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Phonon-dislocation interaction in deformed lithium fluoride

In-Sang Yang* and A. C. Anderson
Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801
and Materials Research Laboratory, University of Illinois at Urbana-Champaign, 104 South Goodwin Avenue,
Urbana, Illinois 61801

Y. S. Kim† and E. J. Cotts‡
Keck Laboratory, California Institute of Technology, Pasadena, California 91125

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The thermal conductivity has been measured over the temperature range 0.06–6 K for a LiF crystal before and after deformation by compression in which all possible dislocation-slip planes were activated, and after reduction in sample size and, finally, following γ-ray irradiation. At temperatures below 1 K the results are in agreement with a model of phonon scattering by fluttering dislocations. At $T \geq 1$ K the data suggest that dislocation dipoles may dominate the scattering of phonons.

I. INTRODUCTION

Thermal phonons in LiF are scattered strongly by dislocations introduced through deformation. The scattering can be monitored experimentally by either thermal conductivity[1] or ballistic phonon[2] measurements. The ballistic measurements provide information on the velocities (modes) and angular distributions of those phonons not scattered. Thermal conductivity data provide an indication of the frequency dependence of scattering processes, since phonons dominant in heat transport typically have a frequency $\nu \approx (10^{11} T)/(1 \text{ Hz/K})$ where T is the temperature of the measurement. For technical reasons, ballistic measurements have been limited to temperatures and equivalent phonon frequencies greater than ≈ 1 K.

To understand phonon transport in deformed LiF, one must take into account the anisotropy of the crystal, which causes phonon focusing,[3,4] plus the strong dependencies in the phonon-dislocation interaction[5,6] on phonon mode, angle of incidence, and phonon frequency. The experimental observations are generally in good agreement with the predictions of a model which assumes a resonant interaction of phonons with "fluttering" dislocations vibrating at the phonon frequency

$$\nu \approx v/L \ , \qquad (1)$$

where v is an average phonon velocity and L is the length of a segment of a dislocation lying between two pinning points. The experimentally observed scattering magnitude and frequency dependence[7] cannot be explained by the alternative scattering mechanism, that provided by "static" dislocations.[8]

There are, however, two questions which remain unanswered for deformed LiF. At temperatures above ≈ 1 K, the observed scattering is too strong to be explained by isolated, fluttering dislocations. Suggested explanations have included the effects of dislocation dipoles[5] and the possible role of impurities[9] or deformation-produced debris, but the nature of the "debris" introduced by deformation is not well understood at this time.[10] Experimentally it is found that, at temperatures $T \geq 1$ K, phonon scattering depends strongly on the condition of the sample prior to deformation.[11] In brief, additional studies are required to understand the effect of deformation on phonon transport at temperatures above 1 K. The work described below suggests that the strong phonon scattering at $T \geq 1$ K may arise from dislocation dipoles.

A second question is the frequency dependence of the phonon-dislocation interaction. Even in samples of heavily deformed LiF, the unscattered phonons have a mean free path of order of the sample dimensions and dominate the conductivity. The only information available about those phonons scattered by dislocations occurs at the lowest temperatures (frequencies) where γ-ray irradiation is shown to pin the dislocations, reducing L in Eq. (1), and thereby suppressing the scattering of phonons by dislocations. A possible resolution to the question of the frequency dependence was revealed in the ballistic-phonon data.[2] It was observed that the phonons were being scattered by dislocations lying on only two dislocation-slip planes. The other slip planes had not been activated during deformation because the samples had been either sheared or bent or, if deformed by compression, the compression jig permitted expansion in only one lateral direction (the jig was used to prevent the sample from buckling during compression). Since the interaction is strongly anisotropic, a fraction of the phonons were not being scattered. Introducing dislocations on all slip planes, therefore, should cause a more complete scattering of phonons.

In the measurements discussed below, the LiF sample was permitted to expand in both lateral directions during compression, thereby activating four dislocation-slip planes. Thus more phonons should be scattered by the dislocations, and the measured thermal conductivity could reveal more fully the frequency dependence of that interaction. This aspect of the project has been only partially successful. Indeed, the dislocation array on four slip planes is more efficient at scattering phonons, yet a significant portion of the phonons are not scattered by the dislocations and continue to have mean free paths of order of the sample dimension.

II. EXPERIMENTAL PROCEDURE

The origin of the $0.62\times0.62\times5.0$ cm^3 LiF samples, the method of deformation along the $\langle 100\rangle$ rod axis, and the procedure for measuring thermal conductivities are described in Ref. 11. The one important exception[12] has been that the present sample was first compressed 2%, then rotated in the jig about the rod axis and compressed another 2%. This activated all four of the available dislocation slip planes. Etch-pit counts were not made on this sample. Prior work[13-15] on LiF deformed by compression indicated that a 4% deformation would provide a dislocation density of $\approx 10^8/\text{cm}^2$. It is assumed that the dislocation density is roughly twice the etch-pit count observed on one surface. A dislocation density deduced from etch-pit counts is roughly equal to the density deduced by other techniques,[16,17] but is thought to be only a lower limit to the actual density.

