

Dislocation Interactions with Phonons in Sodium Chloride in the Temperature Range 70–300 °K*

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The dislocation drag coefficient B in sodium chloride has been measured in the temperature range 70–300 °K. Use was made of a technique for measuring ultrasonic attenuation changes $\Delta\alpha$, at different frequencies, caused by a bias stress. The numerical values of B were obtained from an analysis which does not require any knowledge of the dislocation density or of other geometrical features of the dislocation network. The experimental results agree qualitatively with theoretical predictions of the temperature dependence of B . The dislocation scattering cross section for phonons is deduced from these measurements and compared with theoretical treatments.

I. INTRODUCTION

In spite of a number of experimental and theoretical studies carried out in recent years on the viscous damping constant B of dislocations, many qualitative and quantitative problems remain unanswered. In the case of metals the viscous damping (resistive force proportional to the velocity of dislocations) is attributed to dislocation interactions with phonons and with conduction electrons. In general, a direct separation of the two contributions is not easy. In an earlier study,¹ using ultrasonic techniques, we were able, however, to measure the electron contribution to B in lead by comparing the dislocation damping in the normal and superconducting states of the metal. In the same study we also found that the electronic B does not depend on temperature. In a subsequent study of B in aluminum,² also by ultrasonic methods, the separation of the electron and phonon contributions was carried out indirectly from the temperature dependence of the dislocation damping. The present investigation was undertaken to determine the phonon contribution to B independently, i. e., in the absence of conduction electrons. To this end we measured the dislocation damping in sodium chloride over the temperature range 2–300 °K. Use was made of a previously developed technique which allows one to obtain the value of B without knowing the dislocation density or other geometrical features of the dislocation network.

II. EXPERIMENTAL TECHNIQUE

In connection with the study of B in aluminum² we developed and successfully applied a "dynamic-bias-stress method." This method is a way of extracting the dislocation contributions from the total ultrasonic attenuation by applying a second ultrasonic wave (low frequency and high amplitude) in a direction perpendicular to that of the attenuation-measuring wave. The change in attenuation caused

by the bias-stress wave is measured as a function of frequency at a given temperature and analyzed on the basis of the string model of dislocations developed by Granato and Lücke.³ The merit of this method is twofold: (i) It is possible to extract dislocation contributions without damaging the samples (e. g., without irradiation); (ii) it is not necessary to know the density of dislocations in the samples. Since the details of the experimental techniques and of the method of the analysis were presented in a previous article,² they are not repeated here.

The samples used are single crystals of sodium chloride cleaved from optical-grade ingots supplied by Harshaw Chemical Co. The size of the samples is approximately 7×7×8 mm, and the faces are oriented in $\langle 100 \rangle$ crystallographic direction. After cleaving, two sets of faces of the sample are ground slightly to obtain flat and parallel surfaces for the purpose of ultrasonic wave propagation.

Two quartz transducers are used—a 10-MHz transducer for the measuring wave and a 5-MHz transducer for the 5-MHz bias stress.

Because of the large difference in the thermal expansion coefficients of quartz and sodium chloride it is not possible, with a single bonding agent, to obtain adequate coupling between transducers and the samples for ultrasonic measurements covering the entire temperature range investigated. As a consequence, different bonding agents were used for different temperature ranges: i. e., from room temperature to 200 °K, Nonaq stopcock grease or silicone grease; from 200 to 160 °K, 4-methyl-1-pentene; below 150 °K, 1-pentene. Since pentene is highly volatile at room temperature, bonds were made at temperatures slightly above its freezing temperature.

A conventional cryogenic system, described earlier,² was used to control temperature ranging from room temperature down to 2 °K.

III. RESULTS AND DISCUSSION

An example of the results is shown in Fig. 1, where the attenuation change $\Delta\alpha$ caused by the bias-stress wave applied at various temperatures is plotted as a function of frequency ν . As discussed in connection with the study of aluminum, a maximum is observable in the $\Delta\alpha$ - ν relation (depending on the temperature at which the experiment is performed), and the position of the maximum is shifted to higher frequencies as the temperature is lowered. (If a relaxation type of mechanism is responsible for this effect, the shift of the maximum with temperature should be in the opposite direction.) The curves drawn through the points are the results of the least-squares fitting by computer of the following expression:

$$\Delta\alpha = \frac{\partial}{\partial L_c} \int_0^\infty \alpha(l) l N_c(l) dl (\delta L_c), \quad (1)$$

where $\alpha(l)$, the attenuation per unit length of dislocation, is given by

$$\alpha(l) = \left(\frac{4RGb^2}{\pi^2 Av} \right) \left(\frac{\omega^2 d}{(\omega_0^2 - \omega^2)^2 + (\omega d)^2} \right) \quad (2)$$

and $N_c(l)dl$ is the number of dislocations whose loop length lies between l and $l+dl$; ω_0 is the resonant frequency of a dislocation of length l and is

