SECTION 4. ELECTRICAL ENGINEERING

4.1 The mechanism of thermoactivated dislocation motion in intrinsically defective semiconductor crystals

Studies of the effect of point defects on the mobility of dislocations in crystals have been studied mainly for impurity atoms in terms of their "braking" properties in order to create materials with predictable mechanical properties [224– 227]. It was assumed, local barriers were thought to be associated with point defects. However, unlike Pierrels barriers, which are placed strictly periodically, such barriers are characterized by a chaotic arrangement in the sliding plane of the dislocation. Therefore, the main work on the study of the interaction of moving dislocations with point defects was solved by modeling the thermoactivated motion of dislocations through randomly placed local barriers of different shapes and a certain distribution in height and distance between them. However, attempts to apply this approach to the Peierls model led to the functional dependences of the dislocation velocity on temperature and tension υ (T, τ) in forms that do not agree with the experimental results.

The problem of the influence of point defects of stoichiometry on the kinetics of reproduction and movement of dislocations has not been studied. In this case, the interpretation of the behavior of dislocations in crystals is a priori carried out in the same way as for impurity atoms, which is not correct for intrinsically defective crystals. Therefore, the ***aim*** of this work is to study the role of stoichiometry defects in the thermoactivated motion of dislocations within a wide range of changes in their concentrations and temperature range. Such studies were performed on crystals of solid solutions of $Cd_xHg_{1-x}Te$ (x-molar composition) as model objects. The source crystals after cultivation have significant nonstoichiometry due to the high elasticity of mercury vapor. An important feature of such crystals is also a smooth change in the band gap (from –0.1 to 1.5 eV) with a change in the molar concentration of Cd.

Thermoactivation analysis of the plastic fluidity of crystals of solid solutions of $Cd_xHg_{1-x}Te$ indicates that the movement of dislocations is controlled by the Payers mechanism [228]. However, with a potentially low Peyerls relief for these crystals, the processes of movement and reproduction of dislocations must be significantly influenced by their own point defects, in particular defects in stoichiometry. The effect of such defects on thermoactivated slip dislocations in $Cd_xHg_{1-x}Te$ crystals was revealed in [229].

Experimental methodology.The methods of microhardness (PMT-3 microhardness tester) and uniaxial compression (Regel-Dubov relaxometer) were used. Bridgman-grown single crystals were studied. The identification plane was the chip plane (110). The concentration of intrinsic defects was regulated by annealing samples at controlled mercury vapor pressures p_{Hg} or high-temperature thermal annealing (HTTA) at 623 K. Control of stoichiometric defects was performed by Hall measurements of carrier concentration (T = 77 K) . The temperature dependences of the microhardness H_v (T) of samples of different stoichiometry in the temperature range 77–450 K were investigated. Based on these data, the dependences of the difference concentration (p_{77K} - n_{77K}), microhardness H_{v1} (T = 300 K) and H_{v0} (values corresponding to the initial part of the athermic region of H_v(T) dependence) on p_{Hg} in the process of regulating thermal annealing were constructed. Measurements of H_v(T) were performed on two identical samples: the first was subjected to the annealing cycle with increasing p_{Hg} (T = 573 K), the second – HT AT in saturated Hg vapors at 623 K.

The results of experimental research and their discussion. Figure 1 shows the experimental dependences of carrier concentration (p_{77K} - n_{77K}) and microhardness for the $Cd_{0,24}Hg_{0,76}Te$ single crystal on the mercury vapor pressure p_{Hg} during annealing.

