Comment on "Interaction of a surface wave with a dislocation"

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These are some remarks to the paper of Maurel *et al.* [Phys. Rev. B **75**, 224112 (2007)], which is devoted to deep theoretical analysis of the interaction of acoustic waves (phonons) with dislocations. Taking account of the secondary elastic waves emitted by the vibrating dislocations is an important development of this problem. As a result, the arising dynamic deformation fields are calculated more accurately than before and compared with our experimental results obtained a few years ago for $LiNbO_3$ crystals [Phys. Rev. Lett. **91**, 115506 (2003)]. Our objection is related to the usage in the simulations [Phys. Rev. B **75**, 224112 (2007)] a very high magnitude (not justified) of the dislocation drag coefficient, which makes problematic a quantitative comparison with our experimental results as well as a part of the conclusions drawn on this basis.

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We would like to comment on the recent paper of Maurel *et al.*,[1] which, as is stated by the authors in the abstract and introduction, is at least partially aimed at simulating the results of our experiments.[2] In Ref. 2 we reported on direct visualization of the interaction between high-frequency (0.58 GHz) surface acoustic waves (SAWs) and dislocations in $LiNbO_3$ crystals. This was accomplished by the aid of the specially developed fast stroboscopic x-ray diffraction topography at synchrotron beam line.[3–5] By using this technique we were able to visualize in the same image the SAW traveling across the crystal, the dislocations beneath the crystal surface, and, what is most important, the interaction between acoustic waves (phonons) and dislocations.

As was thoroughly studied in the classical works of Granato and Lücke,[6] the main outcome of this interaction is the phonon-induced vibrations of the dislocation strings. The groups of Maurel and Lund further contributed to the deeper understanding of this interaction by considering theoretically the emission of the secondary elastic waves by vibrating dislocations and the effect of the crystal surface (see Ref. 1, and references therein).

By analyzing the observed distortions of the acoustic wave fronts in the collected x-ray images we have determined the amplitudes of the vibrating dislocation segments, their velocities and, on this basis, extracted dislocation viscosity coefficients in brittle ceramic crystals of $LiNbO_3$. It is important to mention that our analysis gave high dislocation velocities, V, (in significant parts of the shear sound velocity) and, correspondingly, very low coefficients, B, of dislocation viscosity, being about two orders of magnitude lower than the values previously measured in ductile materials by internal friction and similar techniques. A review of the dislocation viscosity issue, including our and early results together with the comprehensive list of relevant references, can be found in our recent review paper.[7]

When comparing their simulations [Fig. 1(a)] with our experimental results [Fig. 1(b)], Maurel *et al.*[1] claimed that the dislocation velocity is much lower and, correspondingly, the viscosity coefficient, B, is much higher than we have obtained in Ref. 2. They conclude "that the unexpectedly high value of the dislocation velocity and the unusual low value of the drag coefficient B announced in Ref. 2 are artifacts of the approximations in the model herein."

In this Comment, we show that this conclusion is not justified. In fact, the papers of Refs. 1 and 2 are focused on somewhat different aspects of phonon interaction with dislocations and, hence, not too much overlap in specific results chosen for comparison.

In brief, by using stroboscopic x-ray diffraction topography we take an instant snapshot of the time-dependent deformation fields evolving near the surface of the crystal. In nearly perfect crystals (such as the $LiNbO_3$ wafers that we used), the probed region is defined by the interplay between the dynamical-diffraction and kinematical-diffraction regimes (see, e.g., Ref. 8). In practical terms, the x-ray penetration depth is between l_e (penetration depth restricted by the x-ray extinction) and l_a (penetration depth restricted by the x-ray photoelectric absorption).[9] For our experimental conditions, $l_e=1.8$ μm and $l_a=7.6$ μm, and it means that the imaged dislocations are located within depth $y<l_a$. Since the SAW attenuation depth is close to the SAW wavelength, $\lambda=6$ μm, the dislocations located a few microns beneath the surface will "feel" the SAW amplitude not very much differing from that one at the crystal surface. As we show below, by taking the surface value of the SAW amplitude for B evaluation, we will receive the upper limit of B magnitude, so, the real B value can be even smaller than we published in Ref. 2.

