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On the nature of ionic crystals' sonoluminescence excitation threshold: point-defect generation

V.M. Loktev, Julia Khalack*

Bogolyubov Institute for Theoretical Physics, National Academy of Sciences of Ukraine, 14-b Metrologichna Str., 252143 Kyiv-143, Ukraine

Abstract

The sonoluminescence (SL) observed in ionic (mainly, semiconducting) crystals under the action of megacycle range ultrasound (US) is explained with the help of an electric field of inhomogeneously moving charged dislocations. The threshold of SL excitation is suggested to be due to the generation of point defects to be excited by the above-mentioned electric field. The main mechanism of point-defect generation (PDG) is supposed to be the motion of jogs in screw dislocations. The potential relief for such a jog is proposed and the threshold value of US amplitude for the start of large amplitude jog motion is calculated. The results of numerical simulations of the driven jog motion showing that a certain number of vacancies should be created by a jog even before the threshold are presented. The possibility to detect these vacancies with the help of sonophotoluminescence spectra are explored. © 1998 Elsevier Science B.V. All rights reserved.

Keywords: Sonoluminescence; Ionic crystals; Dislocations; Point defects

Sonoluminescence (SL) of ionic crystals has been known for nearly 20 yr [1]. Since then it resisted all attempts to explain the very mechanism of the energy transfer from US wave of frequency $\omega_{ac} \sim 10^8$ Hz to optic excitations with frequency $\omega_{opt} \sim 10^{15}$ Hz.

Consideration of direct electron–phonon interaction in the ideal crystal makes no sense because of the large difference in the above frequencies. Therefore, some new agent accumulating the US energy should be taken into account. We supposed [2] that linear crystal defect – dislocations – could be such an agent. In ionic crystals these defects can be charged, therefore the high (up to 10^6 V/cm) electric field can exist in their vicinity. If the charged dislocation is moving through the crystal containing point defects (PD), the last can be excited by the electric field of the former one. The nonzero probability of PD electronic subsystem excitation consists of two parts which can be characterized as follows: (1) probability of electron tunneling in the presence of quasi-constant in time, but spatially inhomogeneous electric field of quasi-static dislocation [3]; (2) probability of electron excitation by a time-dependent (due to the spatial inhomogeneity) electric field of moving dislocation [2].

*Corresponding author. Fax: 38044 266 5998; e-mail: julia@nonlin.gluk.apc.org.

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The first approximation is good for the periods of time when dislocation is relatively far from the PD, and the second one works for the times when the PD is found within the dislocation core. Another possible way of PD excitation is a creation of this defect (see below) in an already excited state. Either way, the dislocation electric field should work.

One of the most specific features of SL is the exclusive threshold character of its excitation [4]. In Ref. [2] an attempt was made to explain this threshold by the motion of dislocation in the Peierls relief. But such an explanation does not work in the case of A_2B_6 compounds, which begin to glow under the US stresses much less than the Peierls one. So we should suppose that thermal overcoming of Peierls barriers takes place, and the threshold is due to something else, e.g. PDG. In fact, the experimental observations [4] show that the number of PD in the crystal after the threshold becomes much higher than before it. Therefore, it is quite reasonable to suggest that the sharp increase of SL intensity is caused by the large increase in the number of exciting objects, i.e., PD.

To obtain the threshold value of the US stress amplitude, let us consider a segment of screw dislocation of the length $2L$ with a jog in the middle. It is well known [5] that such a jog should create PD (vacancies or interstitials) when it moves in transversal direction with respect to the dislocation segment. The equation of the dislocation motion under the US action in the elastic string approximation is [6]

$$M_{\mathrm{dis}} \frac{\partial^2 y}{\partial t^2} + B \frac{\partial y}{\partial t} - T_{\mathrm{dis}} \frac{\partial^2 y}{\partial x^2} = \sigma \boldsymbol{b} \cos \omega t, \qquad (1)$$

