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REGULARITIES OF MACROPLASTIC DEFORMATION OF NARROW-BAND SINGLE CRYSTALS OF CdxHg 1-xTe SOLID SOLUTIONS

ABSTRACT:

The regularities of macroplastic deformation of narrow-band semiconductors of HgTe-CdTe solid solution crystals were studied by the uniaxial compression method on a Regel-Dubov relaxometer. The four-stage character of the strain hardening curve “stress-strain” is established. The influence of stoichiometry, load velocity and temperature on the nature of load curves is investigated. From the experiments on the relaxation of mechanical stresses, a thermoactivation analysis of the kinetics of microplastic deformation was performed. Thermoactivation parameters of dislocation motion are estimated. The criteria for performing the Pierrels mechanism of dislocation motion in these crystals are investigated. The influence of light on the macroplastic fluidity of CdxHg1-xTe crystals is described.

INTRODUCTION.

For today in the literature provides extensive information on macroplastic deformation, as well as the behavior of individual dislocations of semiconductor single crystals [1,2]. Such objects with diamond lattices (Si, Ge) and sphalerite (compounds A^2B^6 and A^3B^5) are characterized by high Pierrells barriers for the movement of dislocations due to the direction of covalent bonds in these materials. The investigated single crystals of solid solutions of HgTe-CdTe on a number of physical and mechanical parameters occupy an intermediate position between classical semiconductors and metals. In particular, these materials are characterized by high fragility at room temperature, which brings them closer to purely covalent semiconductors. However, on the other hand - high densities of dislocations of the "forest" (10^5-10^6 cm^{-2}), a high concentration of point defects, mainly vacancies of mercury,

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reaching within the homogeneity of 10^{19}-10^{20} cm^{-3} [3], mixed ionic covalent nature of the chemical bond with the predominance of the ionic component (~ 60%) - factors that contribute to some extent to the approximation of such materials to metals. For comparison, we note that the concentration of vacancies in Ge, even close to the melting point, is only 10^{15} cm^{-3} [4].

Despite the "exotic" nature of the objects, and their important practical application, the data on the patterns of motion of dislocations and the mechanisms of plastic fluidity are fragmented.

The **aim** of the work is to study the regularities of plastic deformation of crystals of narrow-band semiconductors of solid solutions of HgTe-CdTe (E_g = 0.05-0.22 eV) and to establish the mechanisms of motion of dislocations that cause these processes.

Experimental methodology.

The investigated crystals $Cd_xHg_{1-x}Te$ ($x \leq 0,25$) were grown by Bridgman's methods and solid recrystallization.

Regularities of macroplastic deformation of crystals of solid solutions of HgTe-CdTe were investigated by the method of uniaxial compression on a Regel-Dubov relaxometer. In the process of deformation, the sample was in a quartz self-centering punch with a ball section, which eliminated the influence of possible non-parallelism of the sample ends on the overall course of the load curve.

Monocrystalline samples in the form of a rectangular parallelepiped with $2 \times 2 \times 6$ (mm) dimensions and different crystallographic orientations relative to the compression axis were subjected to uniaxial compressio. The strain rate varied in the range of 5.85-9.4 10^{-2} mm / min. In some cases, the deformation of the samples was performed in a vacuum chamber of a cryostat of special design.

REGULARITIES OF PLASTIC DEFORMATION AND MECHANISMS DISLOCATION MOTION OF NARROW-GAP CRYSTALS OF SOLID SOLUTIONS CdxHg1-xTe.

The primary task of studying the deformation properties of $Cd_xHg_{1-x}Te$ single crystals was to study the influence of various factors on the parameters of their strain hardening curves. Such dependences are well described by the four-stage form of the load curve (Fig. 1), first proposed for f.c.c. crystals in [5].

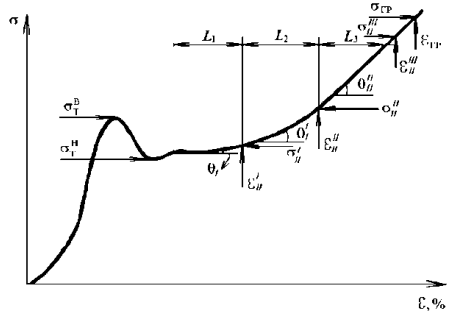

Figure 1. **Schematic four-stage deformation curve strengthening stress – strain**

Uniaxial compression of $Cd_xHg_{1-x}Te$ samples along different crystallographic directions does not reveal significant differences in the parameters of strain hardening curves. This fact follows from the geometry of the dislocations in the structure of sphalerite.