Under these conditions we were able to visualize the periodic (1.7 ns in the time domain and 6 microns in space) deformation field of SAW and its interaction with dislocation strings which are subjected to forced vibrations induced by SAW. The main effect clearly visible in the x-ray diffraction images [see Fig. 1(b)] is the periodic spatial modulation of the shape of dislocation string. The vibration amplitude, ξ, and, closely related to it, the strength of interaction ξ/λ, are extracted from the collected images by using model considerations described in detail in Ref. 2. The idea behind the model is to express the modified dislocation deformation field by using the well-known equation for the edge dislocation deformation field, in which the shape of the dislocation segment is periodically modulated due to resonant interaction with SAW. Certainly, this is a first approximation only, which does not take into account the emission of the second-

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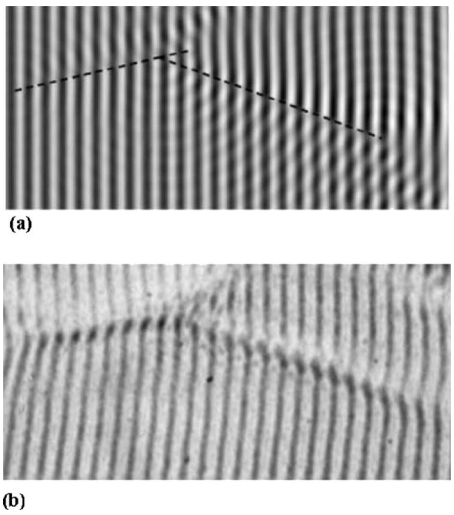

FIG. 1. A comparison between the dynamic deformation fields resulted from the phonon interaction with dislocations: (a)—simulated in Ref. 1; (b)—measured by stroboscopic x-ray topography (Ref. 2). Alternating dark and light vertical lines are acoustic wave fronts, whereas intersecting inclined lines [dashed lines in (a)] are linear dislocations.

ary elastic waves. As was mentioned before, the latter contribution was considered in theoretical works by groups of Maurel and Lund. However, the contribution of the re-emitted waves is more important far away from the vibrating dislocation line, where its own deformation field vanishes. This is also seen in calculations presented in Fig. 1(a). On the contrary, in close proximity to the dislocation line, on which we are focusing in our experiments and where the dislocation deformation field prevails, the approximation used by us should be valid.

The vibration amplitude, ξ, is a fitting parameter of the model, and is extracted from the direct comparison between the measured and simulated images. The effect of the vibration amplitude on the wave-front perturbations is strong and, first of all, is revealed in the inclination angle of these perturbations with respect to the straight wave-front lines far away from the dislocation line [see Fig. 1(b)]. After extracting the vibration amplitude, ξ from the images (for details see Ref. 2), the maximum velocity of the vibrating dislocation segments is found as $V=\omega\xi$, where ω stands for the frequency of SAW. Hence, high dislocation velocities are the result of large amplitudes of dislocation vibrations (up to $\xi/\lambda \approx 0.1$) that follow from experimental data. Extracting high dislocation velocities, implies low viscosity coefficients B, since $B \sim 1/V$ (certainly if we are not too close to the velocity of sound and B is the main factor limiting the dislocation velocity). The lowest value found by us was $B=5 \times 10^{-6}$ P or 5×10^{-7} Pa s (the latter units were used in Ref. 1). Note, that for B determination we use the expression

$$B = \frac{\mu b \varepsilon_0}{\omega \xi}, \tag{1}$$

which follows from the equation for dislocation motion used in both papers of Refs. 1 and 2. In Eq. (1), μ stands for the shear modulus of the material, b for the Burgers vector of the dislocation, and ε_0 for strain value induced by SAW. The latter is proportional to the SAW amplitude. Therefore, by taking its maximal surface value we obtain the upper estimate of the B magnitude and the true value of B may be even lower.

Contrary to our approach, Ref. 1 is focused on calculating the amplitude of the secondary elastic waves emitted by the vibrating dislocation string and then simulating the resulting interference pattern. Not going deeply into simulation details, we stress that these simulations require the knowledge of the dislocation viscosity coefficient, B, a single important parameter not known *a priori* since it depends on the details of phonon-phonon and electron-phonon interactions. Physically, larger B values imply stronger interactions and higher amplitudes of the emitting wave. In their calculations, Maurel *et al.*[1] arbitrary set $B=10^{-5}$ Pa s, i.e., 20 times larger than we obtained experimentally in Ref. 2. In order to do this, they postulate that the B value is more or less the same in all materials, which is not true as we show below. As justification, they apply certain expression for B well above the Debye temperature and estimate several physical parameters of interest. Since we use identical equations for dislocation motion, it is easy to conclude that setting a 20 times larger B value means 20 times smaller dislocation velocity which is indeed calculated in Ref. 1. This is also the basis of their conclusion that they "observed" (i.e., calculated) dislocation velocities equal a few percent of the velocity of sound. Correspondingly, their calculated amplitudes of dislocation vibrations are 20 times smaller than we measured experimentally (25 nm instead about 500 nm that we obtained).