where t is the time, x is a coordinate along a dislocation, $y\,(x)$ is its transversal displacement, M_{dis} is a dislocation mass per unit length, B_{dis} is a friction coefficient, T_{dis} characterizes linear tension, $\boldsymbol{b}$ is a Burgersvector, σ is the US stress amplitude, and $\omega \equiv \omega_{\mathrm{ac}}$. The boundary conditions taking into account the dislocation pinning down at the strong pinning points, are as follows:

$$y(-L) = y(L) = 0. \qquad (2)$$

The equation of motion of a jog can be chosen in the form (see Ref. [7])

$$M_{\mathrm{jog}} \frac{\partial^2 y_{\mathrm{jog}}}{\partial t^2} + B_{\mathrm{jog}} \frac{\partial y_{\mathrm{jog}}}{\partial t} + \frac{\partial W_{\mathrm{jog}}}{\partial y_{\mathrm{jog}}} = T_{\mathrm{dis}} \left(\left.\frac{\partial y}{\partial x}\right|_{+0} - \left.\frac{\partial y}{\partial x}\right|_{-0} \right), \qquad (3)$$

where

$$y_{\mathrm{jog}} \equiv y(x=0), \qquad (4)$$

M_{jog} is a jog mass, B_{jog} is the friction coefficient for it, and $W_{\mathrm{jog}}(y_{\mathrm{jog}})$ denotes the potential energy of a jog. The relief $W_{\mathrm{jog}}(y_{\mathrm{jog}})$ should have a form shown in Fig. 1. It reflects the fact that the jog motion in the positive direction is accompanied by the creation of vacancies, and the motion in the negative direction stipulates the creation of interstitials. Furthermore, this curve is not invariant under translations, because under conditions of fast diffusion of the PD into the bulk, the jog returns to its initial geometry by means of the creation of new PD rather than absorbing an 'old' one of the opposite topological sign.

The critical value of the US amplitude for the start of the jog motion can be estimated in the assumption that the amplitude of the force of a linear tension acting on the jog must be sufficient to pull it out from the local potential minimum:

$$\left| \frac{\partial W_{\mathrm{jog}}}{\partial y_{\mathrm{jog}}} \right|_{\max} = T_{\mathrm{dis}} \left(\left.\frac{\partial y}{\partial x}\right|_{+0} - \left.\frac{\partial y}{\partial x}\right|_{-0} \right)_{\max}. \qquad (5)$$

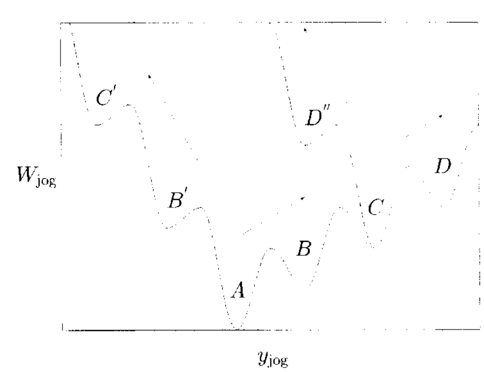

Fig. 1. The general form of the jog potential relief. The way ABCB does not exist; a possible one is ABCD''.

Then from Eqs. (1), (2) and (5) one can obtain

$$\sigma_{\text{th}}(\omega) = \frac{M_{\text{dis}}L}{8bT_{\text{dis}}} \frac{|\partial W_{\text{jog}}/\partial y_{\text{jog}}|_{\max}}{\sqrt{I_1^2(\omega) + I_2^2(\omega)}} \tag{6}$$

with the substitutions

$$I_1(\omega) = \sum_{n=0}^{L/2b} \frac{\Omega_n^2 - \omega^2}{(\Omega_n^2 - \omega^2)^2 + (\omega\Gamma_{\text{dis}})^2}, \tag{7}$$

$$I_2(\omega) = \sum_{n=0}^{L/2b} \frac{\omega\Gamma_{\text{dis}}}{(\Omega_n^2 - \omega^2)^2 + (\omega\Gamma_{\text{dis}})^2}, \tag{8}$$

where $\Omega_n^2 = \pi^2(2n+1)^2 T_{\text{dis}}/M_{\text{dis}}L^2$ are the eigenfrequencies of the dislocation segments ($n = 0, 1, \ldots$), and $\Gamma_{\text{dis}} = B_{\text{dis}}/M_{\text{dis}}$.

