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AMPLITUDE-DEPENDENT ULTRASOUND ATTENUATION DUE TO INCLINED DISLOCATIONS

Julia M.Khalack
Bogolubov Institute for Theoretical Physics
of the Ukrainian National Academy of Sciences
14^b Metrologichna St., 252143 Kyiv–143, Ukraine

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Amplitude dependence of the ultrasound attenuation and change of the elastic modulus due to the dislocations with a certain number of the geometrical kinks at zero temperature is investigated by the numerical simulation of dislocation motion. A decrease of attenuation before the amplitude of stress in a slip plane achieves the Peierls stress value is found.

1. In spite of a long period elapsed since the theory of the damping due to dislocations was formulated by Granato and Lücke [1], this theory remains the most consistent with the experimental data concerned the region of the small amplitudes of motion. But an increase of the ultrasound (US) intensity in the megacycle range has lead to the discovery of the acoustoluminescence (it is a luminescence of the ionic crystals which has an evident threshold dependence on the US amplitude [2]). This phenomenon is accompanied by the quite unexpected from the view of Granato-Lücke theory, fall in US attenuation before the threshold amplitude is achieved.

In order to explain the experimentally observed threshold character of the acoustoluminescence excitation, a model connecting this thresold with the onset of the large-amplitude dislocation motion in the Peierls relief was suggested in reference [3]. Such a motion under an external force is essentially nonlinear, that is why the threshold amplitude of US was computed with the help of the numerical simulations. As a result, a jump of US attenuation was found when an amplitude of the shear stress produced by US reached some critical value that was, in fact, equal to Peierls stress. Before the threshold in the case when the, Peierls relief was sine-like, an attenuation increased with the ancrease of the US amplitude. But when the Peierls relief shape approached step-like one, the attenuation behavior became more complicated: for very small amplitudes attenuation was constant and consistent with the string model [1]; then it fell rapidly by several orders and remained at that level until the threshold amplitude was reached. Such a behavior can be qualitatively explained by the fact, that at small amplitudes dislocation moves in the vicinity of the flattened bottom of the Peierls valley hardly taking notice of barriers existence. When the external force amplitude increases, dislocation spends more and more time in the vicinity of barriers where it is practically motionless, and the attenuation (which in this model is proportional to the mean square of its velocity) decreases. This model, while giving qualitatively correct behavior of the experimentally measured US attenuation, predicts the value of US amplitude at which a transition between two regimes of the dislocation motion takes place equal to $\sim 10^{-3}$ times of the threshold one; the experimental ratio is about 1/2.

However it should be noted that in Ref. [3] the direct dislocations were taken in to account only. At the same time a majority of dislocations in the real crystal are, as a rule, inclined, i.e. consist of the segments with the ends pinned down in different Peierls valleys. Such a dislocation has a certain number of the geometrical kinks, therefore at small amplitudes of US the last causes, in fact, only the motion of existing kinks without generating of the new ones [4]. In such a case the total potential energy of dislocation in the Peierls relief is constant, so one can suppose that dislocation is not affected by this relief, and string model [1] remains valid. Situation changes drastically at larger US amplitudes, when the number of the geometrical kinks becomes insufficient for the dislocation motion as a string, and new kinks are needed. Without the thermal activation (i.e. at sufficiently low temperatures) new kinks cannot be generated till amplitude of the shear stress produced by US is larger than the Peierls stress. That is why a reduction of the US attenuation comparing a constant value given by a simple linear model of the elastic string should be observed before the threshold. But in the contradistinction with the case of the direct dislocation such a reduction can take place at the comparatively large US amplitudes, where a number of the geometrical kinks mentioned above is enough.

It should be noticed that the possibility of the US attenuation reduction due to the exhaustion of kink motion was already considered many years ago by Alefeld [5]. But he had examined the dislocation motion under small-amplitude US and large bias stress only (when the effect of US could be taken into account with the help of the perturbation theory), since the large US amplitudes could not be achieved experimentally at that time. It is just an investigation of the inclined dislocation motion and respective attenuation of the large-amplitude US that are the main topics of of present communication.

2. In order to find out the precise form of the US attenuation dependence on its amplitude for the inclined dislocation, the numerical simulations of the motion of the dislocation segment pinned down in the different Peierls valleys under the action of the US wave of megacycle range were carried out.