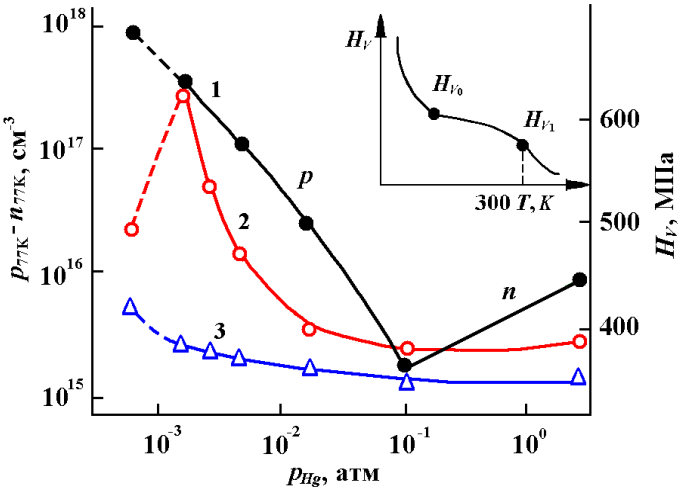

Figure 1. Dependences of carrier concentration (p_{77K} - n_{77K}) (1) and microhardness H_{v0} (2) and H_{v1} (T = 300 K) (3) for the $Cd_{0,24}Hg_{0,76}Te$ single crystal from the mercury vapor pressure p_{Hg} during annealing. The dashed line corresponds to the changes in the sample after HT AT.

The insert shows a schematic dependence of H_v (T) for $Cd_xHg_{1-x}Te$ with characteristic measurement points H_{v0} and H_{v1}

It follows from the figure that the increase in p_{Hg} for the first sample from 1.8 $\cdot 10^{-3}$ at is accompanied by a monotonic decrease in p_{77K}, which in accordance with the conventional model of point defects in $Cd_xHg_{1-x}Te$ means "healing" vacancies in the metal lattice diffusion. The extremum at $p_{Hg} \approx 10^{-1}$ at corresponds to a composition close to stoichiometric, when vacancies [Hg] and [Cd] are mostly absent. A further increase in p_{Hg} is accompanied by an increase in the concentration of interstitial atoms (Hg), as a result of which the crystal acquires an electronic type of conductivity.For the semiconductor composition $Cd_{0,24}Hg_{0,76}Te$ studied in this work, the characteristic regions on the nonmonotonic dependence of H_v (T) (see the insert in figure 1) are relatively more pronounced than for compositions close to semimetallic. For the first sample, when the concentration of vacancies decreases, the value of H_{v0} decreases monotonically, reaching the minimum value at the stoichiometric composition. Further saturation of the Hg sample by increasing the concentration between the nodal mercury does not change the microhardness. The second sample after HT AT (30 min.) shows an increase in concentration to a maximum value of 10^{18} cm^{-3} (H_{v0} in this case decreases

sharply from 63 to 49 kgf / mm^2). It is noteworthy that with increasing concentration of [Hg] crystal hardening is observed only in the low temperature region, i.e. in the athermic region and lower on the H_v (T) dependence, and in the high temperature region there is a slight hardening of both crystals. The minimum value of H_{v1} in this case is reached at stoichiometric concentration and does not change with increasing concentration (Hg).

To assess the contribution of various stoichiometry defects to the process of interaction with moving dislocations in plastic fluidity, the dependences of the yield strength σ_0 at uniaxial compression (293K) and activation volume V_a on the degree of structural perfection were studied compression of samples with different concentrations (p_{77K} - n_{77K}), using the method [230] (T = 293K). In figure 2 shows the following dependences for $Cd_{0,21}Hg_{0,79}Te$ crystals.

