Thermally activated motion of dislocations in irradiated KBr crystals

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Abstract. Dynamics of thermally activated motion of dislocations in real time were studied by recording the pulses of electrical potential on the surface of the KBr crystals (in situ). It is shown that the radiation influence leads to crystals hardening, activation energy increasing and movement of dislocations initial stage shift to higher temperatures.

Keywords: alkali halide crystals, dynamics of dislocations, pulses of electrical potential

1. Introduction
Mechanical stresses in the crystal, powder, ceramic micro - and nanomaterials after pressing, are eliminated by prolonged thermal annealing. Residual stresses occur in these materials after radiation sintering also. Since the relaxation of mechanical stresses in crystalline dielectrics is determined by the motion of charged dislocations, it is necessary to investigate the dynamics of their thermally activated motion, which is extremely time-consuming process.

It is known that the motion of charged dislocations is accompanied by a pulse change of the electric potential on the surface of the crystal [1-3]. Starting temperature and the activation energy of their thermally activated motion is defined by recording the pulses of electrical potential (PEP) on the surface of LiF crystals [4]. In this work, the dynamics of thermally activated dislocations in the radiation-irradiated crystals in real time (in situ) was studied by recording PEP by the example of alkali halide crystals KBr.

2. Experimental techniques
Samples of KBr crystals (size 15×15×0,89…1,0 mm) were prepared from artificially grown from the melt of the crystals. The dislocations density is not more than 10^5 sm^-2 by the etching method. Platinum electrodes, which served as a capacitive sensor antenna, is applied on the pattern surface by the method of cathode sputtering in a vacuum. The using of these type electrodes results to reduce ten times the level of background radiation, due to the near-electrode processes [5]. Electrical signals were amplified using high-frequency broadband amplifier, and then they were observed on the oscilloscope screen and were recorded by counting device counting mode pulse per unit time. Measurements were carried out in vacuum while heating at a constant rate 0,1 К·s^{-1} with a sensitivity of the 350 μV in the frequency range 100…2·10^7 Hz. The samples of crystals were subjected to x-ray irradiation (U=50 kV, I=20 mA, t=1 h).

3. Result and discussion
Figure 1 presents the temperature dependence of the counting rate of the pulses of electrical potential and synchronously measured thermally stimulated luminescence (TSL) of crystals KBr. We can observe two areas differing of the counting rate of the pulses of electrical potential. The first portion (a) is the number of the maximum PEP counting rate that are correlated with TSL. It is due to thermal annealing hole centers with subsequent recombination of holes on the F-centers [6].
Figure 1. The counting rate changing the pulses of electrical potential (a, b) and luminescence (b) by thermal stimulation KBr crystals irradiated by x-rays.

Figure 2. The parameters of the pulse shape of the electric potential of the irradiated x-ray crystals KBr in the field thermally activated motion of dislocations. The speed of the scanner 10 is seconds, the amplitude of the 500 μV/span.

The second part (b), above 220 °C, there has been exponential growth PEP exceed the background level by more than three orders of magnitude. Then the counting rate pulses of electrical potential reaches the maximum value and has some tendency to decrease but it remained high. Non-irradiated crystals have only the second high-temperature portion (b).
The pulses of electrical potential is observed on the oscilloscope screen in the form of signals, both positive and negative polarity, bell-shaped form with the amplitude of 10 mV with a duration of the leading edge 10...20 μs (Fig. 2). Because «jump» of dislocations occur spontaneously, it can be superimposed pulses of electrical potential, resulting in the observed pulses of complex shape.

The sharp increase of the counting rate of pulses on part (b) begins with some “starting“ temperature, which is characteristic for various alkali halide crystals. It coincides with the known research results of dislocations dynamics.

According to modern concepts [7, 8], the motion of dislocations in the crystal becomes possible when the energy of the dislocation is sufficient to thermofluctuation overcoming the retarding its movement stoppers. Since some "starting" temperature the spontaneous dislocations movement occurs and its number increases with temperature. Surrounded by a «cloud» of charged defects the dislocations moves jumply at low speed (<10⁻³ sm c⁻¹) without looking up from his «cloud».

