Abstract

The sonoluminescence of ionic semiconductors were studied. The main attention is paid to threshold phenomena which accompany the light irradiation, namely — point defect creation and nonlinear ultrasound wave attenuation. The model for description of processes under investigation which connects the sonoluminescence excitation with the onset of point defects (vacancies and interstitials) generation by moving under ultrasound action screw dislocation with a jog. The attempt is made to estimate the parameters of crystals which define the jog motion in its crystal relief.
1 Introduction

The problems of dislocation dynamics, especially nonlinear one, and defects in crystals are still of high interest \[1, 2, 3, 4, 5\]. Among them there is well-known effect of acoustic waves on ionic crystals (mainly, semiconductors) which is studied and investigated in details (see, for example, \[6, 7, 8, 9\]). Sound and ultrasound (US) treatment results in change of the various important characteristics of semiconducting media, which, in its turn, can depend upon amplitude of acoustic waves. The most interesting here are those phenomena, when the changes induced by such waves have threshold character, i.e., are observed when wave amplitude reaches the certain value. One of these brightly threshold phenomena is sonoluminescence (SL), which was discovered by Ostrovskii et al. \[10\] (see also \[11\]) and represents a glow of ionic crystals, subjected to an US load of an overthreshold amplitude.

The analysis of SL spectra has allowed to establish \[11\] that the large role in SL excitation is played by the crystal point defects of crystal, number of which essentially increases above the threshold. In such a situation it was natural to suppose generation of point defects, which can be stipulated by the motion of dislocations, to be the reason for threshold. As a whole the sequence of processes can be such that, that US shakes dislocations (edge and screw) available in a crystal, the amplitude of their motion being proportional to the amplitude of US wave. Thus, free segments of the dislocations between the pinning points are oscillating only. However any new defects cannot be generated by them.

There are several ways known for point defects to be created \[12\], one of which is climbing of jogs on screw dislocations. Other ways (for example, intersection with dislocations of the “forest”) in conditions of rather small density of the dislocations should be less effective.

In the present paper an attempt is made to consider the threshold phenomena connected just to generation of defects by a driven jog on a screw dislocation. An equation of such a motion is investigated for US amplitude value up to a threshold and after it. Experimental study on amplitude relations of US damping in ionic crystals is also conducted. The results obtained are compared to the theory.

2 Model of Nonlinear Dynamics of Dislocation with a Jog
2.1 Approach and Equations

The jogs on a screw dislocation can be regarded as some kind of pinning points, which, however, in difference from usual ones, can at some conditions move together with its “own” dislocation. This motion is not free, and any displacement of the jog between its initial position and nearest, final, one is always accompanied by a creation of a point defect — vacancy or interstitial. Already this implies that such positions appear nonequivalent, and consequently the potential \( W_{\text{jog}}(y_{\text{jog}}) \) of a jog proposed in Ref. [13] in difference, for example, with a potential of Peierls relief is not symmetrical under translations (see Figure 1). Just this potential determines the motion of the jogs in a crystal, which we shall consider below. We should notice only that the energy of the point defect creation makes usually a few eV; so the thermal overcoming of appropriate barriers by a jog is improbable. Therefore here the essential role should be played by forces due to oscillating dislocation segments, or, in other words, by forces of linear tension.

Let us consider the simplest case of a segment of a screw dislocation of length \( 2L \) with a jog in the middle, the ends of which are fixed on so-called strong (i.e., immovable) pinning points. Then (in a neglect by a Peierls relief that is fair for the relatively high temperatures) the motion of the free segments of a dislocation in US field is described by well-known model of an elastic string [14]; corresponding equation of a motion may be written in the form:

\[
M_{\text{dis}} \frac{\partial^2 y}{\partial t^2} + B_{\text{dis}} \frac{\partial y}{\partial t} - T_{\text{dis}} \frac{\partial^2 y}{\partial x^2} = -\sigma_{zx}'(t) b,  
\]

where \( x \) is a coordinate along a dislocation, \( y(x) \) is transversal displacement, \( t \) is the time, \( M_{\text{dis}} \) is a dislocation mass per unit length, \( B_{\text{dis}} \) is a factor of a friction, \( T_{\text{dis}} \) is a linear tension of a dislocation string, \( b \) is a Burgers vector, \( \sigma_{zx}'(t) \) is appropriate (active) component of stress deviator, caused by US.

