-organization processes at the macro level in a fragmented crystal. The presence in it of adjacent grains (regions) with different crystallographic orientation, the emergence of new structural elements separated by dislocation sub-boundaries, leads to a specific phenomenon - interphase interaction of bounded regions. This type of interaction occurs, as is known, between heterogeneous volumes, as well as within the same solid body between regions with different mechanical compatibility, that is, which have different Young's moduli E and are separated by a structural boundary [6]. Quantitatively, the intensity of such an interaction is estimated by two main parameters: the interfacial interaction energy γ_m and the interfacial tension σ_m. The basis of the theory is a macroscopic approach, which is based on the relations of non-equilibrium thermodynamics and surface physics, which characterize the thermodynamic state of the contacting system.

For the model in which the interfacial layer consists of two parts, the interfacial energy γ_m and the interfacial tension σ_m at the interface of the bounded regions are determined from the relations:

$$\sigma_m = \int_{-H}^{H} \sigma_y dx\,;\ \sigma_y = \sigma_z\,; \gamma_m = \gamma_e + \xi_m \gamma_s\,;\ \gamma_e = \int_{-H}^{H} w_e dx\,;\ \gamma_s = \int_{-H}^{H} w_s dx\,.$$

where $x = 0$ corresponds to the interface; σ_y, σ_z is normal mechanical stresses in direction to y and z planes, respectively (MPa); γ_e, γ_s – electrical and mechanical components of interphase energy (J/m^2); w_e, w_s are specific electrical and mechanical components of interphase energy; E, ν – Young's modulus and Poisson's ratio of material interfacial layer; Ψ is electrostatic potential (electric field potential in the interphase layer); ξ_m – physical characteristic of the interphase layer; $2H$ - effective thickness of interphase layer.

In detail, the method of estimating interfacial energy γ_m and interfacial tension σ_m and their numerical values for a number of practically important contacting pairs are given in [10]. Evaluation of the interfacial interaction parameters under this method in deformed $Cd_xHg_{1-x}Te$ crystals revealed that when Young's module of bounded regions change due to crystallographic disorientation to the value $E/E_0 = 1.5$, the energy of the interfacial interaction undergoes change up to $2-3\,\%$, and the value of the interfacial tension up to $15\,\%$. For samples close in composition to $CdTe$, this parameter can reach $20\,\%$. As can be seen, the most sensitive parameter to modular changes, which determines the stress state on interfacial surfaces, is interfacial tension. Therefore, without reducing the generality, it can be stated that the process of strain hardening is not only the result of the multiplication and interaction of dislocations generated in the process of plastic yielding, but also a certain contribution of interphase interaction between deformation fragments.

Mechanisms of self-organization of deformed crystals at the micro levels.

Let us consider the transformation of electroactive defects in the near-surface layers of micro- and macroplastically deformed $HgTe-CdTe$ single crystals.

Since the intensity of generation of electroactive defects at all structural levels of crystal deformation is different, in order to establish their mechanisms, it is advisable to monitor synchronous changes in the electrophysical parameters of the deformed crystal at all its stages. This makes it possible to use an independent method to register transitions between structural levels caused by changes in the mechanisms of elastic energy dissipation in the deformation process. Since the newly introduced dislocations are blocked by impurity atmospheres in almost a few minutes or less, it is reasonable to assume that the fixed changes in the Hall coefficient R_H and the specific electrical conductivity $\sigma_0 = f(\varepsilon)$ are to a certain extent caused by "pure" dislocations generated in the crystal at the stages of micro- and macrofluidity.

The most interesting behavior of the parameters R_H, σ_0 with deformation is demonstrated by samples of $Cd_{0.2}Hg_{0.8}Te$ with an initial carrier concentration close to its own ($n \approx p$, $T = 77K$). In fig. 5 shows the results of synchronous measurements of R_H, σ_0 in the process of uniaxial deformation at a constant speed of such samples. Measurements of R_H were carried out according to the standard method in constant magnetic field with induction of $0.8\,T$. Synchronous measurements of σ_0 - direct current measured with four-probe technique.