Since the deformed crystals are nonstoichiometric materials, it is of interest to investigate the effect of deviations from stoichiometry on the parameters of the σ – ε (stress-strain) curves.

In fig. 2 shows the following dependences for samples $Cd_{0,18}Hg_{0,82}Te$ with different concentrations of stoichiometric defects. As the graphs show, this factor significantly affects the nature of the deformation hardening curves. Therefore, one of the reasons for the observed non-reproducibility of the σ - ε diagrams may be the excellent stoichiometry of the studied objects.

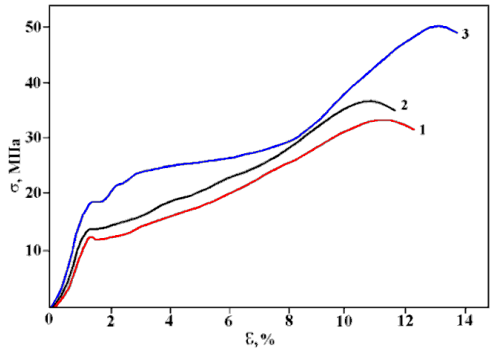

Figure 2. **Curves of deformation hardening of $Cd_{0,05}Hg_{0,95}Te$ crystals with different stoichiometry:**
1 - $p_{77} = 7 \cdot 1017$ cm^{-3}; 2 – $p_{77} = 8 \cdot 10^{16}$ cm^{-3}; 3 - $n_{77} = 2 \cdot 10^{15}$ cm^{-3}.
Deformation rate - $5.85 \cdot 10^{-3}$ mm / min. Temperature - 300 K.

The strain hardening curves of $Cd_xHg_{1-x}Te$ single crystals show a significant difference from the loading rate. In fig. 3 shows typical diagrams of σ - ε crystals of $Cd_{0,2}Hg_{0,8}Te$ deformed at different velocities.

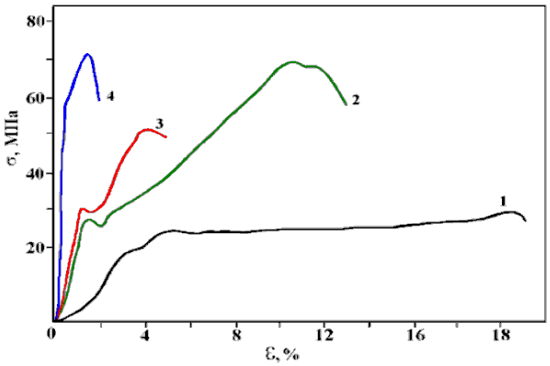

Figure 3. **Curves of deformation hardening of $Cd_{0,2}Hg_{0,8}Te$ crystal at different loading speeds:**
1 - $1{,}46 \cdot 10^{-3}$ mm / min .; 2 - $5.85 \cdot 10^{-3}$; 3 - $1.17 \cdot 10^{-2}$; 4 - $2.34 \cdot 10^{-2}$. T = 300K

As can be seen, the deformation at the extremely low (v = $1.46 \cdot 10^{-3}$ mm/min) and high (v = $2.34 \cdot 10^{-2}$ mm / min) velocities is not accompanied by the manifestation of the "tooth" of fluidity. Increasing the strain rate in the studied interval leads to an increase in the yield strength of the crystal. In addition, the increase in load speed is accompanied by a monotonic decrease in the length of the stage of easy sliding. The value of the maximum deformation for the minimum speed was 21%, and for the maximum - 1.6%. The tensile strength with increasing strain rate increases from 2.85 to 7.15 kgf / mm^2, respectively.

Fig. 4 shows the results of experimental studies of the velocity dependence of the yield strength of $Cd_{0,2}Hg_{0,8}Te$ crystals for temperatures of 77, 293, 388 and 423K. The applied speed interval was $2 \cdot 10^{-6}$ - $9 \cdot 10^{-5}s^{-1}$. The temperature range is 77–423 K. Such dependences, as we see, for the last two temperatures are straight lines with different slope coefficients. The general regularity of the velocity dependence of the yield strength at 77 and 293 K is the presence in them of two sections with significantly different degrees of velocity dependence. The first section of relatively weak dependence occupies the interval of velocities c-1 and is characterized by a linear relationship between and the logarithm of the strain rate.