Let the jog be placed in a point \( x = x_{\text{jog}} \). A condition of a dislocation pinning down (at small US amplitudes) is then

\[
y(x_{\text{jog}}) = 0 \quad (2)
\]

At large amplitudes of an external force (i.e., of the exciting US wave) the condition (2) should be replaced by an equation of a jog motion, which can be written as

\[
M_{\text{jog}} \frac{\partial^2 y_{\text{jog}}}{\partial t^2} + B_{\text{jog}} \frac{\partial y_{\text{jog}}}{\partial t} + \frac{\partial W_{\text{jog}}}{\partial y_{\text{jog}}} = T_{\text{dis}} \left( \frac{\partial y}{\partial x} \right)_{x_{\text{jog}}+0} - \left( \frac{\partial y}{\partial x} \right)_{x_{\text{jog}}-0}, \quad (3)
\]

where \( M_{\text{jog}} \) and \( B_{\text{jog}} \) are a jog mass and friction coefficient for it, correspondingly (they, as well as \( M_{\text{dis}}, B_{\text{dis}}, \) are phenomenological parameters), and \( W_{\text{jog}}(y_{\text{jog}}) \) is Loktev-Khalack
potential (see Figure 1). In general case its form depends upon all previous positions of a jog. For example, if the last has moved from a position A on Figure 1 to position B with a vacancy being created, the branch $AB'CD'$ has ceased to exist. In other words, the jog can return “initial geometry” only passing exactly to $C'$ on the curve $W_{\text{jog}}(y_{\text{jog}})$, for what it needs to overcome a potential barrier, appropriate to the interstitial formation. Thus, it is essential that the energies of the formation of the vacancies and interstitials are definitely different; it naturally makes a potential relief $W_{\text{jog}}(y_{\text{jog}})$ central-asymmetrical one and is reflected in the jog motion under the action of US wave.

### 2.2 Threshold characteristics

Let an US wave with the amplitude of acoustic displacement $u_{\text{ac}}$ and frequency $\omega_{\text{ac}}$ be spreaded in a crystal. Then the force per unit length exerted on the dislocation (see (1)) is

$$-\sigma'_{zx}(t)b = f_{0r}\frac{\omega_{\text{ac}}u_{\text{ac}}b}{v_{\text{us}}}\cos\omega_{\text{ac}}t = \sigma_{\text{us}}b\cos\omega_{\text{ac}}t,$$

where $f_{0r}$ is some factor, dependent on the orientation of an US wave (on its polarization and the direction of propagation in a crystal), and $v_{\text{us}}$ is a sound velocity. Under the action of force (4) free segments of a dislocation begin bowing out and in accordance with the increase of $u_{\text{ac}}$ a situation will set in, when the amplitude of this bowing out (and consequently, pulling forces of a linear tension exerting on the jog) will become sufficient for the jog to overcome the potential relief. The amplitude of this force is determined (see a right term in Eq.(3)) by condition

$$\frac{|\partial W_{\text{jog}}}{\partial y_{\text{jog}}} = T_{\text{dis}}\left(\frac{\partial y}{\partial x} + \frac{\partial y}{\partial x}\right)_{\text{max}}.$$

The solution of equation (1) together with (5) for the case of external force (4) gives the following expression for the threshold amplitude of US produced displacement:

$$u_{\text{ac}}^{\text{thr}}(\omega_{\text{ac}}) = \frac{v_{\text{us}}M_{\text{dis}}L}{\omega_{\text{ac}}^2 f_{0r}bT_{\text{dis}}} \left[I_1^2(\omega_{\text{ac}}) + I_2^2(\omega_{\text{ac}})\right]^{-1/2} \left|\partial W_{\text{jog}}\right|_{\text{max}},$$

with the substitutions

$$I_1(\omega_{\text{ac}}) = \sum_{n=0}^{L/2b} \frac{\Omega_n^2 - \omega_{\text{ac}}^2}{(\Omega_n^2 - \omega_{\text{ac}}^2)^2 + (\omega_{\text{ac}}\Gamma_{\text{dis}})^2}.$$
$$I_2(\omega_{ac}) = \sum_{n=0}^{L/2b} \frac{\omega_{ac}\Gamma_{\text{dis}}}{(\Omega_n^2 - \omega_{ac}^2)^2 + (\omega_{ac}\Gamma_{\text{dis}})^2},$$

and

$$\Gamma_{\text{dis}} = \frac{B_{\text{dis}}}{M_{\text{dis}}},$$

where

$$\Omega_n^2 = \frac{\pi^2(2n+1)^2T_{\text{dis}}}{M_{\text{dis}}L^2}$$

are the eigen-frequencies of the dislocation segments \(n=0,1,...\). The obtained expressions (7), (8) testify that at \(\Gamma_{\text{dis}} < \Omega_0\) the threshold characteristics defined by (6), should have resonant character (see Figure 2).