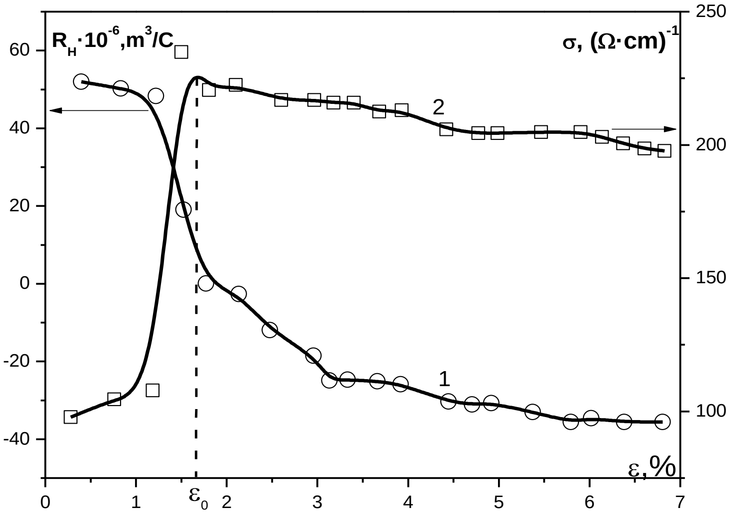

Fig. 5. $Cd_{0.2}Hg_{0.2}Te_{0.8}$ ($p = n$) crystal hall coefficient R_H (1) and electrical conductivity σ (2) us uniaxial deformation at $T = 300K$.

It is believed that such samples are the most structurally perfect, as they have the minimum concentration of donor and acceptor centers. Therefore, from the point of view of the conducted research, this is the most "pure" experiment. As can be seen, the achievement of the critical deformation ε0, that is, the formation of a yield tooth, is achieved in such samples at ($\varepsilon_0 \approx 1.2\,\%$), since in this case there are more favorable conditions for the formation of a "debris" layer. Deformation of such a crystal at the stage of microplasticity (up to ε_0) is accompanied by slight changes in R_H , σ_0 (fig. 5). However, particularly exotic changes of the investigated parameters are observed after reaching the yield point: the Hall coefficient abruptly changes its sign from negative to positive and subsequently changes weakly with deformation, maintaining a positive sign. The electrical conductivity of the deformed crystal, starting from ε_0 , rapidly decreases according to a two-stage dependence, reaching saturation at a deformation of about $6\,\%$. Moreover, its relative change within the limits of deformation in region 1.2 to $6\,\%$ is abnormally large up in 4.5 times.

Thus, the change in the sign of the Hall coefficient R_H at ε_0 indicates structural rearrangements caused, most likely, by a change in the mechanisms of elastic energy dissipation in the deformation process.

Thus, the change in the sign of the Hall coefficient at ε_0 indicates structural rearrangements caused, most likely, by change in the elastic energy dissipation mechanisms at deformation process.

Deformation above ε_0 leads to decrease of Hall coefficient due to the further increase in the concentration of acceptors - the situation is similar to $p-type$ crystals and the original inverted $n-type$ samples. However, the electrical conductivity in this case does not increase, but decreases, since its value is determined, as in the original sample, by conduction electrons that have higher mobility than holes. The concentration of such electrons decreases with sample deformation due to their localization on freshly introduced acceptors.

Self-organization in the "dislocation - point defect" system is realized by the formation of stable impurity atmospheres around freshly introduced dislocations. This process significantly depends on the type of impurity and the temperature of the process. Taking into account the drift flow of impurity to the dislocation and the diffusion flow as a result of the concentration gradient, it is quantitatively described by the equation [11]:

$$\frac{N(t)}{N(\infty)}=1-\frac{4}{\pi}\int_0^\infty \frac{e^{-mx^2}}{x^2}\,\frac{\left\{\left(H_2(x)-J_2(x)-\left(\frac{2}{(\pi x)}\right)\right)\left(1+\frac{1}{3}x^2\right)\right\}}{J_2(x)+y_2^2(x)}dx,$$

where $J_2(x)$ is the Bessel function of the real argument; $H_2(x)$ is the Struve function, and $m=D(\tau)t/r_c^2$

The kinetics of the total concentration change in the impurity cloud is determined by:

$$c(t)=c_0+N(t)/(\pi r_c^2)$$

where r_c^2 is the radius of the dislocation core.

For example, fig. 6 shows the dependence of Cu atoms concentration around the dislocation vs time and temperature.

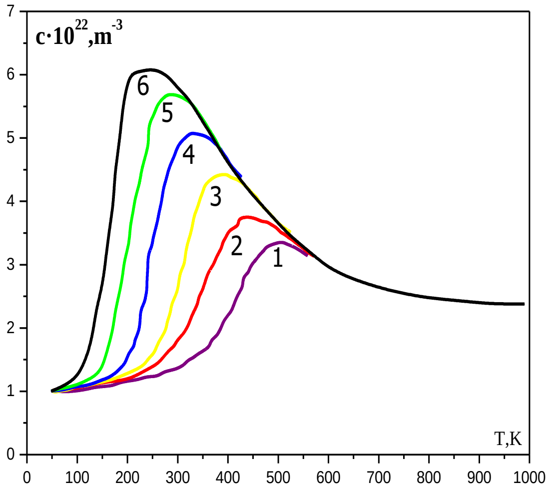

Fig. 6. Temperature dependence of copper atoms concentration c in process dislocation blocking and creating an impurity atmosphere:
$1-10^{-3}$ sec, $2-10^{-2}$ sec, $3-10^{-1}$ sec, $4-1$ sec, $5-10$ sec, $6-10^{2}$ sec