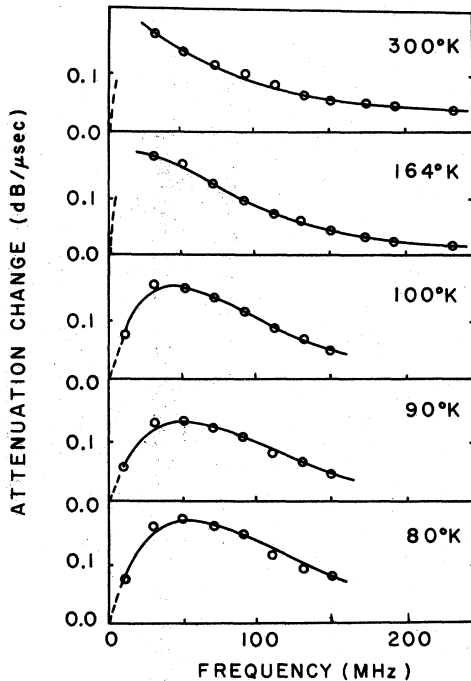


FIG. 1. Incremental attenuation $\Delta\alpha$ as a function of frequency for five representative temperatures. The points represent experimental data; the continuous curves represent computer fits of Eq. (1) to those points. Experimental uncertainty in $\Delta\alpha$ is ± 0.01 dB/ μ sec.

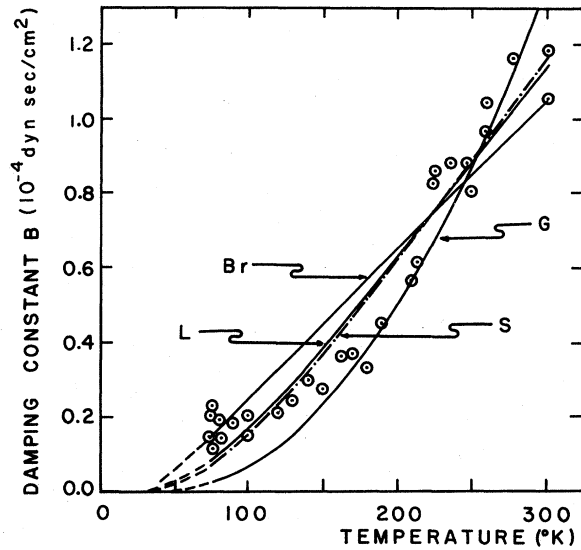


FIG. 2. Damping constant B as a function of temperature. The circles represent the values of B obtained from the curves of $\Delta\alpha(\omega)$. The curves marked L, S, G, and Br represent computer fits of Eqs. (3), (4), (5), and (6), respectively.

given by

$$\omega_0 = (\pi/l)(C/A)^{1/2},$$

where C is the dislocation line tension; ω is the frequency of the applied ultrasonic wave; $d = B/A$, where B is the damping constant and A is the effective mass per unit length of dislocation, assumed to be $\pi\rho b^2$, where ρ is the density of the material and b is the Burgers vector; R is an orientation factor; G is the shear modulus; and v is the velocity of the wave. For the distribution function $N_c(l)dl$, an exponential distribution has been used:

$$N_c(l)dl = (\Lambda/L_c^2) e^{-l/L_c} dl,$$

where Λ is the total length of dislocations per unit volume and L_c is the average loop length of the dislocations. The derivation of this expression is given in Ref. 2. For the least-squares fitting, d and ω_0 are used as the adjusting parameters. The values of the damping coefficient B thus obtained are shown in Fig. 2 (for $A, \pi\rho b^2 \approx 10^{-14}$ cgs is used). Although the experiments were carried out at temperatures down to 2°K, only the results obtained at temperatures above 77°K are presented in Fig. 2. The reason for this is that at temperatures below 70°K contributions from mechanisms other than the viscous damping seem to become appreciable. As a consequence, it may no longer be justifiable to carry out the analysis with expression (1) alone. A report discussing this matter will be presented separately.