### 2.3 Point defect generation

The asymmetrical form of a curve \(W_{\text{jog}}(y_{\text{jog}})\) stipulates that basic conclusion, that a threshold condition (5) for the jog motion with a formation of vacancies begins to hold still before an appropriate condition for the motion with interstitials formation. Then it is easy to see that for the amplitude \(u_{ac}\) between these two threshold values the jog can move and move during an only one halfperiod of every period of the external force action. It means that in the given range of US amplitudes the jog drift happens only in one direction, and a creation of one vacancy corresponds to each its climb.

Already from physical reasons it is clear, that the appearance of vacancy gives premises for lattice relaxation in a vicinity of a defect, which with necessity should be accompanied by an acoustic emission. It is important that such an emission happens before transition of a jog to an oscillatory mode. On the other hand, transfer of the jog into some new position at corresponding value \(u_{ac}\) causes a reduction of resultant forces of a linear tension along the \(x\) axis. As a result this total force will decrease so that further jog climbing will become impossible, and the jog will stay in new, biased rather initial, equilibrium position.

However, such a displacement has also a positive effect, if a reduction of threshold US amplitude necessary for interstitial formation is to be mentioned. This threshold value is determined by the same formula (6), in which instead of value of derivative \(\partial W_{\text{jog}}/\partial y_{\text{jog}}\)|\(_{\text{max}}\), appropriate to interstitial formation, stands a half-sum of appropriate derivatives for two opposite directions; the observable threshold for full oscillatory jog
motion is given by

\[ u_{ac}^{thr}(\omega_{ac}) = \frac{v_{us}}{8\omega_{ac}} \frac{M_{\text{dis}}}{f_{\text{us}}bT_{\text{dis}}} \frac{|\partial W_{\text{log}}/\partial y_{\text{log}}|_{\text{max}}^i + |\partial W_{\text{log}}/\partial y_{\text{log}}|_{\text{max}}^v}{\sqrt{I_1^2(\omega_{ac}) + I_2^2(\omega_{ac})}}. \]  

(11)

Thus, after a beginning of large-amplitude oscillatory jog motion (i.e., after overcoming by the amplitude \( u_{ac} \) of its threshold value (11)) continuous generation of defects of both types begins. The total number of defects generated by jog per one US wave period above the threshold grows proportionally to US amplitude.

### 2.4 US attenuation

Because of real crystals containing the dislocations of different length, let us consider a pure single-crystal with a network of dislocations, as well as a certain quantity of point defects, being the weak pinning centers for the former ones. It is assumed also that initial concentration of the point defects is small enough for the mean distance \( L_c \) between them to be of the order of the network length \( L_N \):

\[ L_c(0) \sim L_N. \]

If the acoustic stress of small amplitude is applied to a crystal, the dislocations are bowing out between pinning points, which results in amplitude-independent US attenuation. At the higher stresses a breakaway occurs, giving rise to hysteresis losses, and consequently to the increase of US attenuation (see [14]).

But in the case under consideration (\( L_c(0) \sim L_N \)) the increase of attenuation due to dislocations unpinning from the weak pinning centers may be negligible, so that the amplitude dependence of the US attenuation is determined by the motion of the jogs on the skew dislocations. When the amplitude of an acoustic stress is sufficient for a creation of the vacancies, the jog merely changes its equilibrium position, not causing hysteresis losses by itself. The attenuation is changed by the newly created vacancies. The last serve as the additional weak pinning centers for the dislocations, so that the attenuation coefficient for low frequency range is given by Granato-Lücke expression [14]

\[ \alpha_H(\omega_{ac}, \sigma_{\text{us}}) = \frac{\omega_{ac} \Lambda L_N^3}{2v_{\text{us}} L_c} \frac{8\mu b^2}{4b\sigma_{\text{us}}L_c} \left[ \frac{\pi f_m}{4b\sigma_{\text{us}}L_c} - 1 \right] \exp \left( -\frac{\pi f_m}{4b\sigma_{\text{us}}L_c} \right), \]  

(12)

where \( \Lambda \) is the dislocation density, \( \mu \) is a shear modulus, \( f_m \) is the maximum value of the binding force. Here the value of \( L_c \) is no longer equal to the initial value \( L_c^{(0)} \), but depends on the amplitude of acoustic stress \( \sigma_{\text{us}} \). In the assumption that the vacancies are
uniformly distributed throughout the volume, \( L_c \approx (N_v(\sigma_{us}) + (L_N)^{-3})^{-1/3} \). The number of vacancies per unit volume is

\[
N_v(\sigma_{us}) = \frac{L_{\text{max}}}{L^v(\sigma_{us})} \int N_{\text{jog}}(L) \frac{Y(L, \sigma_{us})}{y_0} dL,
\]

