

THE PHONON-DISLOCATION INTERACTION

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Thermal conductivity measurements on LiF crystals in the temperature range 0.04 - 30 K have demonstrated that, throughout this range, thermal phonons interact with dislocations via a dynamic or resonant process which is highly frequency and phonon-mode dependent. The results of earlier work are consistent with this interpretation.

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MASTER

66.70.+b

61.70.Le

63.20.Mt

63.20.Pw

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Since the early theoretical papers by Klemens^{1/} in 1955 until the present,^{2/} there has been a continuing controversy in the literature concerning the physical nature of the interaction of thermal phonons with dislocations. The present paper is an attempt to partly clarify the situation through a review of the experimental data on LiF available in the literature.

Figure 1 displays the results of thermal conductivity measurements on deformed single crystals of LiF. The thermal conductivity λ of the deformed sample has been divided by that, λ_B , of the sample prior to deformation. This normalization procedure removes much of the temperature dependence so that the vertical scale can be expanded, and it also emphasizes the changes in λ caused by deformation. No change from the undeformed state is represented by the dashed line at $\lambda/\lambda_B = 1.0$.

Curve A of Fig. 1 represents crystals of LiF deformed by bending.^{3,4/} Crystals deformed by shear have a similar behavior.^{5/} The rise in curve A at temperatures above ≈ 15 K occurs because phonon scattering by isotopes and other causes mask the dislocation scattering.^{6/} It should be noted that, in the undeformed crystals at temperatures below ≈ 15 K, the phonons scatter predominantly from the surfaces of the samples. The temperature dependence of λ_B is therefore T^3 .

The thermal conductivity of curve A is roughly 50% that of the undeformed crystal. This $\approx 50\%$ reduction is (i) independent of the diameter of the crystal and is (ii) independent of the number of dislocations. This observation can be explained in only one way, namely that some fraction of the thermal phonons is scattered so strongly by the dislocations that they make no appreciable contribution to thermal transport. Hence λ is independent of the number of dislocations. In addition, another fraction

of the phonons must be so weakly scattered by the dislocations that they continue to scatter predominantly from the surfaces of the sample. Hence λ of the deformed crystal continues to scale with the dimensions of the sample.

There are many reports in the literature of thermal conductivities for samples of LiF deformed by compression. An example is curve B of Fig. 1.^{7/} Unlike curve A, these results are found to scale inversely with the density of dislocations. Besides the method of sample deformation, the major difference between curves A and B is the density of dislocations, $\sim 10^{11} \text{ m}^{-2}$ for curve A and $\sim 10^{12} \text{ m}^{-2}$ for curve B. It is therefore suggested that, for curve B, the density of dislocations is sufficiently large that even that fraction of phonons which interacts weakly with dislocations is now scattered.

The dotted curve shows the change from curve A caused by prolonged exposure to γ -irradiation.^{4,5/} The dislocations are still present, but the phonon-dislocation interaction has been greatly reduced at $T \lesssim 2 \text{ K}$ by the pinning action of the point defects introduced through γ -irradiation. Pinning caused by the thermal diffusion of impurities produces a similar behavior.^{4,7/} At temperatures above $\approx 2 \text{ K}$, pinning appears to have little influence on the thermal conductivity of deformed samples.

The above collection of empirical observations may now be compared with theoretical models. The original theories related to phonon scattering by the static strain fields surrounding sessile dislocations.^{1,8/} The most appropriate data for comparison are therefore those of the dotted line in Fig. 1, namely the pinned dislocations for $T \lesssim 2 \text{ K}$. These data place only an upper limit on the scattering cross section, but this limit

is consistent with the theory. On the other hand, the theory of Ohashi^{9/} gives too large a scattering cross section.

An attempt has been made to ascribe the temperature independence of curve A to a process of "global" scattering from the average, static distortion fields of all dislocations.^{2/} However, it has already been demonstrated above that the temperature independence of curve A is caused by the scattering of a fraction of the thermal phonons from the surfaces of the sample. Hence the "global" scattering process, if present, certainly is not dominant.

The fact that pinning, by γ -irradiation or heat treatment, reduces the phonon scattering process for $T \lesssim 2$ K suggests that the strong interaction in the deformed but unirradiated crystal may be between a phonon and a dislocation having a resonant mode of the same frequency. The "vibrating-string" model of a dislocation^{10/} does provide, qualitatively, the correct scattering cross section. The effect of pinning is then understood as the shortening of the "vibrating strings", thus increasing the resonant frequency and the temperature at which the dominant thermal phonons attain this frequency. Furthermore, the theory indicates that the slow transverse phonon mode should be scattered most strongly. This accounts for the observed $\approx 50\%$ reduction in λ and the fact that only a fraction of the phonon population is strongly scattered. That the slow-transverse mode is scattered most strongly has been experimentally verified by observation of the attenuation of ballistic thermal phonons in shear-deformed crystals of LiF.^{5/} Even though the success of this vibrating-string model is impressive, it has not been possible to obtain quantitative agreement between experimental data and this model.^{4/}

Still to be explained is why the scattering cross section above ≈ 2 K cannot be reduced by pinning. The cross-section is sufficiently large that a resonant phonon-dislocation interaction is assumed to occur. Perhaps a dislocation can only absorb pinning points until their separation is of order 100 \AA . Or, perhaps the nature of the resonance cannot be described as a vibrating string for frequencies above $\approx 2 \times 10^{11} \text{ Hz}$.^{11/}

In summary, it has been argued that, in LiF, freshly introduced dislocations cause a strong, resonant scattering of thermal phonons, and that the strength of this interaction is strongly dependent on phonon mode and frequency. At temperatures below 2 K (dominant phonon frequencies below $\approx 2 \times 10^{11} \text{ Hz}$) the dislocation resonance can be described as that of a vibrating string but, above 2 K, the resonant nature of the dislocation is not known. At temperatures below 2 K the dislocations can be pinned. The phonon scattering cross-section of such a pinned or sessile dislocation is greatly reduced, and is consistent with the theoretical models appropriate to static dislocations. As a further test of these conjectures, it would be desirable to have additional experimental data for deformed and irradiated crystals at large dislocation densities at low temperatures, see Fig. 1. Finally, it should be noted that these conclusions may not extrapolate to other materials.

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Figure Caption

Fig. 1. The thermal conductivity, λ , of a deformed crystal of LiF divided by that, λ_B , of the undeformed crystal, versus temperature. Curve A is for a sample deformed by bending; curve B is for a sample deformed by compression and having a larger dislocation density. The other curves are discussed in the text.