Following the procedure given in Ref. 2, theo-

retical expressions predicting the values and temperature dependence of the damping constant B are compared with the experimental results. Here, however, the term B_e (contribution from conduction electrons) included in Ref. 2 is set to be zero. The theoretical results are shown in Fig. 2 by the curves marked L, S, G, and Br. The explanation follows.

First, the definitions of the symbols and their values used for the computer fitting are listed: c (Debye average sound velocity) = 2.7×10^5 cm/sec, c_t (velocity of transverse wave) = 2.41×10^5 cm/sec, c_l (velocity of longitudinal wave) = 4.74×10^5 cm/sec, b (Burgers vector) = 4.0×10^{-8} cm, ρ (density) = 2.16 g/cm³, ω_D (Debye frequency) = 3.68×10^{13} /sec, Θ_D (Debye temperature) = 281 °K, γ (Grüneisen constant), ω_{ph} (thermal phonon frequency), T (temperature °K), and \hbar and k_B have the usual meaning.

Curve L: Leibfried's theory⁴ based on the fluttering mechanism of dislocations. The expression for B is given by

$$B_L = \frac{1}{10} (\sigma/c) \bar{\epsilon}, \quad (3)$$

where $\bar{\epsilon}$ is the thermal energy density and is given by

$$\bar{\epsilon} = \frac{3}{2\pi^2 c^3} \int_0^{\omega_D} \hbar \omega^3 \{ \exp[(\hbar \omega_{ph}/k_B T) - 1] \}^{-1} d\omega_{ph}.$$

The scattering cross section per unit length, σ , which is assumed to be independent of phonon frequency, is chosen as the fitting parameter. The best fit is obtained when σ is 8.2×10^{-8} cm, i. e., approximately equal to $2b$.

Curve S: Scattering of phonons caused by the strain field of dislocations. The scattering cross section of dislocations at rest has been calculated by several investigators for the study of thermal conductivity. Aside from numerical constants, they all agree in that the scattering cross section is proportional to the phonon frequency, i. e., $\sigma(\omega_{ph}) = \Gamma \omega_{ph}$. If one substitutes this cross section for σ in the following expression derived by Nabarro,⁵

$$F = \frac{1}{3} (\sigma/c) \bar{\epsilon} v, \quad F = B_s V,$$

one finds

$$B_s = \frac{\hbar \Gamma}{2\pi^2 c^4} \int_0^{\omega_D} \omega_{ph}^4 d\omega_{ph} [\exp(\hbar \omega_{ph}/k_B T) - 1]^{-1}. \quad (4)$$

The best fit of this expression to the data is obtained when Γ is equal to 9.2×10^{-22} cgs. This value of Γ may be compared with the various predictions.

(a) Klemens's expression^{6,7}:

$$\Gamma_k = 6.04 \times 10^{-2} \frac{b^2 \gamma^2}{c} \approx 4.16 \times 10^{-22} \text{ cgs with } \gamma = 1.06.$$

(He revised his estimate of Γ by a factor of 10

upwards in his later publication.⁷)

(b) Carruthers⁸ and Moss's⁹ expression:

$$\Gamma_c = 5.21 \times 10^{-3} \frac{(gb\beta/\rho c^2)^2}{c} \approx 3.4 \times 10^{-20} \text{ cgs},$$

where g is the anharmonic coupling coefficient, $\beta = (1 - 2\nu)/(1 - \nu)$, and ν is Poisson's ratio. These values are tabulated in Ref. 9. (For numerical comparison with our Γ , Γ_k and Γ_c given in Ref. 9 should be divided by c as indicated above.)

(c) Ziman's expression¹⁰:

$$\Gamma_z = \frac{1}{2} \gamma^2 b^2 / c \approx 3.5 \times 10^{-21} \text{ cgs}.$$

(Brailsford¹¹ recently stated that the value Γ_z should be reduced by a factor of 8.)