(13)

where \( N_{\text{jog}}(L) \) is the distribution function for the dislocations with jogs, \( Y(L, \sigma_{us}) \) is the displacement of a jog from its initial position in the US field, \( y_0 \) is a lattice spacing, and \( L^v(\sigma_{us}) \) is the minimum half-length of a dislocation, the jog on which can climb at given value of \( \sigma_{us} \). If we suggest that \( N_{\text{jog}}(L) = N_{\text{jog}} = \text{const} \), then

\[
N_v(\sigma_{us}) = \frac{2N_{\text{jog}}L_{\text{max}}^{3}}{3\pi^{2}T_{\text{dis}}^{2}} \frac{\sigma_{us} - \sigma_{us}^{v}}{(2\sigma_{us} + \sigma_{us}^{v})^{2}},
\]

(14)

For stresses high enough for the jog transition into an oscillatory mode (i.e., for \( \sigma_{us} > \sigma_{us}^{\text{thr}} \)) the attenuation of US is determined by the losses due to creation of point defects. The attenuation coefficient for this case is

\[
\alpha_{\text{jog}}(\sigma_{us}) = \frac{\omega_{ac}^{2}}{2v_{\text{us}}} \mu \left( W_{v} + W_{i} \right) \int_{L^\text{thr}(\sigma_{us})}^{L_{\text{max}}} N_{\text{jog}}(L) \frac{\Delta y_{\text{jog}}(L, \sigma_{us})}{y_0\sigma_{us}^{2}} dL,
\]

(15)

where \( W_{v} \) and \( W_{i} \) are correspondingly the energies of creation of vacancy and interstitial, \( \Delta y_{\text{jog}}(L, \sigma_{us}) \) is the amplitude of the jog oscillations, and \( L^\text{thr}(\sigma_{us}) \) is the minimum half-length of dislocation, the jog on which is oscillating. If we adopt the above assumption \( N_{\text{jog}}(L) = \text{const} \), the amplitude dependence of attenuation is given by the factor

\[
\frac{(\sigma_{us} - \sigma_{us}^{\text{thr}})^{2}(2\sigma_{us} + \sigma_{us}^{\text{thr}})}{\sigma_{us}^{4}}
\]

(16)

(the account is taken of proportionality of \( \Delta y_{\text{jog}}(L, \sigma_{us}) \) to the difference \( \sigma_{us} - \sigma_{us}^{\text{thr}} \)).

The further increase of acoustical stress can activate the Frank-Read sources, as well as additional slip planes (in accordance with the factor \( f_{\alpha} \) in (4)), the last giving rise to new threshold-like peculiarities in the amplitude dependence of US attenuation.

The behaviour of the attenuation during the unloading cycle is determined by the newly created defects. Additional dislocations lead to the increase of losses, while the point defects reduce losses to some extent. It is noteworthy that the amplitude dependence of US attenuation below the threshold in the case of unloading is given by the expression (12) with the constant value \( L_c \), because the jogs are fixed at some new positions and cannot create any point defect. The qualitative form of the curve of the amplitude dependence of US attenuation during the loading and unloading cycles is shown at Figure 3.
3 Experiment and Analysis

The monocrystalline samples NaCl, KCl, and ZnS (sphalerite) were experimentally studied at room temperature. The initial density of dislocations in crystals under investigation not subjected to US treatment made for NaCl about $10^4\text{cm}^{-2}$ and for ZnS — about $5 \cdot 10^3\text{cm}^{-2}$. Longitudinal US waves were excited by piezoceramic transducers of PZT type within a frequency range $1.5 \text{MHz} \lesssim (\omega_{ac}/2\pi) \lesssim 7 \text{MHz}$. The factor $\alpha$ of US attenuation was measured by two techniques: 1) by comparing of the exciting US rf-voltage $V$ with those picked up from receiving transducer, and 2) with the help of a probing pulse by an echo-pulsing method. The US waves were excited by a continuous rf-voltage.

Typical dependence of US attenuation $\alpha$ on US amplitude taken from the sample KCl-1A is shown on Figure 4. Along X axes a rf-voltage $V$ of the frequency $f = (\omega_{ac}/2\pi) = 2.5 \text{MHz}$ is given. US amplitude is proportional to this voltage. It is seen that at a low amplitude $V$ the attenuation of US wave is equal to some value (point A) which remains practically constant at $V$ increase up to a point B ($V \approx 10 \text{ V}$). After this value of $V$ the attenuation begins to decrease (part BC of the curve). This reduction can be explained by the threshold vacancy generation as it was described in Section 2.4.

