PHONON-DISLOCATION DIPOLE INTERACTION IN LiF AT LOW TEMPERATURE
G. Kneezel, A. Granato

To cite this version:
G. Kneezel, A. Granato. PHONON-DISLOCATION DIPOLE INTERACTION IN LiF AT LOW TEMPERATURE. Journal de Physique Colloques, 1981, 42 (C6), pp.C6-250-C6-252. <10.1051/jphyscol:1981672>. <jpa-00221608>

HAL Id: jpa-00221608
https://hal.archives-ouvertes.fr/jpa-00221608
Submitted on 1 Jan 1981

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
PHONON-DISLOCATION DIPOLE INTERACTION IN LiF AT LOW TEMPERATURE

G.A. Kneezel and A.V. Granato*

Xerox Webster Research Center, Webster, New York, U.S.A.
*University of Illinois, Urbana, Illinois, U.S.A.

Abstract.--We compare the effects of isolated dislocations and a somewhat larger density of edge dislocation dipoles on thermal conductivity, specific heat, and ultrasonic velocity and attenuation in alkali halides such as LiF. The motivation for this study is to check the implications of earlier work where it was demonstrated that the effect of deformation on thermal conductivity in LiF could not be accounted for by dynamic scattering by a dislocation density equal to the etch pit density, but could be fit assuming scattering was due to the "optical" mode of vibration of a much larger density of dislocation dipoles.

By irradiating previously deformed LiF [110] rods and remeasuring the thermal conductivity, Anderson and co-workers have demonstrated that the scattering of phonons by dislocations is predominantly dynamic--at least below 2 K. Although their results were qualitatively inconsistent with static strain field scattering they were also not quantitatively fit by previous calculations of dynamic scattering effects. We undertook a calculation based on the vibrating dislocation string model and taking into account several details which others have neglected--including phonon focusing, resonance angle effects, and the resolved shear stress factor for each incident phonon--and confirmed that dynamic phonon scattering by isolated dislocations of a density equal to the etch pit density could not account for observed effects.

It became clear that the defect responsible for scattering was a dislocation-like defect having a higher resonant frequency (with a broader distribution of resonant frequencies) and present in larger numbers. These conditions are met by the dislocation dipole, which is a pair of dislocations of opposite signs on glide planes a distance d apart. Dislocation dipoles are predominantly of edge character, as screw dislocations of opposite sign cross glide and annihilate. Because the members of the dipole attract each other there is a restoring force Dy when the dislocations move in opposite directions (the optical mode of vibration) so that the equation of motion is

\[ \dot{A} \frac{d^2y}{dt^2} + B \frac{dy}{dt} - C \frac{d^2y}{dx^2} + Dy = b_v \cos(kx - \omega t). \]

The optical resonant frequency of the mth normal mode is

\[ \omega_{op}(m) = (\omega_{ac}^2(m) + D/A)^{1/2} = \left[ (m^2 \pi^2 C/L^2 A) + (Gb^2/2\pi A(1-v)d^2) \right]^{1/2} \]

where \( \omega_{ac} \) is the acoustical mode resonant frequency, A is the effective mass, B is the damping constant, C is the line tension, \( \sigma \) is the resolved shear stress, L is the length between pinning points, b is the burgers vector, and \( \nu \) is Poisson's ratio. Thus the optical mode frequency is higher than the acoustical mode frequency, especially for narrow dipoles. Long wavelength (\( \lambda \gg d \)) stress waves excite only the optical mode of vibrations because the dislocations have opposite signs.

Dislocation dipoles are believed to greatly outnumber isolated dislocations in deformed crystals. A reasonable ratio appears to be 10-100, distributed primarily at dipole widths of 3b to 300b with most having widths less than a few hundred Angstroms so that they are not easily detected by electron microscopy or etch pitting techniques. A distribution of this type (for dipole
width nb) is the exponential distribution $A(n) = A_0 \exp(-(n-3)/N_0)$ for $n \geq 3$. The observed thermal conductivity effects were fit by assuming $N_0 = 60$ and a Koehler distribution of lengths with average loop length equal to the ultrasonically determined value of $2 \times 10^{-5}$ cm. If all dipoles are on the (110) planes perpendicular to the rod axis it is found that $7.5 \times 10^8$ cm$^{-2}$ dislocations paired into dipoles are required in order to fit the observed effects. However if some fraction of the dipoles are on the other (110) planes which scatter the predominant heat carrying phonons along [110] LiF rods more effectively, then less dipoles are required. Because of the type of deformation used most dislocations and dipoles are expected to be on (110) so that the number of dipoles required to fit the thermal conductivity data is 10-30 times the observed etch pit density.