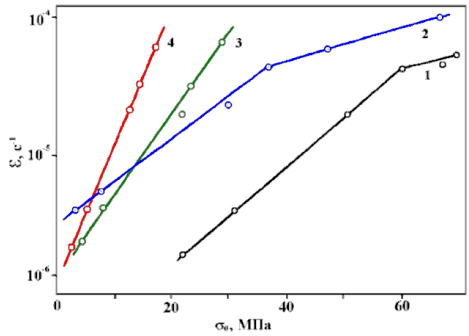

Figure 4. **Dependence of the yield point σ_0 of $Cd_{0,2}Hg_{0,8}Te$ single crystals from the rate of deformation at temperatures:**
1 - 77 K, 2 - 293, 3 - 388, 4 - 423

The second part of the above dependence is characterized by a much stronger velocity dependence of the yield strength. This interval is $4\times10^{-5} - 9\times10^{-5}$ s^{-1}. The dependence of the yield strength on the rate of deformation here is also linear. Comparing the analyzed dependence with similar curves for some BCC metals with a base-centered (b.c.) lattice and alkali-halide crystals, it can be argued that in the second section of the velocity dependence of the yield strength, a certain contribution to the mechanism of dislocation inhibition is made by dynamic effects (rule, at v> ~ 10^{-2} s, where c is the speed of sound). The temperature dependence of the sensitivity of the deforming stress (Fig. 5) in this speed range has a maximum in the region of 300 K. Note that similar studies performed on (b.c.) metals reveal a "bell-shaped" curve with maxima at certain temperatures for each metal. This course of the dependence = f (T), which has a maximum, indicates the thermoactivation nature of plastic deformation.

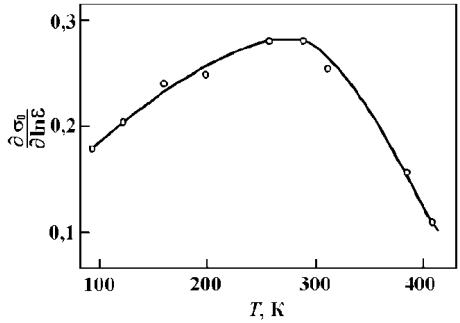

Figure 5. **Temperature dependence of the sensitivity of the deforming stress to the strain rate for single crystals $Cd_{0,2}Hg_{0,8}Te$**

Thus, the velocity dependence of the yield strength of $Cd_{0,2}Hg_{0,8}Te$ crystals in the first section in the temperature range 77–300 K is satisfactorily described by thermoactivation representations mechanisms.

Studies of the temperature dependence of the yield strength of n-$Cd_{0,2}Hg_{0,8}Te$ crystals in the temperature range (120–420 K) at five different loading velocities demonstrate its monotonic drop with increasing temperature (Fig. 6).

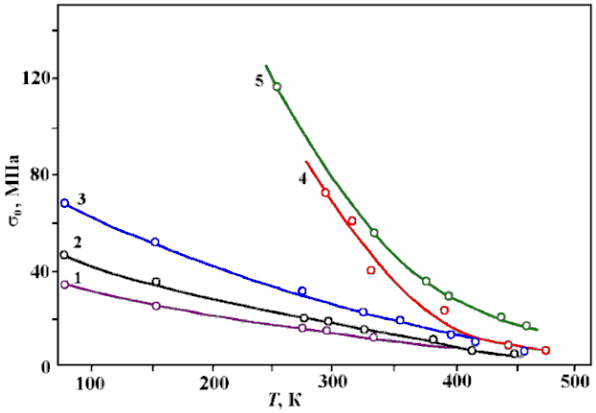

Figure 6. **Temperature dependence of the yield strength of single crystals n-$Cd_{0,2}Hg_{0,8}Te$ at different load speeds:** 1 - $7{,}32 \cdot 10^{-3}$ mm / min., 2 - $1.46 \cdot 10^{-3}$; 3 - $5.85 \cdot 10^{-3}$; 4 - $1.17 \cdot 10^{-2}$; 5 - $0.75 \cdot 10^{-2}$.