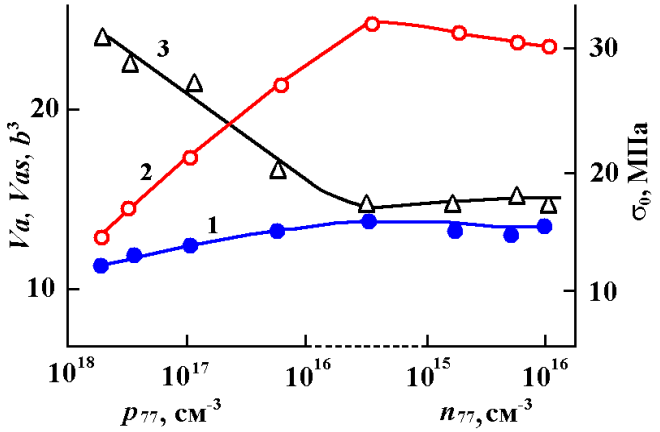

Figure 2. Dependences of dark V_a (1) and light V_{as} (2) activation of dislocation volumes and yield strength σ_0 (3) from the concentration of carriers in single crystals $Cd_{0,21}Hg_{0,79}Te$, obtained from uniaxial deformation tests at T = 300 K

From figure 2 it follows that σ_0 (as well as H_{v1}) decreases monotonically with increasing concentration [Hg], reaching the maximum value at stoichiometric composition. The introduction of type (Hg) defects in the lattice does not affect σ_0. With such a change in the spectrum of point interferences, V_a increases from 11 to 14 b^3, reaching the maximum value in stoichiometric crystals. Subsequent annealing,

which leads to n-type conductivity with an electron concentration of $n_{77K} = 10^{16}$ cm^{-3}, has virtually no effect on V_a. The tendency to change V_a with the concentration of stoichiometric defects is especially clear for the "light" value of the activation volume V_{as} obtained by irradiating the relaxed crystals with light under conditions of negative photoplastic effect.

Let us discuss the results obtained in terms of thermoactivated dislocation motion. The non-trivial nature of H_v (T), as well as the results of the study of the effect of annealing on the parameters H_{v0}, H_{v1}, σ_0 and V_a indicate a specific role of stoichiometric defects in the inhibition of mobile dislocations. In particular, the dominant defects that resist motor dislocations are [Hg] and [Cd]. However, when the crystal temperature changes, the mechanism of interaction [Hg] with mobile dislocations changes: in the region of high temperatures ($T \geq 300$ K) the interaction is mainly elastic, resulting in a slight strengthening of the crystal with increasing [Hg] concentration. This fact is confirmed, as shown above, also by a decrease in V_a with increasing concentration [Hg], which is due to a decrease in the average distance between local stoppers, and thus an improvement in the structural perfection of the crystal. Atoms (Hg) do not have a locking effect on moving dislocations, which is also consistent with the conclusions [229].

Using the activation volume value, we estimate the average distance between obstacles for moving dislocations. Provided that the distance between the obstacles is comparable to their size, the minimum distance between them is equal to:

$$L_{\min} \approx (V_0/b)^{1/2}$$

where V_0 is the activation volume at $\sigma^* = 0$ (σ^* – the thermal component of the applied tension), b is the Burgers vector.

The effective distance between obstacles along the dislocation line depends on the tension (weak obstacles) [231]:

$$L_{\max} = (Gb\, l^2/\sigma^*)^{1/3}$$

where G is the shear modulus.

Estimates of the above formulas show that the stoppers for moving dislocations are defects in the sliding plane of dislocations at distances of approximately 2.0 – 2.4

and 3.2 – 4.6 nm for p- and n-type crystals, respectively. Thus, in n-type samples, the distance between the interferences is almost twice the same distance in p-type crystals, which is due to the "healing" of mercury vacancies during annealing in saturated mercury vapor.

In the region of low temperatures, electrical interaction predominates. In this case, the sliding process of dislocations is accompanied by an increase in their fill factor *f* due to saturation of broken bonds in the dislocation nucleus by electrons of point centers (in our case – ionized [Hg]), "swept" by dislocation when moving in the sliding plane. The probable course of such processes in $Cd_xHg_{1-x}Te$ is evidenced by the results of electrophysical measurements of crystals in the process of their uniaxial deformation [232]. According to this model, as the concentration of [Hg] increases, the charge at the dislocations increases, thus limiting the mobility of the latter, which macroscopically manifests itself in increasing the microhardness of the sample. Therefore, the nonmonotonic nature of the $H_v(T)$ dependence for $Cd_xHg_{1-x}Te$ is due to a similar charge dependence on the dislocations, and hence to the effect on their mobility.

