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Peculiarities of Mechanical Properties and Self-Organization Processes in Deformed Crystals of CdTe–HgTe Alloys

B. P. Koman, R. I. Bihun, V. M. Yuzevych*, and D. S. Leonov**

*Ivan Franko National University of Lviv,
1 Universytets'ka Str.,
UA-79000 Lviv, Ukraine*

**G. V. Karpenko Physico-Mechanical Institute, N.A.S. of Ukraine,
5 Naukova Str.,
UA-79060 Lviv, Ukraine*

***Technical Centre, N.A.S. of Ukraine,
13 Pokrovs'ka Str.,
UA-04070 Kyiv, Ukraine*

Under complex approach by means of simultaneous measurements (during the deformation) of stress–strain diagrams (τ – ε), the Hall coefficient R_H , electrical conductivity σ , temperature dependences of microhardness $H_v(T)$ and quantitative analysis of interfacial interactions (energy of interfacial interaction γ_m and interfacial tension σ_m), the peculiarities of the mechanical properties in $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ solid-solution crystals ($x = 0$ – 0.26) with metal and semi-conductor properties are studied. The special role of point defects and the influence of band structure on the behaviour of mobile dislocations are established. As found, in the process of strain hardening, a significant contribution is made by the interphase interaction between neighbouring structural fragments inherent in the semi-metallic crystal as well as induced in the process of deformation. From the point of view of non-equilibrium thermodynamics, energy parameters of interphase interaction in a fragmented crystal are estimated and a mechanism of self-organization is proposed. The peculiarities of near-surface layers and their role in formation of the elastic–plastic state of the investigated crystals are analysed. As claimed, the crystal under process of deformation should be considered as an open non-

Corresponding author: Bohdan Petrovych Koman
E-mail: koman.bohdan@lnu.edu.ua

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equilibrium thermodynamic system that evolves to minimum entropy not only to preserve its integrity, but also to create new types of structures (defects) capable of more effectively dissipating the added energy.

Key words: deformed crystals, Hall coefficient, microhardness, Young's modulus, interfacial interaction, interfacial tension.

Із застосуванням комплексного підходу, — синхронних мірянь у процесі деформації діаграм напруження–деформація (τ – ε), Голлового коефіцієнта R_H , електропровідності σ , температурних залежностей мікротвердості $H_v(T)$ і кількісної аналізи міжфазових взаємодій (енергії міжфазової взаємодії γ_m і міжфазового натягу σ_m), — досліджено особливості механічних властивостей кристалів твердих розчинів $Cd_xHg_{1-x}Te$ ($x = 0-0,26$). Встановлено особливу роль точкових дефектів і вплив зонної структури на поведінку рухомих дислокацій. Виявлено, що у процесі деформаційного зміцнення істотний внесок вносить міжфазова взаємодія між сусідніми структурними фрагментами, властивими кристалу, а також індукованими у процесі деформації. З позицій нерівноважної термодинаміки проведено оцінки енергетичних параметрів міжфазової взаємодії у фрагментованому кристалі та запропоновано механізм самоорганізації. Проаналізовано особливості приповерхневих шарів та їхню роль у формуванні пружньо-пластичного стану досліджуваних кристалів. Стверджується, що кристал у процесі деформації слід розглядати як відкриту нерівноважну термодинамічну систему, яка еволюціонує до мінімальної ентропії не лише для збереження своєї цілісності, але й з метою створення нових типів структур (дефектів), здатних більш ефективно розсіювати підведену енергію.

Ключові слова: деформовані кристали, Голлів коефіцієнт, мікротвердість, модуль Юнга, міжфазна взаємодія, міжфазний натяг.

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1. INTRODUCTION

The long-term history of the plastic deformation study in crystals indicates the relaxation nature of internal processes under the action of mechanical stresses. The multifaceted nature of structural states inherent in deformed materials testifies to the complex nature of deformation defect formation and the non-trivial nature of dissipation of the energy supplied to the crystal. Therefore, the logical consequence of this situation is the absence of the universal and simple mechanism for the deformation of solid bodies at the moment. In this aspect, increasing the range of research on unique objects contributes to the deepening of the understanding of existing and the formation of new ideas about the mechanisms of deformation of solid bodies.

Single crystals of HgTe–CdTe solid solutions occupy intermediate position between metals and classical semiconductors in terms of physical number and mechanical parameters were studied. With small com-