(d) Ohashi's expression¹²:

$$\Gamma_0 = \frac{1}{2} \left(-\frac{g}{C_{11}} \right) \frac{b^2}{c_l} \approx 3 \times 10^{-19} \text{ cgs}$$

with

$$C_{11} = 5.88 \times 10^{11} \text{ dyn/cm}^2.$$

Order-of-magnitude agreement was obtained between the experimentally determined Γ and the values predicted by Klemens and Ziman. The theories of Carruthers and Ohashi, on the other hand, give values of Γ substantially in excess of the present results relating to B .

Curve G: Gruner's theory. In the above calculations, the scattering cross section of dislocations at rest was estimated first and then the effect of motion of the dislocations with a constant velocity v was evaluated. Seeger and Engelke,¹³ on the other hand, calculated the retarding force on a dislocation using perturbation theory, starting from a Hamiltonian in which the motion of dislocations with velocity v is taken into account from the outset. Their final results (applicable to dislocation kinks), however, were too complicated to be tested by means of the fitting procedure used here. Gruner,¹⁴ following the same approach, derived a simpler expression for the damping constant B when all parts of a dislocation move with the same velocity. The extension of his theory to the case of dislocation kinks was found¹⁴ to agree, except for a numerical factor, with Seeger and Engelke's result for the case of interactions of "light phonons." Gruner's expression is given by

$$B_G = [\bar{\epsilon}_l b T / (c_l \Theta_D)] \alpha^{\text{screw/edge}}, \quad (5)$$

where $\alpha^{\text{screw/edge}}$ is a numerical factor connected with the anharmonicity and $\bar{\epsilon}_l$ is the energy of the longitudinal phonons given by

$$\bar{\epsilon}_l = \frac{\pi^2 k_B^4 T^4}{30 \hbar^3 c_l^3}.$$

Although this theory may be applicable only for low temperatures ($T < \frac{1}{3} \Theta_D$), as Gruner indicated, we arbitrarily extended it to higher temperatures

by using the expression for $\bar{\epsilon}_i$,

$$\bar{\epsilon}_i = \frac{\hbar}{2\pi^2 c_i^3} \int_0^{\omega_D} \omega_{ph}^3 [\exp(\hbar\omega_{ph}/k_B T) - 1]^{-1} d\omega_{ph}.$$

$\alpha^{\text{screw/edge}}$ was chosen as the fitting parameter and was found, for the best fit, to be equal to 6.5. The value of $\alpha^{\text{screw/edge}}$ for NaCl is not known to us. If this value does not differ much from that of copper, i. e., 4.599×10^3 , as quoted by Grüner,¹⁴ then the experimental value obtained here is obviously much too small. If one compares Grüner's original expression with the data at 77 °K (disregarding the computer fitting), one finds for $\alpha^{\text{screw/edge}}$ a value 20, which is still too small.

Curve Br: Brailsford's theory. Brailsford made a detailed study of the drag force acting upon moving dislocations and developed a unified theory which includes and classifies the thermoelastic damping, phonon viscosity, phonon scattering, and reradiation damping. Among these mechanisms, the most relevant one here is the phonon scattering, which is given by the following expression:

$$B_{Br} = \frac{3}{2} \frac{T}{c} \left(\frac{\gamma S^2 b}{2\pi} \right)^2 \int_0^{\omega_D} q^3 C_q dq, \quad (6)$$

where C_q is the contribution of the mode q to the specific heat per unit volume. Using the Debye approximation $\omega_{ph} = cq$ and the relation $C_q = \hbar\omega_{ph}(\partial n/\partial T)$, the curve Br is obtained with γ as the fitting parameter. The value of γ for the best fit was found to be 1.4, which should be compared with the values reported in the literature ranging from 1.55 to 1.61.⁹

Some remarks should be made concerning Brailsford's theory. Expression (6) was derived in terms of a single phonon velocity (longitudinal), and it was pointed out by Brailsford that a numerical correction factor of 22 should be applied to take into account the weighing of each phonon mode by its velocity. We have used here the average velocity (as defined above), thus incorporating from the outset a correction of similar magnitude to that suggested by Brailsford. The same procedure was also used in our previous work on aluminum,² in connection with which his remark was made. It follows that our values of B in aluminum apparently are consistent with Brailsford's calculation, contrary to his assessment. The correctness of Brailsford's theory will have to be tested further, but the fact noted above supports his calculations.