These results indicate that in $Cd_xHg_{1-x}Te$ crystals, within the framework of the main dislocation displacement mechanism (Peierls mechanism), the transformation of the alternative mechanism of interaction of mobile dislocations with point defects takes place when the temperature changes.

The decreased strength of the crystal after HT AT can be explained by the action of the following mechanisms. First, since the final cause of p_{77K} growth after HT AT is currently unknown, a sharp increase in H_{v1} after such annealing indicates that after growth, the studied crystals contain a significant concentration of local stoppers of unknown nature (possibly [Hg] complexes), as a result, the crystals have a high initial microhardness. Annealing destroys such defects and the crystal acquires a more perfect structure for thermoactivated dislocation motion. In the framework of the used dislocation charge model, the drop in microhardness can be explained by a decrease in the energy of formation of double inflections due to a sharp increase in the coefficient *f* of mobile dislocations [233].

After HT AT at the maximum concentration of point defects, distortions of the potential relief and fine structure of dislocation nuclei are possible, as a result of which the strength properties of the lattice also change. To quantify the contribution of intrinsic defects in this process, the calculation of the Peierls tension σ_P – tension of the deactivation motion of dislocations was performed. For Pierre's sinusoidal relief [234]:

$$\sigma_p = \pi U^2 / 16 G a_1 b^3$$

for quasi-parabolic:

$$\sigma_p = 16 U^2 / \pi G a_1 b^3$$

where G is the shear modulus (for $Cd_{0.2}Hg_{0.8}Te$ is 1.8 10^{10} N / m^2), a1 is the distance between two adjacent Peyerls relief grooves), b is the value of the Burgers vector. The most real results of σ_P calculations are obtained for quasi-parabolic relief. In particular, for crystals of different stoichiometry, the specific values are as follows:

p_{77K} = 8 10^{16} cm^{-3} σ_P = 860 MPa

$p_{77K} = n_{77K}$ = 10^{15} cm^{-3} σ_P =770 MPa

p_{77K} = 10^{18} cm^{-3} σ_P = 120 MPa

Satisfactory agreement between the calculated value of Peierls tension and the value obtained from the extrapolation of the temperature dependence of the yield strength to σ_0 (T = 0 K) is observed only in samples with minimal deviation from the stoichiometric concentration (intrinsic). At the maximum concentration of acceptors, the calculated value of σ_P does not correspond to real values. Thus, the above results indicate the possible influence of stoichiometry defects (Hg vacancies) on the Pierrels relief up to its distortion.

Thus, a set of studies to establish the role of intrinsic defects in thermoactivated dislocation motion shows that [Hg] vacancies are the dominant defects that affect the kinetics of motion and reproduction of double bends in the entire temperature range of plasticity of $Cd_xHg_{1-x}Te$ crystals.

The study of thermally activated sliding dislocations in such crystals in a wide range of temperatures synchronously with the control of their electrophysical

parameters $R_H(T)$ found that plastic deformation is determined by the equilibrium state of their electronic subsystem [232]. This situation is typical of narrow band semiconductors due to the presence of stoichiometric defects, creating an acceptor level in the band gap near the valence band ceiling with low activation energy E_A = 0.02 eV and a donor near the bottom of the conduction band (activation energy close to zero). Therefore, a certain thermodynamic state of the electronic subsystem will determine the charge state of its own stoichiometric defects - vacancies [Hg] and [Cd] and interstitial atoms (Hg_i). The latter will always be in the ionized state and due to their coordination in the internodal positions will not, as confirmed above, inhibit the dislocations due to the lack of lattice dilatation. Thus, a change in temperature in a relatively small range will be accompanied by recharging of the local centers associated with [Hg] and their corresponding levels in the restricted zone. Thus, within the main mechanism controlling the plastic fluidity, the change in crystal temperature, synchronously with the change in its conductivity type, will also be accompanied by a change in the mechanism of interaction of moving dislocations with point defects of the crystal lattice.