Vibrating dislocations and dipoles are expected to contribute to the specific heat of a deformed crystal. The contribution by isolated dislocations (and also by the acoustical mode of dipoles which obeys the same equation of motion) at temperatures above $T_0 = h\omega_1/k_B$ is

$$C_{ac} = \frac{n^2}{3Z\theta}$$

where $\omega_1$ is the lowest normal mode frequency, $a$ is the lattice vector, $Z$ is the number of atoms per unit cell, $\theta$ is the Debye temperature (723 K in LiF) and $p$ is the average sound velocity divided by $d\omega/dk$ for the dislocation modes. At lower temperature the contribution falls off exponentially. For a delta function dislocation length distribution $L = 2 \times 10^{-5}$ cm in LiF, $T_0 \sim 0.5$ K and

$$C_{ac} \sim 2.0 \times 10^{-15} \Lambda N K_B T/\theta.$$ (4)

This same asymptote is approached at higher temperatures by the dipole optical mode contribution $C_{op}$. This can be seen from equation (2) in that for the higher order modes ($m > 1$) $\omega_{op} \sim \omega_{ac}$. For a delta function distribution $L = 2 \times 10^{-5}$ cm and $d = 60b$, $T_0 \sim 1.5$ K.

The background to which $C_{op}$ and $C_{ac}$ must be compared is the lattice specific heat at low temperature $C_L = 234 N K_B (T/\theta)^3$. Because of their linear temperature dependence the vibrating dislocation dipoles make their largest relative contribution at low $T$. At 1 K the asymptotic dipole contributions are less than 1% of the total specific heat for $\Lambda = 7.5 \times 10^8$ cm$^{-2}$. At lower temperatures the linear asymptotic expression is no longer valid and a numerical calculation of the dipole contributions to the specific heat was performed with two objectives: 1) observe the form of the curves below the asymptote, and 2) determine the effect of assuming exponential distributions of dipole lengths and widths as in the thermal conductivity calculations.

For a delta function distribution of lengths and widths it was found that the asymptote (4) was approached to within about 10% by $C_{ac}$ and $C_{op}$ around 0.5 K and 1.5 K as expected. The results of the calculations incorporating the exponential distributions of lengths and widths are shown in figure 1 assuming $\Lambda = 7.5 \times 10^8$ cm$^{-2}$. Relative to the delta function case, it is found that $C_{ac}$ is increased at all temperatures while $C_{op}$ is increased below $\sim 0.3K$ and decreased above $0.3K$. In the approximately linear regime above 1 K, $C_{ac} + C_{op} \sim (1.5 + 1.0) \times 10^{-6} N K_B T/\theta$. At 1 K the dipole contribution for that defect density is $\sim 0.5\%$ of the lattice contribution and at higher temperature the relative contribution is proportional to $1/T^2$. This is consistent with recent experimental work in which no change was observed (to within the 1% experimental accuracy) in the specific heat of a sample deformed in compression by 4.5%.
Comparison of the predicted effects of dipoles and isolated dislocations can also be made for ultrasonic velocity and attenuation. In particular the relative velocity change $\Delta v/v$ is proportional to $1/\omega_1^2$ and the logarithmic decrement $\Delta$ is proportional to $\omega^2/\omega_1^4$ for $\omega \ll \omega_1$. For dipoles only the optical mode of vibration is expected to be excited by the long wavelength stress waves.

Numerical calculations were made to compare the effects of a Koehler distribution of screw dislocations ($L = 2 \times 10^{-5}$ cm) and of the edge dipole distribution used in fitting thermal conductivity measurements ($L = 2 \times 10^{-5}$, $N_0 = 60$). Normalized to the same defect densities it was found that the screw dislocation contribution was 10 times greater for $\Delta v/v$ and 100 times greater for $\Delta$ than the edge dipole contributions. If the dipole density is an order of magnitude greater, dipole effects should certainly be observable—although not dominant. Irradiation pinning experiments should especially be able to discriminate between dislocation and dipole contributions because $\omega_1$ of the dislocations is proportional to $1/L$ while that of the dipole is given in equation (2). The length varies during irradiation according to the relation (5)

$$L = L_0/(1 + \beta t).$$

Thus the time dependence of the velocity and attenuation changes during irradiation pinning should be less rapid if dipole effects are important. For an LiF sample deformed in [001] compression and measured by 10 MHz longitudinal waves at 4.2 K the irradiation pinning results suggest that there are not an order of magnitude more edge dipoles than screw dislocations. However for this sample the deformation was much less so that the dislocation density was about $1 \times 10^6$ cm$^{-2}$, and it is likely that the dipole density and width distribution is somewhat different for small deformation.

In conclusion we have considered the implications of assuming a large density of edge dipoles (previously deduced from thermal conductivity measurements) on the specific heat and ultrasonic velocity and attenuation in LiF. We have found the specific heat is relatively insensitive to dislocations and dipoles in the expected densities. We also found that irradiation pinning ultrasonic measurements should show the optical mode effects of edge dipoles if they are in fact present in numbers an order of magnitude greater than isolated dislocations. Such measurements should be carried out on specimens deformed by a few percent. If possible it would be useful to measure the thermal conductivity effects on the same sample. In this case, kilohertz ultrasonic measurements would be more applicable to the typically rod-shaped thermal conductivity samples.

References

5. (a) A. Granato and K. Lücke, J. Appl. Phys. 27, 583 (1956).
(b) A. Granato and K. Lücke, J. Appl. Phys. 27, 789 (1956).