A comparison of the load curves shows that an increase in temperature affects the parameters of the curves similar to a decrease in the strain rate.

Since the plastic deformation of the investigated crystals is a thermally activated process, the activation parameters of the dislocation motion were evaluated to identify the mechanisms controlling the rate of plastic deformation.

Thermoactivation analysis of the kinetics of microplastic information of CdHgTe single crystals from stress relaxation experiments was performed according to the method [6]. According to the theoretical foundations of this technique, the stress relaxation in the crystal is described by the equation:

$$\ln\left(-\sigma^*\right) = \frac{V_a}{kT}\left(\sigma - \sigma_\mu\right) + \delta, \qquad \text{here} \quad \delta = \ln\left(Kb\rho L\vartheta_0\right) - \frac{U}{kT} \qquad (1)$$

Here b, ρ, are the Burgers vector, density and velocity of dislocations, respectively; L is the average free path length of dislocations; ϑ_0 - Debye

oscillation frequency of atoms (internal long-range voltage, athermic component). Thus, the slope of the line in the coordinates determines the magnitude of the activation volume V_a, And the values of the segments δ cut off along the coordinate axis at different temperatures - the magnitude of the activation energy U.

Due to the fact that the studied compounds are non-stoichiometric, the thermoactivation analysis was performed taking into account such imperfections of the lattice, as they must affect the processes of movement and reproduction of dislocations.

Samples of $Cd_{0,19}Hg_{0,81}Te$ with an initial concentration of $p_{77} = 8 \cdot 10^{16}$ cm^{-3}, obtained by a modified method of band solid recrystallization, were studied. The concentration of carriers was regulated by low-temperature annealing in saturated mercury vapor. Relaxation tests of the samples were performed in the temperature range (273–400 K). Fig. 7 shows the results of such tests for samples of different deviation from stoichiometry.

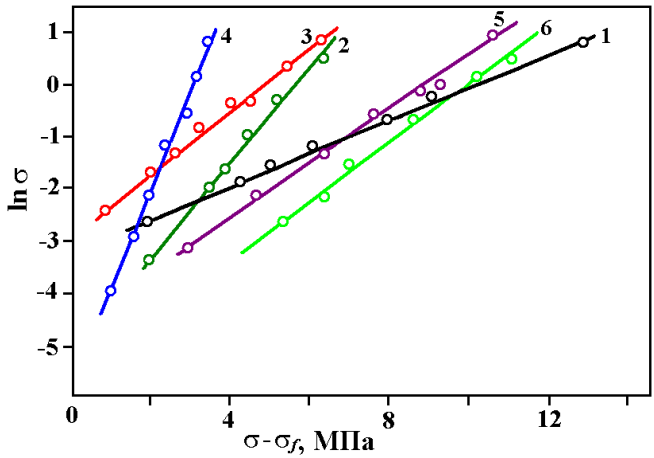

Figure 7. **Experimental stress relaxation curves of $Cd_{0,2}Hg_{0,8}Te$ single crystals at different temperatures with different stoichiometry in the coordinates ln** σ - (σ – σf): p77 = 8 · 1016 cm-3, 1 - 293 K, 2 - 380 K; n77 = 2 · 1015 cm-3, 3 - 293 K, 4 - 378 K; p_{77} = 1018 cm-3, 5 - 293 K, 6 - 374 K

In the table 1 shows the results of calculations of activation parameters of the studied crystals.

Table 1. Activation parameters of dislocation motion in $Cd_xHg_{1-x}Te$ crystals

Table 1

№	Crystal	Type of conductivity	Concentra-tion of charge carriers $см^{-3}$ (T = 77 K)	Activa-tion volume, V_a, b^3	Activa-tion energy, U, eV	Yield strength, kgf/ mm2 (T = 300 K)
1.	$Cd_{0,19}Hg_{0,81}Te$	p	$8 \cdot 10^{16}$	14	0,37	2,73
2.	$Cd_{0,19}Hg_{0,81}Te$	p	$4 \cdot 10^{17}$	11	0,41	3,20
3.	$Cd_{0,19}Hg_{0,81}Te$	p	$1 \cdot 10^{18}$	22	0,14	2,65
4.	$Cd_{0,19}Hg_{0,81}Te$	n	$2 \cdot 10^{15}$	19	0,35	1,54
5.	$Cd_{0,19}Hg_{0,81}Te$	n	$1 \cdot 10^{16}$	19	0,35	1,56
6.	$Cd_{0,19}Hg_{0,81}Te$	n	$1 \cdot 10^{16}$	18	0,32	1,48