The surfaces of the sample were lightly abraded with 27-μm air-borne powder to enhance boundary scattering of thermal phonons. Following the initial measurements, the deformed rod was sectioned lengthwise with a commercial diamond saw to reduce the lateral dimensions. Prior to the final conductivity measurement, the sectioned sample was γ-ray irradiated by a Cs source to a total of 5×10^5 rad to partially pin the dislocations.[18] This amount of irradiation does not introduce, in a LiF sample,[19] phonon-scattering defects which are effective below ≈ 1 K.

III. RESULTS AND DISCUSSION

The measured thermal conductivity κ of the LiF sample, prior to deformation, is shown in Fig. 1. The conductivities have been divided by T^3 to allow the vertical scale to be expanded, and to display the approximate temperature (frequency) dependence of the phonon mean free path l since, roughly, $\kappa/T^3 \propto l$. The data for the sample prior to deformation are scattered, but were obtained only to establish that the phonons had long mean free paths of the order of the sample dimensions (0.6 cm). The solid line resulted from a computation which assumed boundary scattering of phonons and took into account the effects of phonon focusing and the finite length of the sample.[5,20] The conductivity expected for scattering only by sample surfaces assuming the Casimir approximation of an isotropic sample would lie about 25% below the solid line. The rough agreement between data and the computations indicates a crystal reasonably free of defects active in phonon scattering at temperatures below 1 K.

The thermal conductivity following 4% deformation is also shown in Fig. 1, and is compared with results from Ref. 11 for a sample that underwent 4.5% and 9% deformation, but with only two of the four dislocation-slip planes activated. Clearly, for essentially the same total deformation, activation of four slip systems is much more effective in reducing the conductivity.

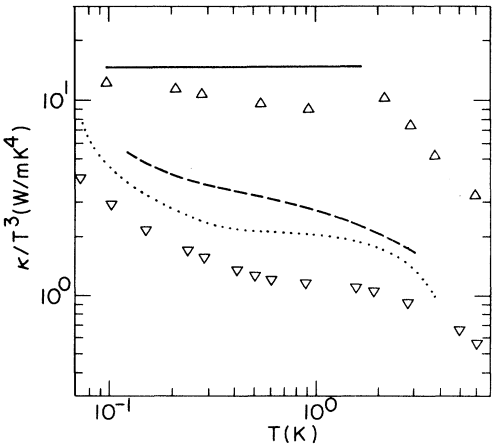

FIG. 1. The thermal conductivity κ, divided by the cube of the temperature T, vs T for a LiF crystal before (△) and after (▽) 4% compressive deformation allowing four dislocation-slip systems to be activated. The solid line represents the conductivity expected with only boundary scattering of phonons present, taking into account the crystal anisotropy and finite length of the sample. Data from Ref. 11 are represented by the dashed (4.5% deformation) and dotted (9% deformation) lines when only two slip planes are activated.

The sample was next sliced lengthwise to reduce its lateral dimensions by a factor of 2, to 0.31 cm. The results are shown in Fig. 2. Reduction in the size of the deformed sample has reduced the conductivity by $>30\%$, indicating that a fraction of the phonons are still being

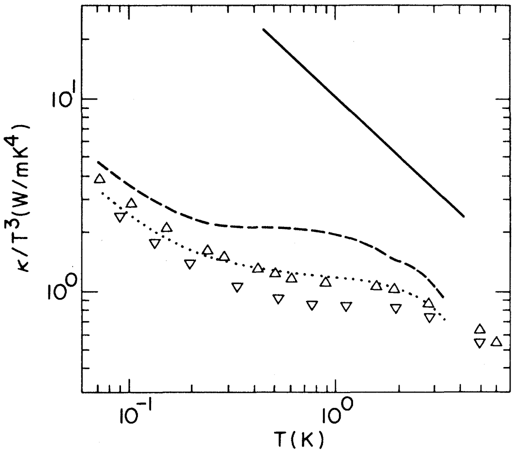

FIG. 2. Thermal conductivity κ, divided by T^3, for the present 4% deformed LiF sample before (△) and after (▽) the lateral dimensions were reduced by a factor of 2. The dashed and dotted lines show the reduction in conductivity caused in a sample deformed 10%, with only two slip planes activated, when the lateral dimensions were reduced by a factor of 2 (Ref. 11). The solid line represents the κ/T^3 expected for static, strain-field scattering from a dislocation density of $10^9/\text{cm}^2$ (Ref. 7). Clearly this mechanism is too weak to explain the present data for a sample having a dislocation density of $10^8/\text{cm}^2$.

scattered by the sample surfaces. If all phonons had the same mean free path due to dislocations, the reduction in κ/T^3 with sample size would be less than 10%. Therefore, activation of the four slip systems has not resulted in the scattering of all phonons. Also shown in Fig. 2 for comparison are data from Ref. 11 for a sample deformed 10% while activating only two slip planes, both before and after the lateral dimensions had been reduced by a factor of 2.