When jumping motion of a charged dislocations relatively to compensating its charge cloud of the Debye-Hückel due to the separation of the centers of gravity of the charges, an electric dipole moment. The appearance of the pulses of electrical potential on the surface of the crystal caused by the oscillations of the electric dipole moment

Caused by pulse of electric potential dipole moment \( P_i \) is determined by the expression

\[
P_i = \eta \times q \times d \times \xi,
\]

where \( \eta \) is the number of dislocations segments, making simultaneous jump,
\( d \) is the length of the segment,
\( q \) is the linear charge density per unit length of dislocations,
\( \xi \) is the offset dislocations relative to the compensating its charge cloud.

The magnitude of the electric potential \( \phi \) on the crystal surface, at a distance \( r \) is determined by formula

\[
\phi = (P \times r) / 4\pi \varepsilon_0 \varepsilon r^3
\]

Given for alkali halide crystals the average evaluation values included in this ratio (\( q \approx 3,1 \times 10^{-11} \) K/m, \( d \approx 6,6 \times 10^{-6} \) m, \( \xi \approx 1,0 \times 10^{-6} \) m [7, 8]) we obtain the minimum detectable value of the dipole moment \( P_i \approx 1,0 \times 10^{-21} \) K•m and the potential on the surface (\( r \approx 5 \times 10^{-4} \) m), corresponding to the sensitivity threshold detection scheme \( \phi \approx 350 \) μV at \( \eta \approx 3 \).

It is quite possible the simultaneous collective movement of a large number of the dislocation segments [3].

Due to the thermally activated dislocations motion, counting rate changing the pulses of electrical potential described by the formula [4]:

\[
N \approx A N_0 \exp \left(- \frac{E_a}{kT}\right),
\]

where A is the coefficient, generally depends on the density of mobile dislocations, the dislocations in the number of jumps per unit time, concentration of stoppers, etc.

According to this formula, the dependence \( \lg N = f (1/T) \) should be a straight line. Indeed, the experimental point of high-temperature portion for the temperature dependence counting rate changing the pulses of electrical potential is a straight line, its declination corresponds to the thermally activated dislocations motion energy (Fig.3). The change of activation energy reflects the dislocations dynamics and their interactions with local stoppers.

The dislocations motion in non-irradiated crystal KBr begins since \( \approx 180 \) °C, but in crystals irradiated by x-rays since \( \approx 220 \) °C, wherein in "start-up" stage, the activation energy in the irradiated crystals reaches 1.26 eV. Starting values of energy thermally activated motion of dislocations in all probability can not be less than the bond energy center fastening with dislocation.
Figure 3. Changing the values of energy of thermally activated dislocations motion in non-irradiated (a) and irradiated by x-rays (b) KBr crystals

Experimentally we observe the values of the starting temperature at which breakaway of dislocations from the stopper occurs only due to the thermal motion in radiation irradiated and non-irradiated alkali halide crystals correspond to the definitions produced by the method of internal friction by extrapolation based the activation energy at zero amplitude deformation [7].

Further changes in the activation energy occurs in several stages and then reaches its minimum value of 0.23…0.28 eV. The values of activation energy, for example, in deformed crystals KBr ≈ 0,3 eV, obtained by different methods, probably correspond to the "above-barrier" dislocations motion [9] when their interaction energy with stoppers is not affected to the dislocations moving, because it is overcome by the power of external mechanical, electrical, or heat exposure in our case.

Jumping motion of charged dislocations cannot be explained only by the presence of random barriers along the path of motion. Jumping motion of charged dislocations is their own property and, therefore, it is determined by the state of the dislocations and its "atmosphere" - the clouds surrounding the charged defects [10]. Irradiation of the crystals by x-rays leads to the appearance of charged radiation-induced defects in the crystal, which also interact with dislocations, represent itself as stopper.

4. Conclusions
The temperature dependence counting rate the pulses of electrical potential of in alkali halide crystals at high temperatures reflects the dynamics of thermally activated dislocations motion.

This is confirmed by the literature and experimental data on the dynamics of dislocations in alkali halide crystals obtained by other methods (etching of the surface, internal friction, and others). Irradiation of crystals ionizing radiation leads to the increase of activation energy of their thermally activated motion. It indicates the dislocations pinning and strengthening crystal. This method can be very effective to study the influence of radiation and thermal processes at strengthening crystals (including ceramic) materials in real time (in situ).
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