An equation of motion fitting the case of the inclined as well as direct dislocation can be written as[1] [3,6]:

$$M_{\rm dis}\frac{\partial^2 y}{\partial t^2} + B\frac{\partial y}{\partial t} - T_{\rm dis}\frac{\partial^2 y}{\partial x^2} + \sigma_{\rm P} b \sin 2\pi\frac{y}{y_{\rm P}} = \sigma_{\rm us} b\cos\omega_{\rm ac} t, \qquad (1)$$

where x is a coordinate along Peierls valley, $y \equiv y(x)$ is a transverse displacement of dislocation, t is a time, $M_{\rm dis}$ is a dislocation mass per unit length, B is the friction constant, $T_{\rm dis}$ is the line tension, $\sigma_{\rm P}$ is the Peierls stress, $y_{\rm P}$ is a period of Peierls relief, $\mathbf{b}$ is a Burgers vector, and $\sigma_{\rm us} b$ stands for the amplitude of the force due to US wave with frequency $\omega_{\rm ac}$ per unit length. A possible spatial US inhomogeneity for given US length is considered to be weak and is not taken into account.

After proceeding to the convenient dimensionless variables $y \to 2\pi y/y_{\rm P}$;

[1] The form of the Peierls relief is assumed here to be sinusoidal, since the deviation from this form, as it follows from our estimations (cf. [3]), would give a correction of the order of 0.1% the to maximum US amplitude at which dislocation yet moves as a string.

$t \to (M_{\rm dis} y_{\rm P}/2\pi\sigma_{\rm P} b)^{1/2} t$; $x \to x/a$ equation (1) becomes:

$$\frac{\partial^2 y}{\partial t^2} + \gamma \frac{\partial y}{\partial t} - C_{\rm dis} \frac{\partial^2 y}{\partial x^2} + \sin y = f \cos \omega_{\rm ac} t, \tag{2}$$

where $\gamma = B\sqrt{y_{\rm P}/2\pi\sigma_{\rm P} b M_{\rm dis}}$, $C_{\rm dis} = T_{\rm dis} y_{\rm P}/2\pi a^2 \sigma_{\rm P} b$, $f = \sigma_{\rm us}/\sigma_{\rm P}$, a is a lattice period along x axis, and coefficient before $\sin y$ is equal to 1 due to the choice of variables.

To carry out the numerical simulations, the length of dislocation was divided into N identical segments with the length equal to lattice period, what lead to the system of equations exactly corresponding to the equations of motion for the system of coupled pendulums:

$$\begin{cases} \frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + \gamma \frac{\mathrm{d}y}{\mathrm{d}t} - C_{\rm dis}(y_{i+1} + y_{y-1} - 2y_i) + \sin y = f \cos \omega_{\rm ac} t, \\ y_i = y(x_i), \qquad x_i = i, \qquad i = 0, \ldots, N. \end{cases} \tag{3}$$

The fact that dislocation is inclined is taken into account by the boundary conditions:

$$y_0 = 0, \qquad y_N = 2\pi N_k, \tag{4}$$

where N_k is a number of geometrical kinks in the inclined dislocation (in other words, N_k is equal to the number of Peierls barriers crossed by dislocation).

To solve system (3) with boundary conditions (4) the 8-th order Runge-Kutta method with changing step was applied. Simulations were made for $\gamma = 1$, $C_{\rm dis} = 100$, $N = 1000$, $\omega_{\rm ac} = 10^{-3}$, which are close to the values usually used in the acoustoluminescence experiments. Twelve periods of external force were studied.

The data obtained during the two last periods (when the motion of dislocation could be regarded as totally set up) were used to compute the integral quantities

$$\alpha_{\rm dis}(f) = \frac{\gamma}{N f^2} \int\limits_{20\pi/\omega_{\rm ac}}^{24\pi/\omega_{\rm ac}} \left(\sum_{i=0}^{N} \dot{y}_i^2 \right) dt, \tag{5}$$

and

$$\delta(f) = \frac{\omega_{\rm ac}}{2\pi N f} \int\limits_{20\pi/\omega_{\rm ac}}^{24\pi/\omega_{\rm ac}} \left(\sum_{i=0}^{N} y_i \cos \omega_{\rm ac} t \right) dt, \tag{6}$$

which determine the amplitude dependence of US damping and the modulus defect $\Delta\mu/\mu$, respectively, due to dislocations. The experimentally measured values are related to these dimensionless ones by expressions

$$\alpha_{\rm dis}(\sigma_{\rm us}) = \frac{\omega_{\rm ac}}{2\pi v_{\rm us}} \frac{\Lambda \mu M_{\rm dis} y_{\rm P}^2}{\sigma_{\rm P}^2} \alpha_{\rm dis}(f)$$

for the attenuation coefficient, and

$$\frac{\Delta\mu}{\mu} = \frac{2\Delta v_{\rm us}}{v_{\rm us}}(\sigma_{\rm us}) = -\frac{\Lambda \mu b y_{\rm P}}{\sigma_{\rm P}} \delta(f)$$

for the modulus defect (the last expression is valid for the edge dislocation in the field of the transversal US wave [1]). Here, μ is a shear modulus, $v_{\rm us}$ is US velocity, Λ is a density of dislocations.