Finally, our sliced sample was γ-ray irradiated. This irradiation, as in previous work, caused the thermal conductivity to increase at the lowest temperatures (see Fig. 3). The increase is indicative of added pinning points on fluttering dislocations, thus decreasing the length L of Eq. (1) and increasing the average resonant frequency of the dislocation segments. As a result, the scattering of low-frequency phonons is suppressed even though the dislocation density remains unchanged. In brief, the γ-ray irradiation reveals the presence of a strong dynamic interaction between thermal phonons and fluttering dislocations in deformed LiF.

From Fig. 1 it may be noted that the conductivity at temperatures below ≈ 0.1 K ($\nu < 10^{10}$ Hz) is reduced less by deformation. This is true independent of the amount of deformation, or if the deformation is by bending, shear, or compression, or if two or four slip planes are activated. This implies, from Eq. (1), a maximum value for the spectrum of loop lengths L which happens to be essentially the same for all LiF samples. An alternative possibility is that the dislocations move within a weak Peierls potential[21,22] which establishes a low-frequency limit to the dislocation resonance spectrum. This latter possibility was first suggested in Ref. 1 and is discussed in greater detail there.

Figure 4 compares the ratio of the measured conductivities before and after deformation (the solid line) to the computed ratio using the model of fluttering, isolated dislocations[5,12] (the dotted line) assuming all four slip planes have been activated, that there is an exponential distribution in loop lengths L with an average loop length [Eq. (1)] of 300 Å, and that the dislocation density is $1\times10^8/\text{cm}^2$. In this computation, the slow-transverse-phonon mode makes essentially no contribution to thermal transport. The theoretical curve reveals a deep minimum, in contrast to the measurements which indicate a much stronger phonon scattering at higher temperatures (i.e., frequencies), a scattering which serves to mask the expected minimum.

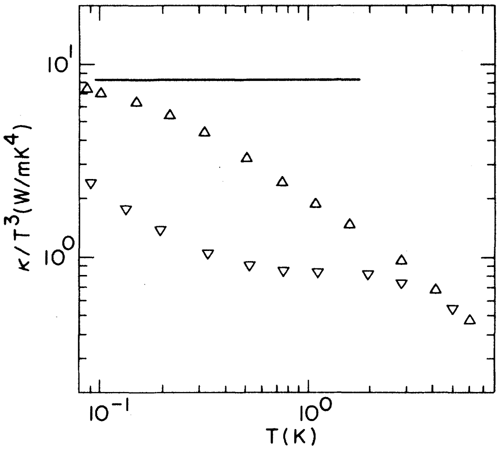

FIG. 3. The thermal conductivity κ, divided by T^3, for the 4% deformed LiF sample before (▽) and after (△) 5×10^5 rad of γ-ray irradiation. The horizontal line represents κ/T^3 if only boundary scattering were present.

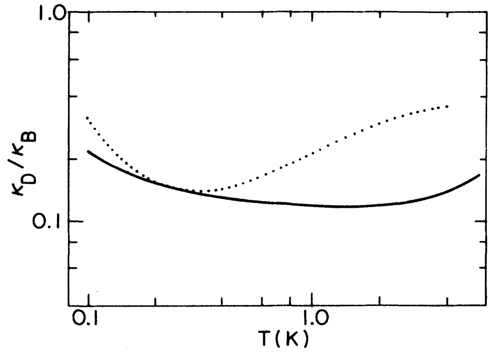

FIG. 4. The ratio of the thermal conductivity κ_D of the deformed sample divided by the conductivity κ_B of the sample prior to deformation. The solid line represents the experimental ratio while the dashed line is the theoretical ratio based on phonon scattering from isolated, fluttering dislocations with only the average dislocation loop length L as an adjustable parameter. Decreasing L would not provide better agreement with experiment at higher temperatures.

Although the source of this high-frequency scattering remains unidentified as mentioned in the Introduction, the present work does suggest that this scattering over the range $\approx 1-3$ K may be caused by dislocation dipoles.[5] In Fig. 3 the scattering within the interval 1–3 K is suppressed by γ-ray irradiation,[11,23] suggesting that vibrating dislocations are involved. Also in Fig. 1 the phonon scattering over 1–3 K is enhanced by deformation on four slip planes, relative to the same deformation on two slip planes, just as for the range below 1 K. It is unlikely that these two observations could be associated with other debris produced by deformation.

In summary, we have measured the thermal conductivity of LiF crystals deformed by activation of four dislocation-slip systems. For $T < 1$ K, the results are in satisfactory agreement with a model of phonon scattering by individual, fluttering dislocations. For $T \geq 1$ K, our results suggest that the observed strong phonon scattering is also caused by vibrating dislocations, perhaps in the form of dipoles. Insufficient knowledge of the density and nature of such dipoles precludes a comparison of model and data.

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[*] Present address: Room 24-257, IBM Thomas J. Watson Research Center, P.O. Box 218, Yorktown Heights, NY 10598.

[†] Present address: Jet Propulsion Laboratory 301-476, 4800 Oak Grove Drive, Pasadena, CA 91109.

[‡] Present address: Department of Physics, State University of New York at Binghamton, Binghamton, NY 13901.

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