position of CdTe ($x = 0.11-0.16$), according to their electrical characteristics, these crystals show semi-metallic properties. These materials are characterized by high brittleness at room temperature, which brings them closer to purely covalent semiconductors. However, on the other hand, there are large densities of 'forest' dislocations ($10^5-10^6 \text{ cm}^{-2}$), a high concentration of point defects, mainly mercury vacancies, reaching electron concentration values of $10^{19}-10^{20} \text{ cm}^{-3}$ within the homogeneity region, mixed ionic-covalent character of the chemical bonds with the predominance of ionic component ($\cong 60\%$)—factors that bring such materials closer to metals. Let us note that the concentration of vacancies in Ge, even close to the melting temperature, is only 10^{15} cm^{-3} . Moreover, the analysis of a number of conducted studies on the deformation behaviour of mixed crystals shows that they are characterized by some contradictory properties that are not characteristic of typical semiconductors but of metals. In combination with low values of Peierls barriers, the studied crystals show a relatively high fragility characteristic of classical semiconductors. On the other hand, there is a high sensitivity of the yield point to the rate of deformation; a significant dependence of their mechanical parameters on temperature brings these crystals closer to metals. Such behaviour cannot be explained within the framework of the traditional mechanism of thermally activated dislocation motion. The multistage deformation curves and the revealed fragmentation of the macrostructure of the deformed crystal indicate not only a significant transformation of the defective structure, but also complex mechanisms of energy dissipation. 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 [1]. Thus, along with microdeformation (moving dislocations), macroplastic fluidity takes place, in which three-dimensional structural elements take part. Such features of the structure are caused by self-organizing processes at the micro- and macrolevels, which correspond to different mechanisms of energy dissipation in the loaded crystal at different stages of its deformation [2]. That is, with a complete description of the mechanisms of crystal deformation, the problem should be solved only taking into account the hierarchy of structural levels of deformation. Therefore, it is important to find out the mechanisms of self-organizing processes at the macro- and microlevels at different stages of strain hardening during uniaxial deformation.

Despite such 'exotic' objects and their important practical application, data on the patterns of dislocation movement and mechanisms of plastic flow are fragmentary. The role of other non-dislocation mechanisms of plastic flow has also not been established. Therefore, the study of the patterns of microdeformation of these crystals is an urgent practical and fundamental task.

The aim of the work was to establish in elastic-plastically deformed crystals of $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ solid solutions ($x = 0-0.26$) at the macro- and microstructural levels of deformation, the laws of energy relaxation and their plastic deformation, taking into account the zone structure, features of point defects and the role of interphase interactions and self-organizing processes.

2. EXPERIMENTAL METHOD

Crystals grown by the Bridgman method and solid-state recrystallization were used. The regularities of microplastic deformation of crystals of HgTe-CdTe solid solutions were studied using uniaxial compression methods on a Regel-Dubov relaxometer in the temperature range of 77–450 K. Measurements at temperatures below room temperature were carried out in a special vacuum cryostat. The dimensions of non-oriented samples were of 3 mm. 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 the process of uniaxial deformation of the load curve ‘stress–strain’ ($\tau-\varepsilon$). In the process of deformation, the sample was placed in a self-centring quartz punch.

The measurement of the Hall coefficient R_H during deformation was carried out according to the standard method in a constant magnetic field with an induction of 0.8 T. The Hall magnetic field was created by an electromagnet (NS) with the direction of the induction lines perpendicular to the axis of deformation. Synchronous measurements of specific electrical conductivity σ were at direct current using the four-probe method using a point pair of contacts. The potential difference was recorded with digital voltmeter.

3. RESULTS AND DISCUSSION

3.1. Analysis of Microplastic Deformation Dislocation Mechanisms in $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ Crystals

The traditional description of plastic deformation mechanisms in crystals is based, on the dislocation mechanisms of nucleation and propagation of dislocations. In this regard, we will consider the patterns of microplastic deformation of crystals of HgTe-CdTe solid solutions.

The primary task of the research was to study the influence of various factors on the parameters of the strain hardening curves ‘stress τ –strain ε ’. It was established: 1) the dependences $\tau-\varepsilon$ are described by a typical four-stage shape of the load curve with a characteristic yield ‘tooth’, first proposed for f.c.c. metals, 2) uniaxial compression of

$\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ samples along different crystallographic directions does not reveal significant differences in the parameters of the strain hardening curves. This fact follows logically from the geometry of dislocation movement in the sphalerite structure [3], 3) the stoichiometry of the crystals significantly affects the process of strain hardening and, accordingly, the parameters of the σ - ε curves, 4) strain hardening curves show great sensitivity to loading speed (Fig. 1).

In particular, as can be seen, deformation at extremely low ($1.46 \cdot 10^{-3}$ mm/min) and high ($2.34 \cdot 10^{-2}$ mm/min) velocities is not accompanied by the detection of characteristic fluidity 'tooth', the nature of which in these crystals is described in [4].

An increase in the loading rate in the studied interval leads to an increase in the yield strength of the crystal and a decrease in the length of the easy sliding stage. It was established that the value of the maximum deformation for the minimum speed was 21%, and for the maximum—1.6%. The yield strength increases from 2.85 to 7.15 kHz/mm² as the rate of deformation increases.

For the investigated crystals, it was established that the activation energy of the dislocation movement lies within the range 0.14–0.41 eV, and the activation volume value is $(11-22)b^3$ (where b —Burgers vector) [5]. According to [6], the given values of the activation parameters of dislocation movement correspond to the Peierls mechanism of displacement and propagation of dislocations.