Based on uniaxial deformation studies, it is established that the general trend in the thermoactivated motion of dislocations during the transition of the crystal from the impurity region of conductivity to its own is an increase in the activation volume and activation energy of dislocations. Activation volume is known to be the first sign that separates the mechanism of thermoactivated dislocation motion. In particular, the low value of V_a in the region of impurity conductivity indicates the dominant role of mechanisms that require the movement of atoms from or to the dislocation in the overall process of movement of dislocations.

Therefore, the thermoactivated motion of dislocations in $Cd_xHg_{1-x}Te$, obviously, should be considered as the imposition of mechanisms of conservative motion of dislocations and sliding dislocations. The increase in the activation volume during the transition from the impurity region to its own indicates an increase in the contribution of net slip over crawl in the overall mechanism of dislocation movement.

In general, we associate the observed correlation between the yield strength and microhardness with the equilibrium state of the electronic subsystem, first, with the different role of stoichiometry defects in the interaction with mobile dislocations at certain equilibrium states of the electronic subsystem of samples and, secondly, when the crystal passes from one mechanism to another in a certain temperature range.

In the region of impurity conductivity, a fixed concentration of temperature corresponds to a certain concentration of ionized intrinsic acceptor point defects. Any change in temperature unambiguously affects the change in the concentration of electrons localized at the acceptor level E_a. The movement of dislocations in this temperature range is carried out mainly due to the creep of dislocations with the participation of their own point defects, in particular vacancies Hg and Cd. This process is accompanied by the filling of dislocation zones with electrons, "swept" from ionized acceptors, as a result of which the mobility of dislocations is reduced. An increase in the crystal temperature is accompanied by an increase in the electron concentration at the acceptor level of the eigenpoint defects. However, the number of such carriers "swept" on the dislocation line decreases due to the thermal release of electrons from the dislocation to the conduction band. Thus, the plastic deformation of $Cd_xHg_{1-x}Te$ crystals in the region of impurity conductivity is carried out by the movement (mainly conservatively) of charged dislocations with simultaneous “sweeping” of electrons from ionized acceptors into dislocation zones.

Further increase in temperature is accompanied by a change in the mechanism of conductivity of crystals. In the mixed conduction region, most point acceptors are ionized, and in their own, all defects of this type are in the ionized state. Plastic deformation in these cases is carried out by the interaction of charged dislocations moving (mostly in a non-conservative way) in the sliding plane, with ionized defects of the lattice. The latter fact, in our opinion, may be one of the reasons for the relatively high plasticity of the studied crystals. In this case, as suggested in [233], the energy of formation of the double inflection on the charged dislocation decreases due to the electrostatic repulsion of the inflection from the rest of the dislocation. reduction of the

energy of formation of double inflection, due to long-range Coulomb forces of interaction between charged defects and dislocations:

$$E = 8\pi/15\varepsilon\, a\, (e^2 / kT\, a \ln c^{-1})^{1/2}$$

where ε is the dielectric constant; e - electron charge; c is the concentration of point defects. This fact leads to the conclusion that increasing the concentration of ionized defects causes an increase in the rate of dislocations, that is hardening of the crystal.

Conclusions. Thus, based on the results of complex studies of concentration and temperature dependences of microhardness, yield strength and activation volume from uniaxial deformation tests, the role of stoichiometry defects in thermally activated motion of dislocations in narrow-band crystals $Cd_xHg_{1-x}Te$. dislocations. It is shown that at high concentrations of mercury vacancies their influence on the Pierrels relief of the lattice occurs. The influence of the equilibrium state of the electronic subsystem of narrow-band semiconductors on the behavior of dislocations in them in the process of plastic fluidity is established. When the temperature changes, within the framework of the main mechanism of dislocation motion, the dominant mechanisms of interaction of dislocations with the imperfections of the crystal lattice change.