Al'shits^{15,16} also calculated B , and obtained the same temperature dependence as Brailsford,¹¹ but different numerical constants. However, his approach is strictly valid only in the regime of fast-moving dislocations ($v > 10^{-3}c$), which is well outside the region investigated in the present study.

The values of B obtained in this experiment are now compared with the experimental results of other investigators.

The methods used by these investigators can be divided into three categories: Two of these involve ultrasonic techniques and the third consists of measuring dislocation displacements under the influence of short-duration stress pulses. The essential steps in those measurements are, by category, as follows. (i) Measure the ultrasonic decrement as a function of frequency, obtain the background decrement by immobilizing the dislocations through irradiation, obtain the decrement due to dislocations by difference, estimate the dislocation density by etch-pit count, and use the following approximate expression for analysis:

$$\text{decrement } \Delta = \left(\frac{8Gb^2}{\pi^3 C} \right) R \Lambda L_c^2 \frac{\omega\tau}{1 + \omega^2\tau^2}, \quad (7)$$

where $\tau = BL_c^2/\pi^2 C$. There are, however, at least three significant sources of error in this technique: (a) the instrumental difficulty of returning to the same tuning condition, at each frequency, after irradiation; (b) the uncertainty in the relation between the etch-pit count and the dislocation density responsible for ultrasonic attenuation; (c) use of Eq. (7) in which the ultrasonic frequency ω used is neglected relative to ω_0 [see Eq. (2)]. (In our experiments the values of resonant frequency ω_0 corresponding to the average loop length L_c were found to be temperature dependent and range from 100 to 300 MHz. The effective resonant frequency then should be $1/3.31$ of ω_0 ,³ which falls easily in the experimental frequency range.)

(ii) Measure the ultrasonic attenuation and velocity, obtain the dislocation density from etch-pit counting, use Eq. (7) with the corresponding equation for velocity to perform the analysis. This method is subject primarily to errors of type (b).

(iii) Measure the dislocation displacement x resulting from the application of a stress pulse of duration t and magnitude S , and obtain B from the relation

$$Bv = Sb \quad \text{with } v = x/t.$$

This method is subject to uncertainties resulting from the fact that measurable displacements x are much larger than those involved in ultrasonic experiments. The value of v thus obtained is very likely, therefore, to be lower than the intrinsic values, because the moving dislocation may be held up by obstacles for a considerable fraction of the measured time t .

Moog,¹⁷ who used method (i), reported seven different values of B in NaCl ranging from 2.5×10^{-4} to 10.5×10^{-4} cgs at room temperature. When one of his data (specimen FG) was analyzed with our computer-fitting method, a value of 7.6

$\times 10^{-5}$ cgs was found, which is much smaller than the quoted value of 2.5×10^{-4} cgs, but close to the results of this experiment. Korowkin and Soifer¹⁸ reported 4×10^{-4} cgs for B at room temperature using the same technique. Fanti, Holder, and Granato,¹⁹ who used method (ii), reported a value of 1.6×10^{-4} cgs, which is very close to our value. Gutmanas, Nadgorny, and Stepanov,²⁰ who used method (iii), reported 2×10^{-4} cgs at room temperature. Ermakov and Nadgorny,²¹ on the other hand, reported (using the same technique) 5×10^{-4} at room temperature, 4×10^{-4} at 150 °K, 2.8×10^{-4} at 100 °K, and 1.7×10^{-4} at 77 °K. Obviously, the temperature dependence of their results does not agree with the present results. They also reported that the value B increased by a factor of 1.5 with 5×10^8 -rad ⁶⁰Co irradiation. This last point suggests that their value of B may include the contribution of point defects interacting with the moving dislocations.

IV. CONCLUSIONS

The results of this study on the dislocation drag constant B in sodium chloride bear on three problems: the absolute value of B at a given temperature, the temperature dependence of B in the range investigated, and the dislocation scattering cross section for phonons.

With regard to the first point, it should be noted that the present analysis yields the quantity B/A , where A is the effective mass of the dislocation. The numerical value of B depends, therefore, on the value adopted for A (we used $A = \pi \rho b^2 \approx 10^{-14}$ cgs). In addition, theoretical predictions of B include the anharmonic phonon-phonon coupling coefficient. This parameter is often represented by the average Grüneisen constant or by a combination of second- and third-order elastic constants, derived from an assumed model of the interaction. The difference, if any, between the above and a rigorously derived coupling is not known. Furthermore, the calculated results for B depend on a high power of the sound velocities and are therefore very sensitive to the values used. Thus the experimental values of B can be compared with pre-

dictions only to within these uncertainties.