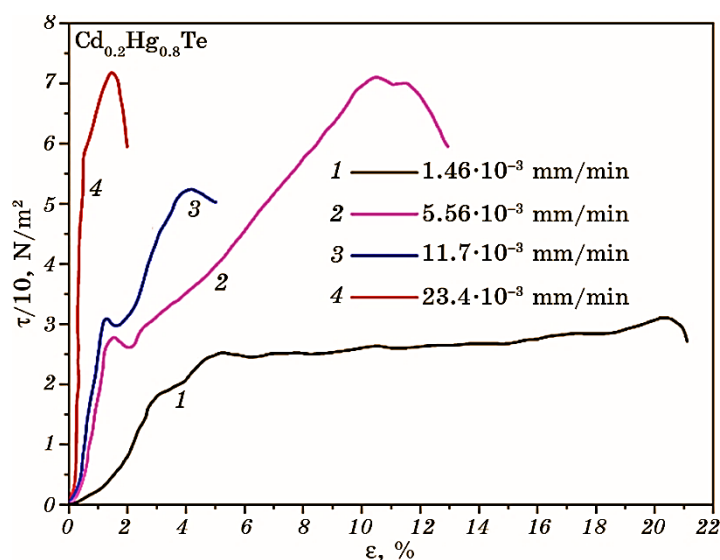


Fig. 1. Strain hardening curves ($T = 293$ K) of $\text{Cd}_{0.2}\text{Hg}_{0.8}\text{Te}$ crystals at different loading rates (mm/min): 1— $1.46 \cdot 10^{-3}$, 2— $5.56 \cdot 10^{-3}$, 3— $11.7 \cdot 10^{-3}$, 4— $23.4 \cdot 10^{-3}$.

Considering the non-stoichiometric nature of the investigated crystals, the special role of stoichiometry defects in the processes of retardation and propagation of dislocations must be taken into account when analysing the mechanisms of plastic deformation. An increase in the concentration of vacancies is accompanied by a natural decrease in the activation volume and a slight increase in the activation energy. This behaviour can be explained within the framework of the mechanism of inhibition of mobile dislocations by local obstacles caused by mercury vacancies. That is, in $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ crystals, within the framework of the main mechanism of displacement of dislocations (Peierls mechanism), [Hg] vacancies are the dominant defects affecting the kinetics of movement and propagation of double kinks. However, the role of point defects (mercury vacancies) in the investigated crystals is not limited to the elastic interaction of mobile dislocations with such imperfections. Obviously, one should expect certain features in such an interaction, which are caused by the features of the zone structure of crystals. In particular, in narrow-band crystals $p\text{-Cd}_x\text{Hg}_{1-x}\text{Te}$ ($E_g \cong 0.1\text{--}0.2\text{ eV}$), stoichiometric defects create acceptor levels in the band gap near the ceiling of the valence band. In this regard, relatively small changes in temperature lead to local centres recharging with corresponding levels in the forbidden zone. Thus, within the limits of the main deformation mechanism that controls the behaviour of dislocations, a change in crystal temperature is accompanied, along with a change in the electrical conductivity mechanism, by a change in the alternative mechanism of interaction of mobile dislocations with point defects of the crystal lattice. Thus, it can be asserted that, in addition to the described factors, the equilibrium state of the electronic subsystem of the crystal has a significant influence on the behaviour of dislocations.

For this purpose, the thermally activated sliding of dislocations in a wide temperature range was studied synchronously with the state control of the electronic subsystem. In particular, we studied the behaviour of the yield strength τ_0 with temperature for a series of crystals of the same type $p\text{-Cd}_{0.2}\text{Hg}_{0.8}\text{Te}$ (Fig. 2).

To identify the state of the electronic subsystem, the figure also shows the temperature dependence of the Hall coefficient of a typical sample from this series of crystals used in deformation experiments. As can be seen, in the area of impurity conductivity of the crystal (conductivity is carried out by 'impurity' acceptors: vacancies of mercury, cadmium or their complexes), τ_0 rapidly decreases with an activation energy of $\cong 0.04\text{ eV}$. In this temperature range, a significant concentration of acceptors is in an electroneutral state, and only a small amount of them is ionized. As the temperature increases, the number of electrons localized at the acceptor level increases. Conduction in this interval is carried out by impurity holes, as well as by own electrons. The yield strength of crystals in this region varies relatively little with temperature.

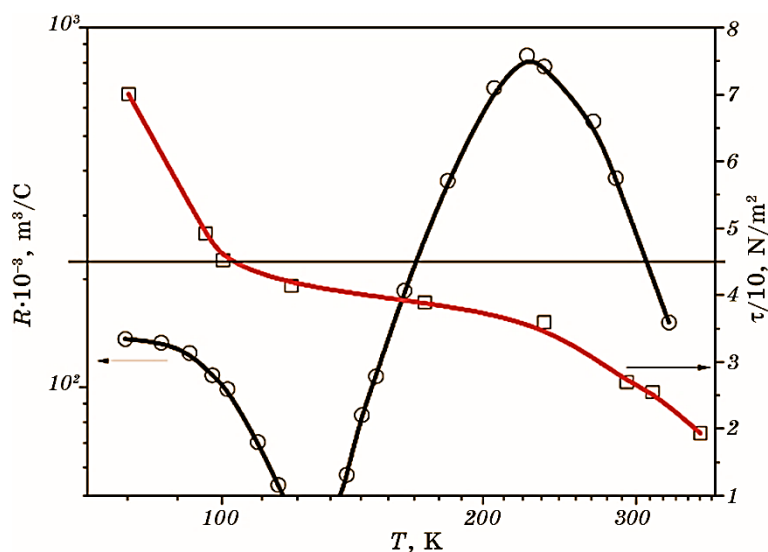


Fig. 2. Temperature dependence of yield strength τ and Hall coefficient R_H of p - $\text{Cd}_{0.2}\text{Hg}_{0.8}\text{Te}$ crystal.