3. The results of numerical simulations for the attenuation coefficient (5) are plotted at figure 1, from which it follows that the existence of geometrical kinks in the dislocation causes the attenuation to be almost amplitude-independent and coinside with the value given by the linear string model [1] in the range of small amplitudes (for f less than some critical amplitude $f_{\rm cr}^{(N_k)}$). The value of $f_{\rm cr}^{(N_k)}$ is approximately proportional to the number of kinks. When the force amplitude increases from $f_{\rm cr}^{(N_k)}$ to $f_{\rm thr} \approx 1$ the attenuation coefficient (5), as seen, gradually decreases, since the part of the time period that kinks are located near pinning points increases. After the point where the force amplitude reaches its threshold value the attenuation grows sharply and then asymptotically approaches its initial level which is characteristic for small amplitudes. Immediately before the threshold the attenuation coefficient is proportional to N_k, and, at least, by three orders of magnitude greater then in the case of direct dislocation, so that a jump in attenuation becomes less sharp on the achievement of threshold US amplitude than in that last case.

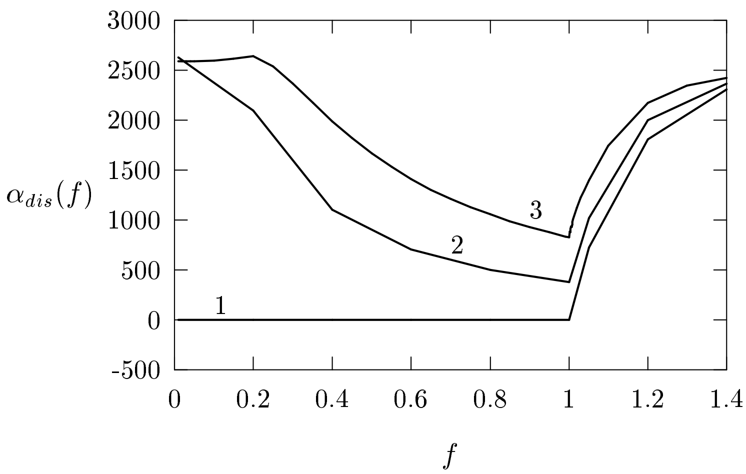

Figure 1. Amplitude dependence of US attenuation for dislocations with 0 (1), 50 (2), and 100 (3) kinks.

The amplitude dependence of the modulus defect (6) (shown at figure 2) resembles qualitatively the corresponding dependence for attenuation (cf. figure 1). Again three regions of with the different behavior are present: (a) region of practically constant δ ($f \lesssim f_{\rm cr}^{(N_k)}$, string motion of dislocation); (b) region of δ decreasing due to the exhaustion of kink motion ($f_{\rm cr}^{(N_k)} \lesssim f < f_{\rm thr}$); (c) overthreshold region with δ again increased (corresponds to the overbarrier motion of dislocation).

4. As a conclusion, it must be noted that the numerical simulations in each case were carried out for one dislocation with a certain number of kinks. But in real crystal the dislocation segments with different numbers of kinks are present, therefore the results of this computations should be averaged in some way with respect to the dislocation orientation in the slip plane. At figure 3 the US attenuation coefficient obtained by adding the corresponding values for dislocations of the same length $L = 1000a$ but with different number (namely, 0, 1, 2, 4, 10, 25, 50, and 100) of kinks