As far as the temperature dependence of B is concerned, in the range investigated here ($T \gtrsim \frac{1}{4} \Theta_D$), current theories yield essentially the same result, namely, $B \propto T$. The proportionality constant of the relation $B \propto T$ differs, however, from model to model. As can be seen in Fig. 2, curve L and curve S are almost indistinguishable, and are in fairly good agreement with the data. Curve G seems to be too steep and curve Br appears to be too flat. The real test of the models, however, might come from measurements at lower temperatures, where Leibfried's theory (curve L) predicts T^4 dependence of B , while the scattering, Gruner's, and Brailsford's theories, curves S, G, and Br, respectively, should give T^5 dependence. Furthermore, Brailsford¹¹ suggested that his theory predicts T^6 dependence when applied to dislocation kinks. Lothe,²² on the other hand, suggested that for kink mobility the cutoff temperature $\Theta'_D = \Theta_D/\eta$, instead of Θ_D , should be used where η is the ratio w/b , w being the kink width. The effect of this is to lower the temperature at which B approaches its asymptotic temperature dependence (linear in T).²³ All these temperature dependences, however, should show up below 77 °K, and for the reason mentioned earlier the subject will be discussed in a separate publication.

Finally, we consider the dislocation scattering cross section for phonons obtained in this study. Most of the calculations of this cross section aimed either at predicting or at accounting for the thermal resistivity contributed by dislocations. Earlier calculated values of this cross section were systematically much lower than those estimated from thermal resistivity measurements,¹² but are of the same order of magnitude as the one deduced here. It is suggested that the cross-section values obtained from thermal-resistivity measurements are generally too large, because of the considerable uncertainty in evaluating the total dislocation density (the measured density is always a lower limit of the actual density). By contrast, the present method, which is independent of dislocation density, is likely to yield a more realistic scattering cross section.

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Role of Longitudinal and Transverse Phonons in the Thermal Conductivity of Alkali Halides

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In the present paper we have explained the temperature dependence of the thermal conductivity of KCl and NaCl by considering the separate contributions of longitudinal and transverse phonons. It is found that the transverse phonons make a major contribution towards thermal transport in these alkali halides.

INTRODUCTION

The low-temperature thermal conductivity of doped and undoped alkali halides has been studied extensively from both an experimental and a theoretical viewpoint by two different groups, one under Pohl at Cornell and the other under Klein at Illinois. The work of the Cornell group has been reviewed by Pohl in three different review articles.¹⁻³ The group at Illinois has also done a large amount of work⁴⁻⁶ of which the most recent and important is the work of Rosenbaum *et al.*⁷ Many other workers have also studied the thermal conductivity of doped and undoped alkali halides.⁸⁻¹⁰ These workers have been successful in explaining the experimental results using the Callaway model¹¹ in which no distinction is made between longitudinal and transverse phonons. This distinction is, however, essential in view of the different dispersive natures and different relaxation times for the two types of phonons. Using both a variational method¹² and a relaxation-time approach,¹³⁻¹⁵ it has been shown that in semiconductors most of the heat is probably carried by transverse phonons. Such a possibility also exists for alkali halides. Therefore, it is desirable to

estimate the separate contributions of transverse and longitudinal phonons towards the phonon conductivity of alkali halides. This is possible either with the Holland model¹⁶ or the Sharma, Dubey, and Verma (SDV) model^{14,15} of phonon conductivity. In the variational method a provision to estimate the separate contributions due to longitudinal and transverse phonons exists in the technique given by Hamilton and Parrott.¹² However, the variational method is very difficult to apply owing to the complexity of the calculations involved. In the present paper we have used the Holland model to estimate the separate contributions of transverse and longitudinal phonons towards the phonon conductivity of alkali halides. As typical examples of alkali halides, we have considered KCl and NaCl.

THEORY

In the Holland model the lattice thermal conductivity K is given by

$$K = K_L + K_{T_1} + K_{T_2}.$$

The subscripts T and L indicate transverse and longitudinal phonons.

In alkali halides the longitudinal phonon spectrum