These results indicate the following situation. A small increase in the concentration of acceptors after high-temperature heat treatment (HT HT) to $p = 4\ 10^{17}$ cm^{-3} leads to the strengthening of the crystal. The value of the activation volume V_a decreases from 14 to 11 b^3, and the activation energy increases slightly. When reaching the maximum concentration of holes for a given sample ($p = 10^{18}$ cm^{-3}), its yield strength decreases, and the value of V_a exceeds the corresponding value for the original sample by almost 1.5 times. The activation energy is reduced from 0.37 eV for the original sample to 0.14 eV. As we can see, the differences in the activation parameters of n – type samples are insignificant. The latter suggests that interstitial mercury atoms do not act as local stoppers for mobile dislocations.

Thus, for the studied samples, the activation energy of dislocation motion, depending on the stoichiometry of the crystal, is in the range (0.14 - 0.41 eV), and the value of the activation volume is (11–22 b^3). The study of the velocity dependence of the yield strength in the temperature range 77–420 K revealed that the dependence $\ln\varepsilon = f(1 / T)$ for p-$Cd_xHg_{1-x}Te$ single crystals consists of two sections with sharply different slopes (Fig. 8).

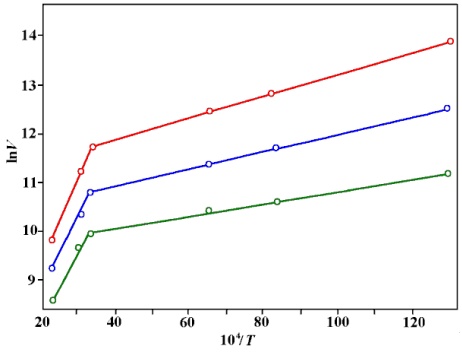

Figure 8. **Dependence of the logarithm of the strain rate on the inverse temperature for crystals $Cd_{0,2}Hg_{0,8}Te$ at σ = const**

Estimation of the activation energy in the low-temperature region (77 - 303 K) gave a value of 0.02 eV, and in the high-temperature region - 0.1 eV.

The values of the activation parameters of the dislocation motion correspond to the Peierls mechanism of dislocation movement. However, when analyzing the mechanisms controlling the process of plastic deformation of $Cd_xHg_{1-x}Te$ crystals, it is necessary to take into account the role of stoichiometry defects in inhibition and propagation of dislocations. From the above data of the velocity dependence of the yield strength in a wide temperature range, it follows that the plastic deformation of $Cd_xHg_{1-x}Te$ crystals within the main Peierls mechanism is obviously controlled by several mechanisms, the contribution of each of which may vary depending on the operating temperature range.

One of the criteria for fulfilling the Pierrells mechanism of motion and propagation of dislocations is known to be the independence of the activation volume from the degree of deformation, as well as its rapid increase at low stresses. Such dependences obtained for the studied crystals of solid solutions (Figs. 9, 10) indicate the possibility of interpreting the plastic deformation of ternary crystals within the Peierls model, but taking into account the peculiarities of plastic fluidity of near-surface layers, band structure and stoichiometry of the studied crystals.

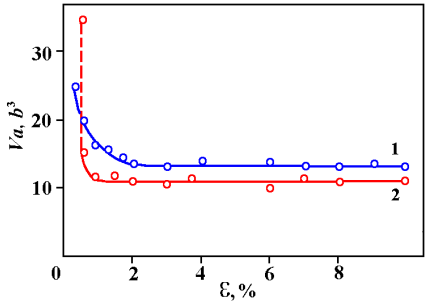

Figure 9. **Dependence of the activation volume on the degree of deformation for n-$Cd_{0,2}Hg_{0,8}Te$** (1-direction of the compression axis <111>, 2 - <110>)

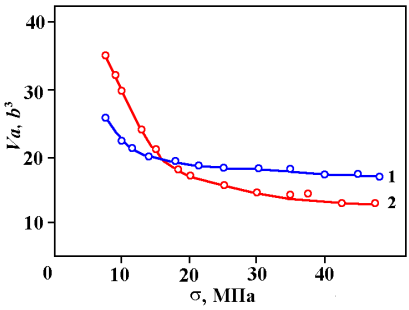

Figure 10. **Dependence of activation volume on voltage for n-$Cd_{0,2}Hg_{0,8}Te$** (1 - direction of the compression axis <110>, 2 - <100>)

INFLUENCE OF LIGHTING ON PLASTIC FLUIDITY.