A further increase in temperature transfers the crystal to the region of its own conductivity, within which electrical conductivity is carried out by its own electrons and holes formed as a result of 'zone-zone' thermal excitations. All acceptor states here are ionized. The yield strength in this region decreases with an increase in temperature with an activation energy of 0.3 eV. Such dependencies are typical for semiconductor crystals. Characteristic values of the activation parameters of dislocation movement for each analysed region are given in Table 1.

It can be seen that the general trend in the heat-activated movement

TABLE 1. Characteristic values of the activation parameters of dislocation movement for each analysed region.

Sample	Area of electrical conductivity	Activation energy, eV	Activation volume,	Energy position of the acceptor level, eV
$\text{Cd}_{0.3}\text{Hg}_{0.7}\text{Te}$, $p_{77} = 4 \cdot 10^{16} \text{ cm}^{-3}$	Own: 350–430 K	0.32	11	0.085
	Mixed: 180–290 K	0.07	3	
	Impurity: 77–180 K	0.04	0.4	
$\text{Cd}_{0.2}\text{Hg}_{0.8}\text{Te}$, $p_{77} = 10^{17} \text{ cm}^{-3}$	Own: 210–400 K	0.3	10	0.028
	Mixed: 100–210 K	0.08	2	
	Impurity: 77–100 K	0.04	0.3	

of dislocations during the transition of crystals from the impurity region of conductivity to their own is an increase in the activation volume and activation energy of mobile dislocations.

Thus, taking into account the behaviour of the activation parameters in the studied crystals, the thermally activated movement of dislocations in $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ can be considered as an overlap of the mechanisms of conservative movement of dislocations and pure slip. The growth of the activation volume during the transition from the impurity region to its own indicates the growth of the contribution of pure slip over creep in the general mechanism of dislocation movement. The last mechanism is quite complex and requires several types of defects and two types of atoms to implement. As can be seen, the atomic structure of the studied crystals is quite favourable for such a mechanism. Extensive studies of the processes of conservative movement of dislocations have shown that dislocation creep is facilitated in materials saturated with point defects [7]. This situation is typical for crystals of $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ solid solutions.

In the light of the outlined concept of the influence of the state of the electronic subsystem on the behaviour of dislocations, a convincing and vivid example is the results of studies of the temperature dependence of $H_v(T)$ of the investigated crystals with different band gap width E_g and spectrum of point defects. Microhardness was measured according to the standard method using the ПИМТ-3 device. In Figure 3, the following dependences for p -type ($x \cong 0.19$, $E_g \cong 0.1$ eV) and n -type ($x \cong 0.26$, $E_g \cong 0.15$ eV) compositions are shown.

The peculiarity of these experiments is that the behaviour of dislocations in the entire temperature range is followed on one sample, which is characterized by a certain type of point defects inherent only to this crystal. As follows from the given results, all the above-described regularities of the influence of the electronic subsystem on the behaviour of the yield strength with temperature are clearly fulfilled also for microhardness. In particular, the dependence of $\tau(T)$ (Fig. 3) has three characteristic sections: in the first section (77–133 K, the region of impurity conductivity), τ decreases sharply with increasing temperature, reaching at the border of the section a value almost equal to the corresponding value at room temperature. The second region (133–293 K, region of mixed conductivity) is characterized by an almost athermal dependence of $\tau(T)$. The plastic flow of the crystal in this region is insignificant. The third section (293–450 K, the region of intrinsic conductivity) is characterized by a rapid increase in the plasticity of the sample with increasing temperature. It is important that the activation parameters of dislocations in the described experiments lie within the limits of the values given above for uniaxial tests, which indicates the adequacy of the above-discussed interpretation of the behaviour of dislocations in intrinsically defective CdHgTe crystals.