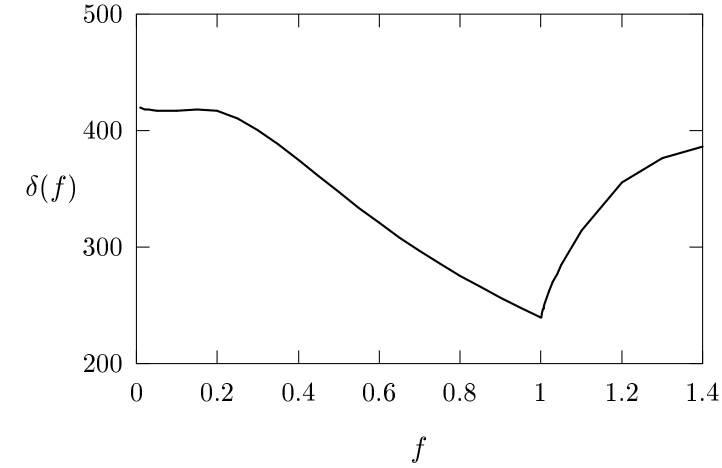

Figure 2. Amplitude dependence of modulus defect $\delta(f)$ for dislocation with 100 kinks.

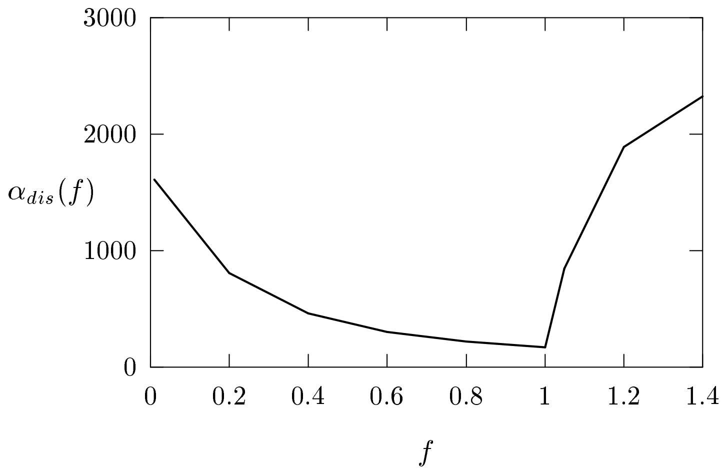

Figure 3. Averaged US attenuation versus US amplitude.

is shown. It is worth noting that such an averaging results in attenuation value above the threshold, which is less then its small-amplitude limit, while experimental picture is found to be inverse. Probably, this points out that the greater part of dislocations in crystal are the direct ones[2] (they give appreciable contribution above the threshold only).

Besides, our consideration does not take into account the possible breakaway of dislocation from the weak pinning centers and the following generation of the point defects, which can take place at the US amplitudes greater

[2]Remind that the potential energy of the inclined dislocation in Peierls relief is more than that of the direct one.

than the threshold one, while these phenomena have to cause the additional nonlinear absorption of US energy.

It is must be emphasised that the probability of the double-kink generation due to the thermal [4] and quantum [7] fluctuations which give rise to the possibility for dislocation to be pulled out into the new Peierls valleys even at stresses less than the Peierls one is not taken into account in present paper. These processes should be a subject of the further investigations.

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References

[1] Granato A., Lücke K. Theory of mechanical damping due to dislocations. // Journ. Appl. Phys., 1956, vol. 27, No 6, p. 583-593.
[2] Ostrovskii I.V. Acoustoluminescence and crystal defects. Kiev, Vyshcha Shkola, 1993 (in Russian).
[3] Loktev V.M., Khalack Ju.M. On the acoustoluminescence of crystals. Model, qualitative analysis and numerical calculations. // Ukr. Fiz. Zhurn., 1997, vol. 42 (in Ukrainian).
[4] Hirth J., Lothe J. Theory of dislocations. N.Y., 1968.
[5] Alefeld G. Dislocation kink chain model versus string model. // Journ. Appl. Phys., 1965, vol. 36, No 9, p. 2642-2651.
[6] Kosevich A.M. Dislocations in theory of elasticity. Kiev, Naukova Dumka, 1978 (in Russian).
[7] Natsik V.D., Kirichenko G.I., Pustovalov V.V., Soldatov V.P., Shumilin S.E. Influence of electronic viscosity and impurities on quantum motion of dislocations over the Peierls barriers. // Fizika Nizkih Temperatur, 1996, vol. 22, No 8, p. 965-984 (in Russian).

АМПЛІТУДНО ЗАЛЕЖНЕ УЛЬТРАЗВУКОВЕ ПОГЛИНАННЯ НАХИЛЕНИМИ ДИСЛОКАЦІЯМИ

Ю.Халак

Чисельним моделюванням руху дислокацій досліджується амплітудна залежність ультразвукового поглинання та зміна модулів пружності дислокаціями із заданою кількістю геометричних птель.