As can be seen, at high temperatures, the start and end of the blocking process occurs faster than at lower temperatures, and the steady-state concentration of defects in this temperature range is smaller. Dislocation blocking by copper atoms occurs at room temperature in $10-100\,\text{sec}$. Impurity atmospheres made of Au, Ag and In atoms are formed in much longer periods of time: $10^5-10^6\,\text{sec}$. Such significant difference in blocking time is explained by the higher diffusion coefficient of Cu atoms in $Cd_xHg_{1-x}Te$ crystals compared to the similar parameter of the analyzed impurities.

The described blocking processes of newly introduced dislocations by point defects after crystal deformation are accompanied with an increase in its thermodynamic stability and generally leads to decrease in its configurational entropy.

Conclusion.

1. Deformation of $Cd_xHg_{1-x}Te$ crystals, along with translational dislocation slip, is accompanied by rotational component of lattice deformation and the emergence of new structural deformation elements that take part in the deformation process as independent.
2. New types of dissipative structures were found in investigated $Cd_xHg_{1-x}Te$ crystals: a) spherical regions with dislocation slip lines in the form of concentric circles and dislocations decorated on certain segments of them, which indicates local plastic deformation of the lattice by twisting around an axis perpendicular to the crystal plane; b) fragmented dislocation structures in cells form of regular geometric shape bordering each other by means of dislocation boundaries.
3. The mechanism of fragmentation of deformed crystal is powerful elastic stresses, the sources of which arise at intergrain boundaries and their joints. In essence, fragmentation is the result of plastic accommodation, the inhomogeneity of which in the volume of the grain manifests itself in the form of a fragmented understructure.
4. The change in the sign of Hall coefficient R_H in the process of deformation at ε_0 indicates structural rearrangements caused, most likely, by change in the mechanisms of elastic energy dissipation at deformation process.
5. Self-organization in the "dislocation - point defect" system is realized by formation of stable impurity atmospheres around newly introduced dislocations.

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ТРАНСФОРМАЦІЯ СТРУКТУРИ ТА ПРОЦЕСИ САМООРГАНІЗАЦІЇ В ДЕФОРМОВАНИХ КРИСТАЛАХ

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У роботі досліджено закономірності процесів самоорганізації в деформованих напівпровідникових кристалах твердих розчинів HgTe-CdTe. Стверджується, що кристал у процесі деформації слід розглядати як відкриту нерівноважну термодинамічну систему, яка еволюціонує не тільки для збереження своєї цілісності, але й для створення нових типів структур (дефектів), здатних більш ефективно розсіювати підведену енергію. Результатом є утворення в кристалі синергетичної структури з мінімальною ентропією. Відкрито нові типи дисипативних структур. Проаналізовано механізми ефективної дисипації пружної енергії. Закономірності релаксаційних процесів у деформованих кристалах на різних етапах кривої деформації $\sigma-\varepsilon$. На основі електрофізичних досліджень проаналізовано трансформацію електроактивних дефектів у приповерхневих шарах мікро- та макропластично деформованих монокристалів $HgTe-CdTe$. Самоорганізація в системі «дислокація - точковий дефект» реалізується шляхом утворення стабільних домішкових атмосфер навколо свіжовведених дислокацій. Цей процес істотно залежить від типу домішок і температури процесу.

Поява нових дислокації у структурі кристалу є термодинамічно незбалансованими дефектами кристалічної решітки, які призводять до значної структурно-динамічної трансформації дефектної підсистеми. Також, виявлено бездислокаційні механізми пластичної деформації кристалів з дефектними структурами нового типу. Багатоступеневі криві деформації та фрагментація макроструктури деформованого кристала свідчать не лише про значну трансформацію дефектної структури, а й про складні механізми розсіювання енергії. Свідченням є унікальні макродефекти у напружених кристалах, які виникають внаслідок процесів самоорганізації дефектної підсистеми під час динамічного навантаження. Пошук відповіді на питання про рушійні сили таких процесів та механізми їх реалізації носить фундаментальних характер. Напружений кристал слід розглядати як відкриту термодинамічну систему, яка дисипує ефективну енергію розсіювання процесу деформації, що створює дефектна структура. Ця енергія постійно надходить в об'єкт через відкриті канали.

В роботі встановлено закономірності процесів самоорганізації та механізмів релаксації енергії на макро- та мікрорівнях у пружно-пластично деформованих кристалах $Cd_xHg_{1-x}Te$ ($x = 0 - 0.18$) з різною структурою дефектів.

Ключові слова: напівпровідникові кристали $HgTe - CdTe$, структурні дефекти при деформації, пружна енергія деформації.

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