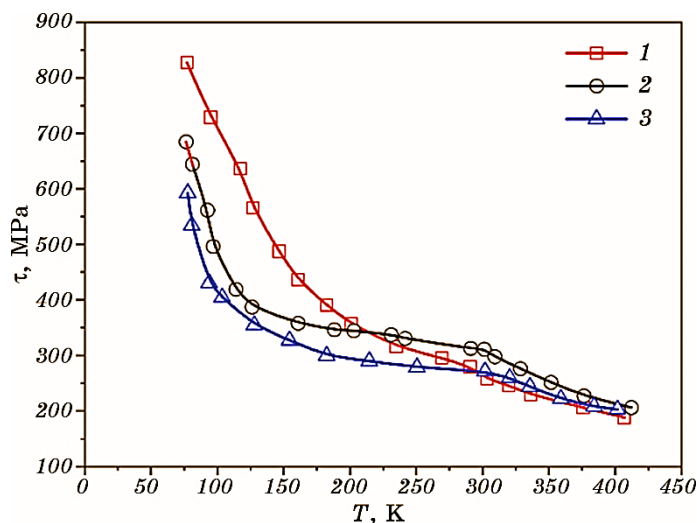


Fig. 3. Temperature dependence of the microhardness of p - $\text{Cd}_{0.19}\text{Hg}_{0.81}\text{Te}$ crystals: 1—concentration of acceptors $p_{77} = 10^{20} \text{ m}^{-3}$, 2— $p_{77} = 2 \cdot 10^{19} \text{ m}^{-3}$ and 3— n - $\text{Cd}_{0.26}\text{Hg}_{0.74}\text{Te}$ ($n_{77} = 10^{19} \text{ m}^{-3}$).

As follows from Fig. 3, the behaviour of the dependence of $\tau(T)$ in n -type crystals is significantly different from the similar one for p -type, since the spectrum of point defects in these crystals is significantly different ($n \gg p$). It is characterized by a monotonous decrease in microhardness with increasing temperature without characteristic areas inherent in p -type crystals. The dominant defects in this temperature range in n -type crystals are ionized internodal mercury atoms. Therefore, in the studied temperature range, the charge state of local stoppers for dislocations does not change. The temperature change in microhardness mainly occurs due to the change in the height of the Peierls barriers and the probability of throwing out double kinks of dislocations.

Note that the result of the interaction in the system ‘an ensemble of point defects—moving dislocations’ is determined not only by the properties of point defects, but also by the properties of linear defects (dislocations) that carry out thermally activated movement in the slip plane. To obtain such information, synchronous measurements in the process of uniaxial deformation of the specific electrical conductivity and the Hall coefficient are relevant.

As follows from Fig. 4, the uniaxial deformation of the p -type crystal is accompanied by a monotonous decrease with an increase in the degree of deformation of the Hall coefficient R_H and an increase in its electrical conductivity σ . Moreover, the Hall coefficient has a negative value, since in the region of mixed conductivity, within which the

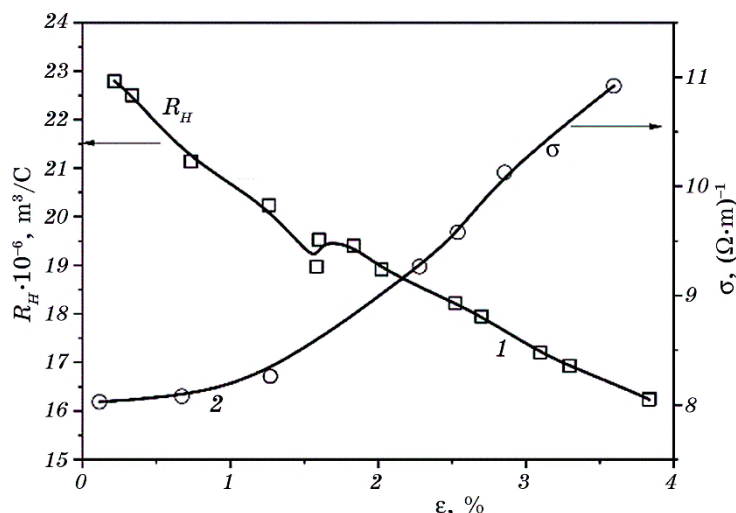


Fig. 4. Change in the Hall coefficient (1) of the $p\text{-Cd}_{0.2}\text{Hg}_{0.8}\text{Te}$ crystal and its electrical conductivity (2) in the process of uniaxial deformation ($T = 300$ K).

measurements were made, the mobility of electrons greatly exceeds the mobility of holes. A significant increase in the electrical conductivity of the p -type sample is observed, as can be seen, after reaching the 'tooth' of fluidity. Therefore, at the stage of deformation to the 'tooth' ($\epsilon < \epsilon_0$), the electrophysical changes of the crystal are determined by the processes responsible for the formation of the 'debris' layer. The transition to the stage of macrofluidity (above ϵ_0) is accompanied by the delocalization of defect formation processes, *i.e.*, the 'drawing in' of the crystal volume into the deformation process. Therefore, changes in electrophysical parameters in the process of deformation at this stage will already be caused mainly by dislocation processes that will occur in the 'internal' crystal, modified in relation to the original sample.

The simultaneous decrease in the Hall coefficient and increase in electrical conductivity in p -type crystals during uniaxial deformation, recorded experimentally (Fig. 4), can be explained within the framework of the mechanism of thermofield ionization of charged centres. Since strong electric fields are associated with dislocations in A^2B^6 crystals ($E \cong 10^6$ V/cm at a distance of $\cong 30$ Å from the dislocation core), regions are formed in the zone of a strong electric field of a moving dislocation in which the dynamic equilibrium in the electronic subsystem is shifted in side of the thermal generation of electrons from local levels to the conduction zone. At the same time, electrons 'ejected' by the field from the centres (Hg vacancies, ionized impurities) enter the conduction zone and increase, accordingly, the concentration of free electrons. Estimation of the thermal deionization time of the ac-

ceptor centre with $E_A \cong 0.03$ eV gives a value of $\cong 2 \cdot 10^{-7}$ s. For comparison, the localization time of the centre near a moving charged dislocation significantly exceeds this value: $t \cong R_{\text{ekr}}/V_d \cong 10^{-2}$ s $\gg 10^{-7}$ s (R_{ekr} is the radius of the Ridov cylinder of the dislocation line $\cong 4 \cdot 10^{-5}$ cm), which indicates the assumption benefit have made.

In connection with the alternative properties of point defects in p - and n -type crystals, the plastic deformation will differ significantly due to the significant influence of electronic subsystem on the behaviour of mobile dislocations.

3.2. Interphase Interaction and Self-Organization Processes in the Volume of a Deformed Crystal

A complete description of elastic-plastic deformations should analyse the deformed crystal as an open thermodynamic system that evolves in the process of deformation in the direction of creating structures of effective energy dissipation, which continuously enters the object through open channels [1, 2]. 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. 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 factors in such processes are mechanisms of energy dissipation, which can change during the evolution of the system.

The self-organization of the deformed crystal experimentally manifests itself in the gradual change of the macroscopic parameters. In structures with existing interphase boundaries (heterogeneous systems), the efficiency of energy dissipation is determined by the intensity of interphase interaction. Therefore, the goal of self-organization in the deformation process is not only the preservation of the integrity of the crystal at this stage, but also the generation of new types of structures capable of effectively dissipating the added energy during the further 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 leading to minimum entropy.

In this regard, we will discuss the mechanism of self-organization processes at the macro level in such a fragmented crystal. The presence in it of adjacent grains (areas) with different crystallographic orientation, the emergence of new structural elements separated by dislocation sub-boundaries, leads to a specific phenomenon—interphase interaction of bounded areas. 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, *i.e.*, which have different Young's moduli E and are separated by a structural boundary [8]. It should be noted that the fragmentation of the crystal during uniaxial deformation begins at the stage of its elastic-plastic deformation during the formation of the debris layer. As shown in Fig. 5, the microstructure of a deformed crystal at different stages of deformation, which demonstrates the sequential process of crystal deformational fragmentation with the formation of such separated structures by dislocation boundaries.

When the crystal is loaded, the volume of the crystal is 'drawn' into the deformation process of new deformation fragments formation. This indicates an increase in the quantitative contribution of interphase interaction to the mechanisms of crystal deformation. Quantitatively, the

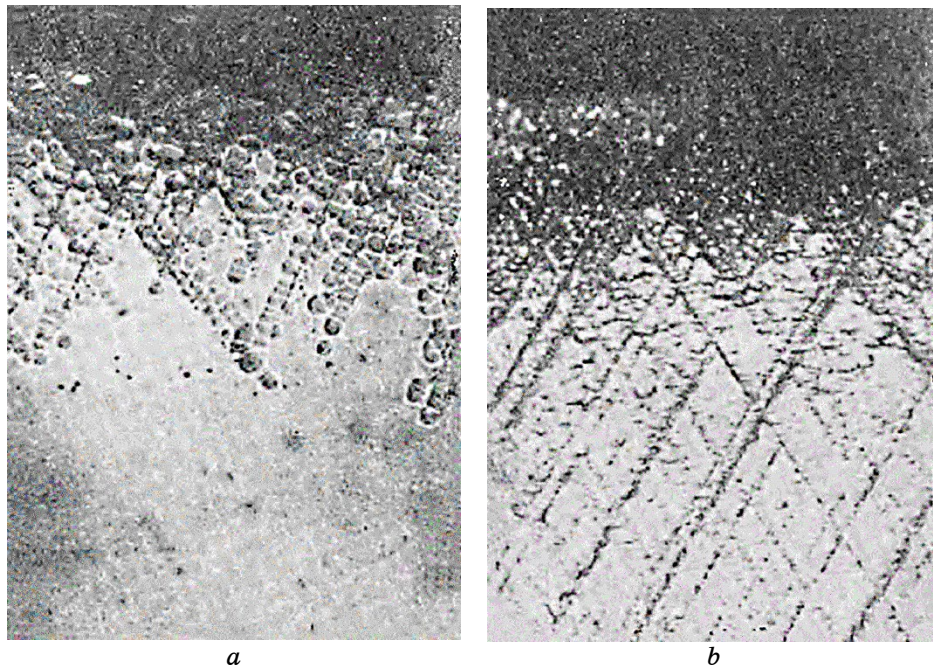


Fig. 5. Formation of a gradient layer near the surface of a deformed crystal: $\varepsilon = 0.6\%$ (*a*), $\varepsilon = 1.2\%$ (*b*).

intensity of such interaction is estimated by two main parameters: the interfacial interaction energy γ_m and the interfacial tension σ_m .

A detailed method of estimating the interfacial energy γ_m and interfacial tension σ_m and their numerical values for number of practically important contacting pairs is given in Ref. [9]. The evaluation of the parameters of the interfacial interaction according to this method in deformed $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ crystals revealed: when the Young's moduli of the bounded regions change as a result of crystallographic misorientation to the value $E/E_0 = 1.5$, the energy of interfacial interaction changes to 2–3%, and the value of interfacial tension—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 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 interfacial tension between deformation fragments.