On account of the ('ratchet') asymmetry of the potential W_{jog}, the critical amplitude, Eq. (6), for the jog motion with generation of vacancies is less than that for interstitials. So for the force amplitude between these two values the jog can move in one direction only. The numerical simulation of Eqs. (1)–(4) show that such motion is not continuous in time (see Fig. 2). This fact is easily understood if one takes into account the geometric decrease of the resultant force of linear tension with the change of the jog position. It means that at some equilibrium position this force becomes insufficient for further jog motion, and the whole number of vacancies generated remains finite.

The large amplitude continuous in time (see Fig. 2) jog oscillations take place when the creation of interstitials is possible. The above geometric considerations give rise to the following expression for the threshold US stress amplitude:

$$\sigma_{\text{th}}^{i}(\omega) = \frac{M_{\text{dis}}L}{16bT_{\text{dis}}} \frac{|\partial W_{\text{jog}}/\partial y_{\text{jog}}|_{\max}^{i} + |\partial W_{\text{jog}}/\partial y_{\text{jog}}|_{\max}^{v}}{\sqrt{I_1^2(\omega) + I_2^2(\omega)}}, \tag{9}$$

where we distinguish between relief derivatives for the jog motion with vacancy (v) and interstitial (i) generation. Since the generation of PD of both types becomes continuous, Eq. (9) defines the threshold for SL excitation. As it is seen from Eqs. (7) and (8), the frequency dependence of the threshold amplitude, Eq. (9), can have the experimentally observed [4] quasi-resonant character only if $\Gamma_{\text{dis}} < \Omega_0$ (see Fig. 3). It is to be noted that the number of PD generated per one period of US wave is proportional to US amplitude (see Ref. [7] for the details of numerical calculations).

The vacancies are generated before the threshold can be detected, e.g., by sonophotoluminescence spectra. In fact, the experimentally observed [4] in CdS increase of the intensity of red line associated with the vacancy V_S^+ radiation along with the decrease of the intensity of green line which is due to interstitials Cd_i^+ just before the threshold can naturally be explained by US-induced vacancy generation.

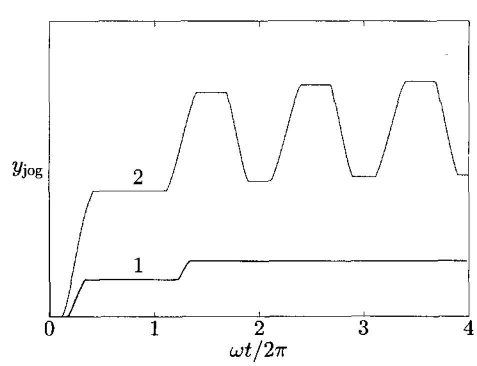

Fig. 2. Typical temporal behaviour of the jog displacement for the force amplitude above the first (1) and the second (2) threshold.

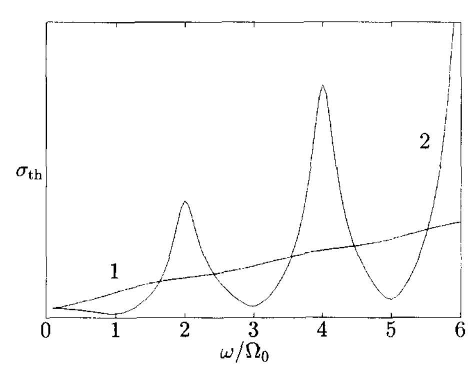

Fig. 3. The dependency of the threshold amplitude σ_{th} on the frequency. (1) $\Gamma_{\text{dis}} = 3\Omega_{\text{dis}}$; (2) $\Gamma_{\text{dis}} = \Omega_{\text{dis}}/3$.

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