The studied crystals are also characterized by a change in the process of uniaxial dynamic compression of the stress of plastic fluidity under the action of light. This phenomenon is called - photoplastic effect (PPE). Since PPE is a typical phenomenon for crystals of broad band compounds A^2B^6, and the component of the solid solution CdTe - has a positive effect, it was advisable to investigate the presence and nature of this effect in narrowband crystals of ternary compounds $Cd_xHg_{1-x}Te$ semiconductor composition (x = 0.16-0.22) with E_g ~ 0.1 eV.

For the first time, the general regularities of negative PPE (NFPE) in narrow-band $Cd_{0,2}Hg_{0,8}Te$ crystals deformed at a constant velocity on a Regel– Dubov relaxometer at room temperature were observed in [7].

A typical diagram of σ - ε with the effect of photostrengthening of the crystal is presented in Fig. 11. It demonstrates that when the crystal is illuminated with white light from an incandescent lamp in the process of its uniaxial deformation at the stage after the fluidity tooth, the yield strength decreases rapidly and the crystal continues to deform with the previous coefficient of strain hardening. Turning off the light switches the crystal deformation to the previous mode. The phenomenon can occur repeatedly until the destruction of the sample.

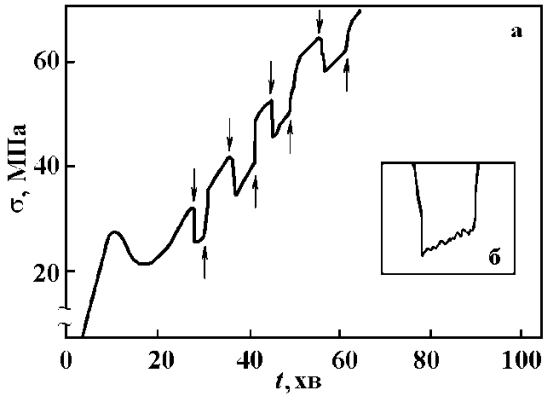

Figure 11. **Negative photoplastic effect of $Cd_{0,2}Hg_{0,8}Te$ crystal** (↑ - light on, ↓ -exclusion; V = 5.85 10^{-3} mm / min, T = 300 K; white light from an incandescent lamp)

It should be noted that the detection of PPE in narrow-band crystals when illuminated by light from the visible spectral range is a fact that was not expected in materials with a narrow band gap (~ 0.1 eV). An attempt to explain

this phenomenon based on ideas about the generation of nonequilibrium carriers using known mechanisms for wide-gap materials, did not give positive results.

Nature of NPPE in narrow bandgap CdHgTe crystals is related to the reduction in mechanical stress under the influence of light due to the decrease of the embedded positive charge at interphase 'intrinsic oxide –semiconductor" boundary [8]. This is accompanied by the decrease in the deformation barrier EMU for the exit of generated dislocations on the surface of the crystal, resulting in reduced level of fluidity stress in the crystal deformed at a constant rate under irradiation.

CONCLUSIONS.

Based on the thermoactivation analysis of the deformation process of CdxHg1-xTe solid solution crystals of different stoichiometry, it was found that the motion of dislocations is controlled by the Peierls mechanism with characteristic process parameters: U = 0.14–0.41 eV and Va = 10–21 b3. The load diagram is described by a four-stage dependence and has a characteristic "tooth" of fluidity. A set of studies of the deformation behavior of mixed crystals indicates that they have some contradictory properties that are not typical of typical semiconductors. In particular: in combination with low values of Pierrels 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 strength to the strain rate, a significant dependence of their mechanical parameters on temperature brings these crystals closer to metals. Illumination of the crystal with white light in the process of uniaxial deformation is accompanied by a decrease in the stress of plastic fluidity of the crystal (capacitive photoplastic effect).

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