Generally, the simulations performed in Ref. 1 [see an example in Fig. 1(a)] do not capture the most important experimental feature: strong wave-front distortions of acoustic waves in close proximity to dislocation lines [see Fig. 1(b)]. As we show in Ref. 2, these distortions reveal the phonon-induced dislocation vibrations and are well reproduced when calculating the quasistatic deformation field of such wavy dislocation lines. In contrast, the calculations in Ref. 1 miss this main effect because the dislocation velocity is very much underestimated as a result of the large B value. At the same time, the simulations in Ref. 1 greatly overestimate the strength of the secondary acoustic waves far away from dislocation lines [see Fig. 1(a)], which hardly appear in experimental images [Fig. 1(b)]. We think that it is therefore worth repeating the simulations of Ref. 1 with a 20 times smaller B value, i.e., $B=5 \times 10^{-7}$ Pa s, and after that to compare the simulated and experimental images.

The source of the major discrepancy, between papers in Refs. 1 and 2, is in the postulation in Ref. 1 that $B=10^{-5}$ Pa s in most materials. This assumption is definitely incorrect and, in fact, the B values may strongly differ for metals and ceramics. In this connection we indicate two important facts. First, in insulating ceramics, as compared to metals, there is practically no electron-phonon interaction. This being so, the B value in ceramics should be generally smaller than in metals (at least at low temperatures). More important is that the Debye temperatures, Θ_D, in ceramics can be two to three times higher than those for typical ductile metals, in which the dislocation viscosity has been measured

by the internal friction technique. For example, at room temperature, Θ_D=95 K, 225 K, 316 K, and 395 K for Pb,[10] Ag,[11] Cu,[12] and Al,[13] respectively. In contrast, for $LiNbO_3$ Θ_D=560 K,[14] and definitely the high-temperature approximation for B value used in Ref. 1 in order to estimate the room-temperature B value in this material is not valid. As another illustration of possible diversity between materials, we indicate that the μb^3 value (the measure of dislocation energy) stated arbitrary as "1 eV for most of materials" in Ref. 1, for $LiNbO_3$ equals 62 eV [taking μ=60 GPa and b =0.55 nm (Ref. 7)].

However, the most direct evidence of the potential large-scale diversity in the B values in different materials is given by the fact that the ultrasonic attenuation, α, at the same frequency, ω, strongly differs in metals and ceramics. For example, at room temperature the attenuations for longitudinal sound waves in Al and Cu at 1 GHz are α =7500 dB/m (Ref. 15) and α=27 000 dB/m,[15] respectively, whereas α=45 dB/m for $LiNbO_3$ (Ref. 16) under the same conditions. Since ultrasonic attenuation, α, and dislocation viscosity, B, are originated from the same general crystal viscosity phenomenon (i.e., phonon-phonon and electron-phonon interactions), it is clear that B values in ceramics and metals may differ by orders of magnitude, in contrast to what is claimed in Ref. 1.

In summary, we consider the theory[1] as a serious step forward in describing the interaction of acoustic waves with dislocations since it takes into account the emission of secondary acoustic waves by vibrating dislocations. At the same time, a comparison between simulated images[1] and experimental images obtained by us in Ref. 2 has been performed at very dissimilar (differing by 20 times) magnitudes of the dislocation drag, B, making the conclusions based on such a comparison worthless. Therefore, the key issue of our Comment is the way in which the comparison between experiment[2] and theory[1] is done and conclusions are drawn. Namely, Maurel *et al.*[1] compared two images, one taken from our paper[2] and the second simulated by the theory,[1] find them similar, and, on this basis, claim a strong difference (20 times) between the drag coefficient, B, introduced *a priori* into their theory, and the value extracted by us from experimental images. Contrarily, we point out that the simulated and experimental images are very different and this difference stems from the 20 times larger B value (as in metals) used in the theory[1] without any serious justification. As we show in this Comment, the B value in $LiNbO_3$ ceramics may be much lower than in metals, and it is worth repeating the simulations[1] for 20 times smaller B values (i.e., similar to those extracted experimentally in Ref. 2) and then comparing the simulated and experimental images again.

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