3.3. Nucleation of Dislocations and Interphase Interaction in Near-Surface Layers of Deformed Crystals

Despite the Peierls mechanism of generation and propagation of dislocations, the studied crystals have a relatively low yield stress that indicates the nucleation of dislocations and, accordingly, the beginning of microplastic flow, at very small values. It is obvious that this behaviour is due to the peculiarity of the behaviour of the surface sources of dislocations inherent in these crystals. The investigated crystals are characterized, in particular, by the presence on the surface of a wide range of natural oxides CdO , CdTeO_3 , TeO_2 , HgTeO_3 , HgTe_2O_5 , which form a stable dielectric structure with the semiconductor crystal—a semiconductor.

The presence of a stable oxide layer on the surface of a semiconductor crystal creates a classic dielectric-semiconductor contact with the corresponding structural elements inherent in such a structure (Fig. 6). In Figure 7, a typical zone diagram of such a contact is shown. A feature of the structure is the presence of a strong electric field in the oxide-semiconductor transition layer, which can reach values of 10^3 – 10^4 V/cm, caused by the localization of a positive built-in charge in the border layer of the oxide [10]. Therefore, the existing electric field, localized in the boundary layers of the semiconductor crystal and the dielectric, will significantly affect the probability of the nucleation of dislocation loops and their further behaviour.

Microscopic studies of deformed samples of $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ in the pseudo-elastic stage indicate that the slip bands do not originate directly

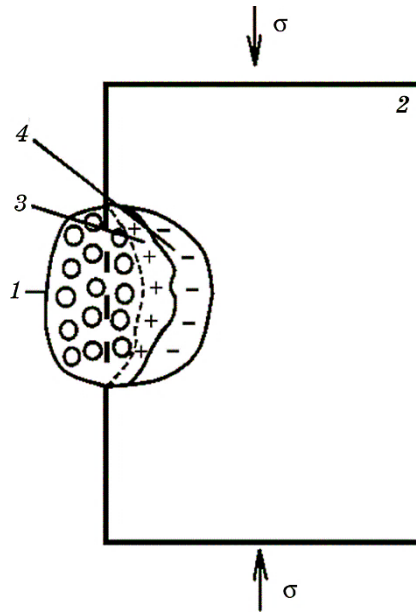


Fig. 6. Model representation of a fragment of the oxide layer (1) on the surface of the deformed crystal (2) and the area of the space charge created by the positive built-in charge in the oxide (3) and the negative charge (4) in the semi-conductor.

from the surface, but originate at some distance from it. This indicates that the formation of the near-surface gradient of dislocations at the initial stage of deformation occurs mainly not with the participation of purely surface sources (ribbons, microuniformities, *etc.*), but near-surface sources. Such sources of dislocations are the accumulation of point defects in the form of clusters or loops (vacancy and internodal types), which are formed during deformational supersaturation. In particular, under conditions of uniaxial compression, the equilibrium concentration of vacancies on the surfaces to which the normal compressive stress is applied decreases to the value $c = c_0 \exp(-\sigma \vartheta_a / kT)$, where c_0 is the equilibrium concentration of vacancies in the unloaded crystal, ϑ_a — atomic volume. At the same time, the equilibrium concentration of internodes, on the contrary, increases to the value $c_i = c_{i0} \exp(\sigma \vartheta_a / kT)$. This leads to oversaturation with vacancies and to undersaturation in internodes. At the same time, vacancies migrate to drains and form clusters and loops, which act as sources of further propagation of dislocations. Since the vacancy formation energy in the near-surface layers of the crystal is significantly lower than in the bulk, and the equilibrium concentration is correspondingly higher, it becomes obvious that the specified processes of condensation

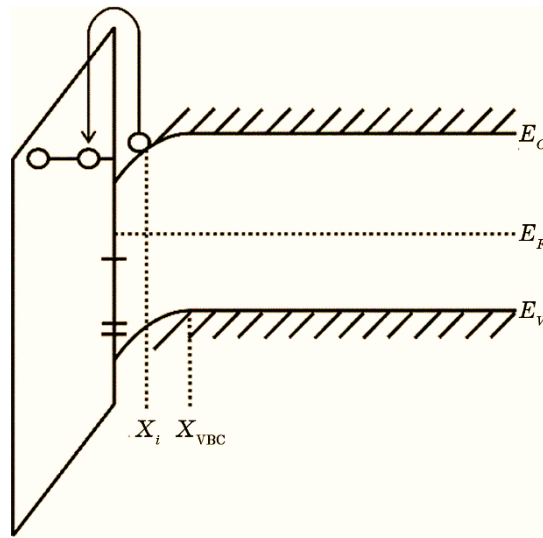


Fig. 7. A typical dielectric–semiconductor energy band diagram showing the characteristic properties of an oxide layer on the surface of a deformed semiconductor.

of point defects will take place primarily and primarily in these elements of the crystal. The predominant formation of loops in the near-surface layers will also be facilitated by the concentration of stresses near the oxide–semiconductor interface due to the difference in elastic moduli and coefficients of thermal expansion.

The critical size of the nucleus r_c for stable growth of the vacancy cluster has the form: $r_c = 2\gamma/c$, where γ is the surface tension [11]. For the investigated crystals, the nucleus size according to calculations is $r_c \cong 0.12$ nm, which mean to real values.

Thus, at the initial pseudo-elastic stage of deformation, vacancy clusters and clusters can form, which later play the role of the main sources of dislocations near the free surface. Therefore, the formation of the primary embryos of nucleation actually begins not directly from the surface, but at some distance from it, that is, in a thin near-surface layer.

4. CONCLUSION

1. Within the framework of the thermoactivation dislocation mechanism of deformation of $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ solid solution crystals, it was established that the movement of dislocations is controlled by the Peierls mechanism with characteristic process parameters. The influence of stoichiometry defects and features of the band structure on the thermally activated movement of dislocations in narrow-band crystals has

been clarified. Due to the alternative properties of point defects in p - and n -type crystals, their plastic deformation is significantly different due to the significant influence of the equilibrium state of the electronic subsystem on the behaviour of mobile dislocations.

2. It was established that the presence of a strong electric field associated with dislocations leads to an increase in the electrical conductivity of p - $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ crystals in the process of deformation as a result of thermofield ionization of electrons from charged centres in the field of a moving dislocation.

3. Deformation of $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ crystals, along with translational dislocation slip, is accompanied by the emergence of new structural deformation elements that take part in the deformation process as independent ones. The presence of adjacent grains (areas) with different crystallographic orientation, the emergence of new structural elements separated by dislocation sub-boundaries, leads to a specific phenomenon—interphase interaction of bounded areas. This type of interaction occurs between heterogeneous volumes, as well as within the same solid body between regions with different mechanical compatibility, *i.e.*, which have different Young's module E and are separated by a structural boundary. It is claimed 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 interfacial tension between deformation fragments. According to estimates, the contribution of this mechanism can reach up to 20%.

4. The onset of microplastic yielding in $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ crystals occurs at stresses much lower than the macroscopic yield strength. This is caused by the presence on the surface of the deformed crystal of a wide range of natural oxides CdO , CdTeO_3 , TeO_2 , HgTeO_3 , HgTe_2O_5 , which form a stable structure of a dielectric—a semiconductor with a semiconductor crystal containing an electric field localized within the transition layer. The last factor will influence the probability of nucleation in the near-surface layer of dislocation loops. The process of formation of vacancy clusters and clusters in the near-surface layers of the deformed crystal is analysed, which later play the role of the main sources of dislocations near the free surface. Therefore, the formation of the primary embryos of nucleation actually begins not directly from the surface, but at some distance from it, that is, in a thin near-surface layer.

5. In the case of weak adhesion of the oxide layer to the surface of a semiconductor with excellent Young's moduli, when the crystal is loaded, a process of interphase slip occurs with the formation of defects of the type of mismatch dislocations at the interphase boundary. In the presence of strong adhesion of the oxide layer to the surface of the semiconductor at the stage of pseudoelastic deformation, an interphase interaction occurs, respectively, which is the cause of strong mechanical stresses in the interphase boundaries and thus facilitates the

nucleation of dislocation loops in the near-surface layers of the deformed crystal.

REFERENCES

1. B. P. Koman, *Metallofiz. Noveishie Tekhnol.*, **39**, No. 8: 1129 (2017).
2. G. Nicolis and I. Prigogine, *Self-Organization in Nonequilibrium Systems. From Dissipative Structures to Order through Fluctuations* (New York–London–Sydney–Toronto: J. Wiley and Sons: 1977).
3. T. Suzuki, *Dislocation Dynamics and Plasticity: Overview* (New York: Springer-Verlag: 2011).
4. B. P. Koman, *Solid State Phys. Chem.*, **12**: 1018 (2011) (in Ukrainian).
5. B. Koman and V. Yuzevych, *State, Trends and Prospects of Land Sciences, Environment, Physics, Mathematics and Statistics Development* (Dallas: Primedia eLaunch LLC Dallas: 2020), p. 47.
6. S. Verheyden, L. Deillon, and A. Mortensen, *Acta Mater.*, **234**, No. 8: 118037 (2022).
7. D. B. Holt and B. G. Yacobi, *Extended Defects in Semiconductors: Electronic Properties, Device Effects and Structures* (Cambridge: Cambridge University Press: 2007), ch. 5, p. 412.
8. B. P. Koman, *Patterns of Interphase Interaction in the Near-Surface Layers of the Structure of Solid-State Electronics* (Lviv: 2017) (in Ukrainian).
9. B. P. Koman and V. M. Yuzevych, *J. Nano-Electronic Phys.*, **7**, No. 4: 04059 (2015).
10. David K. Ferry, Lex A. Akers, and Edwin W. Greeneich, *Ultra Large Scale Integrated Microelectronics* (New Jersey: Prentice-Hall Inc.: 1998).
11. P. M. Sopronyuk and V. M. Yuzevych, *Energy Characteristics of Surface Layers* (Lviv: SPOLOM: 2005) (in Ukrainian).