Part CD of this curve corresponds to attenuation growth when the generation of vacancies as well as interstitials begins (cm. parts BC and CD of the theoretical curve at Figure 3). It is interesting to notice that according to the calculations the very onset of vacancies generation is accompanied by some small attenuation increase. It can be interpreted as a result of competition between hysteresis losses grows due to the dislocations breakaway near the “old” pinning centers and generation of new ones (vacancies), which cause free dislocation segments slowing down. It seems that observable peak at the part AB of the experimental curve can be qualitatively ascribed to the effect reminded. The relatively strong additional growth of attenuation (part DE) is possibly provoked by activation of dislocations with jogs motion in another slip plane, what results in one more threshold value \[15\].

Figure 5 represents the results of the same study of the sample KCl-2 under US of $f = 1.75 \text{ MHz}$. There were two cycles of a loading. In the first case a voltage raised up to a point C below the threshold (curve 1), and then lowered to zero (curve 2). In the second case $V$ increased up to a value above the threshold (point D', curve 3). It is seen that for both samples a hysteresis character of attenuation dependencies is evidently observed. However the concrete shape of the curves depends directly on the maximum amplitude of the acoustical wave propagating in the sample. If the last is larger than the threshold one, then the US attenuation during the unloading is greater than that for the loading because of additional dislocation density. But if the maximum US amplitude is less than
the threshold one (though is sufficient for vacancy generation), then the unloading curve is found below the loading one, in accordance with the greater number of weak pinning centers present at the moment.

As a whole, observable US attenuation meets rather good qualitative agreement with the predictions of the model proposed. One of the most important ones among them is the coincidence of the threshold of the SL excitation with that of the point defect generation. Figure 6 confirms this supposition: such an equality, in fact, takes place (see curve 1 for SL and curve 2 for US attenuation, both of which are sharply changed at the same value of US amplitude).

As to quantitative agreement of experimental and theoretical curves, it should be emphasised that their shape depends strongly on the dilocation length distribution, the character of which is not known for samples under investigation. The single quantity to be derived from this studies exactly is a ratio of the threshold values of US amplitude for continuous point defects generation and for creation of vacancies. It gives a ratio of activation energies of interstitial and vacancy creation by a jog by means of the following expression, as it easily can be obtained from (6) and (11):

$$\frac{W_i^*}{W_v^*} = 2\frac{u_{ac}^{thr}}{u_{ac}^v} - 1.$$  \hspace{1cm} (17)

Results of our experiments shown on the Figure 4 and 5 give this ratio to be about 3. Indeed, as it seen from these figures, $(u_{ac}^{thr}/u_{ac}^v) \sim 2$, where $u_{ac}^{thr}$ corresponds to 1, and $u_{ac}^v$ is $\approx 0.5$ in relative units. The correlation between $W_i^*$ and $W_v^*$ well satisfy the values found from radiation experiments [16].

4 Conclusions

The main results of the given work can be formulated as follows:

1. The model for point defect generation by moving under US wave action jog on skrew dislocation is proposed. It predicts the threshold character of this motion which is defined by energies of creation of the vacancy or interstitial. It must be however noticed that in the simplest above approximation we restricted ourself to one sort of vacancies and one sort of interstitials. In fact, the jogs in real crystals can generate different point defects of one type which can differ, for example, by their charges (valencies). Namely that can be a reason for observation of various impurity center spectra as SL.

2. The US wave nonlinear absorption as a function of US amplitude reveals before threshold minimum which was explained above by supposition that new (generated by
jog) point defects (vacancies) become the additional pinning centers for free dislocation segments.

3. The experimental study of some semiconducting compounds showed that observable dependencies need satisfactory agreement with predictions of the model developed. It allows to estimate some energetical crystal parameters which are in agreement with data obtained from independent investigations.

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Figure captions

Figure 1: Potential relief of jog in a crystal. The right and left sides of this relief correspond to jog motion with generation of vacancies and interstitials.

Figure 2: The dependence of threshold US amplitudes upon its frequency. The upper and lower curves describe the threshold values for interstitials and vacancy generation, correspondingly.

Figure 3: The general behaviour of US absorption under loading and unloading produced by US wave.

Figure 4: Experimental behaviour of US absorption by 1st KCl sample.

Figure 5: Experimental behaviour of US absorption by 2nd KCl sample.

Figure 6: The comparison of threshold US amplitudes for SL excitation and for continuous point defect generation.
Figure 1:
Figure 2:
Figure 3:
Figure 4:
Figure 5:
Figure 6: