FLUTTERING MECHANISM AND RESONANT SCATTERING IN InSb CONTAINING Ga

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The relaxation rate of phonons due to vibrating dislocations (fluttering mechanisms) which appear during the crystal growth, is analysed with the help of the expressions presented by Ninomiya, Nabarro and Granato. The relaxation rate frequency spectrum is studied in the lattice thermal conductivity counterpart. These mechanisms associated with the thermal resistance of dangling electrons play a very important role in thermal conductivity at low temperatures where the point defect scattering is unimportant. The variation of phonon resonances as a function of temperature and frequency is studied at the resonant frequency 5.8×10^{12} rad s^{-1} of the resonant mode of InSb containing Ga impurities. It is found that the resonant scattering properties are enhanced by the dislocation concentration, which, in turn, effectively plays a dominant role in phonon conductivity.

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1. *Introduction*

The anharmonicities of lattice forces govern the thermal transport by lattice vibrations, by the external boundaries and by various types of imperfections in solids. The free electrons also contribute in the lattice component of thermal conduction in many solids, e.g.; metals and semi-metals. The effects of imperfections on the lattice component of the phonon conductivity of metalic alloys are qualitatively the same as their effects on the phonon conductivity of insulators.

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Phonons transporting heat energy in crystals containing irregularities of lattice, such as impurities, a dislocation or more complex imperfections (which can scatter the thermal waves) are scattered through various mechanisms and the lattice heat conduction is restricted to a definite amount. These restrictions are governed by anharmonic interactions arising in the crystal potential energy [1–6]. At low temperatures the plastic deformations are observed to decrease the lattice thermal conductivity remarkably. This phenomenon is basically attributed to the scattering of phonons by dislocations which are developed during the crystal growth or deformation. Klemens [7, 8], and Carruthers [9] have given a very good account for these scattering processes. The scattering of phonons due to dislocations is of various types, e.g., strainfield dislocation [8], core dislocation [8], oscillating dislocations [10–12], dislocations with kink oscillations [13] etc. Imperfections have a dramatic effect on the phonon conductivity of solids at low temperatures. In a number of cases a localized mode is created and lowers the conductivity of solids considerably giving rise to the phonon resonance scattering.

The anisotropic nature of the fields of dislocations makes the problem much more complicated. This anisotropy makes the relaxation times independent of the angle of scattering. Moreover, an experimental situation may lead to this aspect, if one considers a sufficient number of dislocations oriented at random angles, which give rise to the angle--independent relaxation time.

In the present paper we shall deal with the relaxation time phenomena for the oscillating dislocations and the phonon resonant scattering from imperfections. The fluttering mechanisms attributed to the oscillating dislocations and phonon resonant scattering for InSb is studied. The expression reported by Nabarro [11], Granato [10] and Ninomiya [12] has been analysed from different angles and deviations in the relaxation rates are shown on different graphs.

2. *Phonon scattering due to oscillating dislocations*

Ninomiya [12] has discussed the theory of oscillating dislocations. He assumed that the phonons are being scattered due to oscillating dislocations. The dislocations are oscillating in a potential field, a consequence of which is that the potential energy associated to the field is a square function of the displacement of dislocation from its equilibrium state. If the edge of the dislocation scatters only the transverse phonons, then the relaxation time can be given by

$$\tau_d^{-1}(\omega)|_{Ni} = Nv\langle F(\omega)\rangle. \tag{1}$$

where N is the number of dislocations, v — the phonon velocity and $\langle F(\omega)\rangle$ represents the expectation value of scattering width and is expressed by

$$\langle F(\omega)\rangle = \frac{\omega^3 v}{8[(\omega_0^2-\omega^2)^2+(\omega^4/16\pi^2)]}. \tag{2}$$

Here ω_0 represents the frequency of dislocation. In the denominator of Eq. (2), for analytical purposes, we replace $(\omega_0^2-\omega^2)$ by $(\omega_0^2 \sim \omega^2)$. Hence Eq. (1) yields

$$\tau_d^{-1}(\omega)|_{Ni} = \frac{Nv^2\omega^3}{8[(\omega_0^2 \sim \omega^2)^2+(\omega^4/16\pi^2)]}. \tag{3}$$

The expression for the relaxation rate of phonons due to vibrating dislocations is also given by Nabarro [11] and Granato [10] in the form:

$$\tau_d^{-1}(\omega)|_{NG} = \frac{2\pi^2 v^2 N}{\omega[\ln(4v/b\omega)-1.077]^2}, \tag{4}$$

where b represents the Burgers vector. The expression $[\ln(4v/b\omega)-1.077]^2$ in the denominator can be replaced by $[\ln(4v/b\omega) \sim 1.077]^2$ from the analytical point of view.

Viewing expression (3) and (4) carefully, it is obvious to say that the inverse relaxation rates must approach infinity at a certain value of ω, conversely, the relaxation time vanishes for a particular value of ω and these values of ω are

$$\omega_{Ni}^2 = \frac{4\pi\omega_0^2}{16\pi^2+1}(4\pi \pm i) \tag{5a}$$

$$|\omega_{Ni}| = \left(\frac{16\pi^2 \pm 1}{16\pi^2}\right)^{1/4} \omega_0 \tag{5b}$$

and

$$\omega_{NG} = 0, (4v/b)\exp(-1.077). \tag{6}$$

For phonon velocity $v = 3.2\times10^5$ cm/s^{-1} the value of ω_{Ni} is found to be equal to $\pm 1.41\ \omega_0$ and the value of ω_{NG} to 0 and 3.25 ω_0. From this one concludes that the frequency spectrum of relaxation time will go to infinity at the frequencies 1.41 ω_0 and $-1.41\ \omega_0$ for Ninomiya's expression. But the negative value of frequency seems to be unusual and hence only 1.41 ω_0 is acceptable. In case of Nabarro and Granato both the values are acceptable because the smallest value of the frequency is zero.

3. Phonon resonance scattering

Griffin et al. [14] have made use of the perturbation theory in the deformation potential approximation, and they suggested that the inverse of the relaxation rate for phonon resonance scattering is proportional to ω^4 and is given by

$$\tau_R^{-1}(\omega) = \frac{D\omega^2 T^3}{(\omega^2-\omega_0^2)^2}, \tag{7}$$

where D is some adjustable parameter. Eq (7) indicates that $\tau_R^{-1}(\omega)$ has an infinite value at the resonant frequency. The theory of resonance scattering reported by Griffin et al. was developed for elastic scattering only. Kwok [15] extended it for the problems of inelastic scattering and thermally assisted phonon absorption processes. However, the elastic scattering of phonons remains dominant, if one considers the Kwok's extension, and the frequency dependence of the relaxation rate holds to the ω^4 dependence. The theory presented by Kwok is based on thermodynamics with the Green's function technique. The resonance denominator based on the Green's functions is $(\omega-\omega_0)^2$. However, for the sake of comparison he replaces it by $(\omega^2-\omega_0^2)^2$. In the present paper we shall not discuss Kwok's theory but shall analyse the rate

$$\tau_R^{-1}(\omega) = \frac{D\omega^2 T^3}{(\omega^2 \sim \omega_0^2)^2} \tag{7a}$$

extensively. Pohl [16–18], Walker et al. [19], Seward et al. [20] have discussed the resonant scattering in details with a deeper insight for their experimental observations.

The resonant scattering of phonons is able to explain the dips in the thermal conductivity curves in the region around 20K or below. This can be seen better in references [21, 22].

4. *Discussion and conclusions*

The analysis of thermal conductivity around 20K and below 2K shows discrepancies. The dislocation densities affect these results remarkably. Near 20K the point defect type of the imperfections plays a prominent role to contribute much in thermal conductivity, but below 2K discrepancies can be removed by accounting for the scattering of phonons due to dangling electrons located at the dislocation core.

In present paper we have analysed the above cited relaxation rates of InSb for the experiments reported by Guckelsberger et al. [22]. The various constants and parameters

TABLE I

Ga Concentration PPM	b Å	N $cm^{-3}\times 10^{17}$	v $cm\ s^{-1}\times 10^5$	D $s^{-1}\times 10^{24}$	$rad\ s^{-1}\times 10^{12}$
0	2.304	0.2	3.2	9.1	5.8
500	2.304	0.9	3.2	189.0	5.8
2000	2.304	1.7	3.2	310.0	5.8

used in the analysis are furnished in Table I. Fig. 1 shows a typical plot of $\tau_d^{-1}(\omega)|_{Ni}$ vs ω. As the frequency increases gradually the inverse relaxation rate increases rapidly till the frequency reaches 5.5×10^{12} rad s^{-1}. The relaxation rate becomes infinite as the frequency approaches 5.8×10^{12} rad s^{-1}, the resonance frequency. Closer to the vicinity of the resonance frequency it approaches $\omega = 6.5\times 10^{12}$ rad s^{-1}, the relaxation rate falls rapidly and becomes more gradual above it, than in the low frequency region. This clearly shows that the relaxation time is highly effective at the frequencies appearing comparatively farther than the resonant one. This relaxation time will not contribute in the vicinity of resonance dips of thermal conductivity, but will contribute efficiently at lower temperatures which will be more justified by Nabarro and Granato expressions. The dislocation concentration affects the relaxation rates to a large extent. Higher dislocation densities make higher relaxation rates, e.g., curves A, B, C, are relatively at increasingly higher dislocation densities, respectively.

Fig. 2 shows another typical plot for the relaxation rates vs ω. The curves A', B', C' are for the relaxation rate $\tau_d^{-1}(\omega)|_{NG}$ and the others are for those of Fig. 1. A general

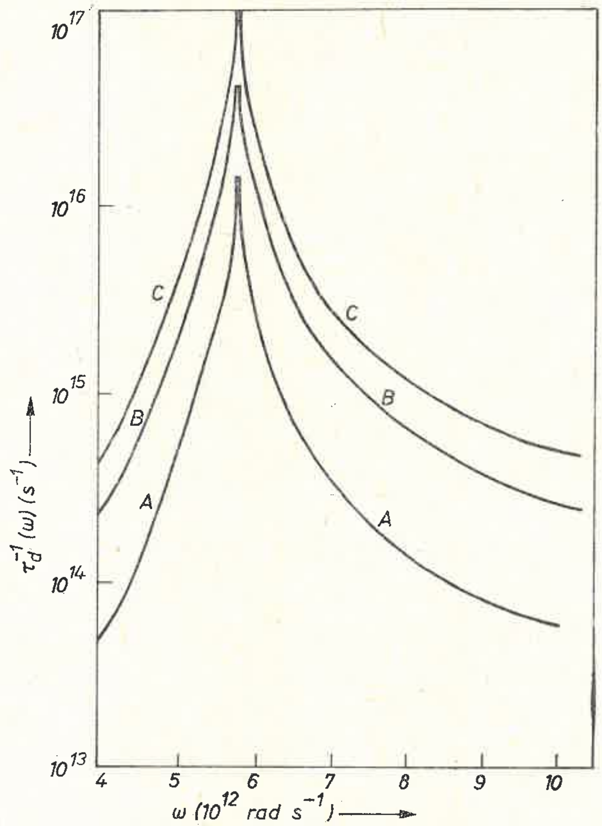

Fig. 1. Variation of $\tau_d^{-1}(\omega)|_{Ni}$ with ω for InSb-Ga. A — InSb-Ga 0.0 PPM, B — InSb-Ga 500 PPM, C — InSb-Ga 2000 PPM

insight into these curves obviously shows te discrepancies between the two relaxation rates. The $\tau_d^{-1}(\omega)$ for Ninomiya's expression shows its infinite value at the frequency 5.8×10^{12} rad s^{-1}, while the Nabarro and Granato expression shows this at the frequencies zero and 18.85×10^{12} rad s^{-1}. The change of dislocation densities show nearly the same behaviour in both the expressions. But between the frequency range 2×10^{12} to 4.5×10^{12} rad s^{-1} the relaxation time shows a slight variation and becomes a most efficient contributor to the thermal conductivity, because it appears not as $\tau_d^{-1}(\omega)$ but as $\tau_d(\omega)$ in Callaway's expression [23] for lattice thermal conductivity.

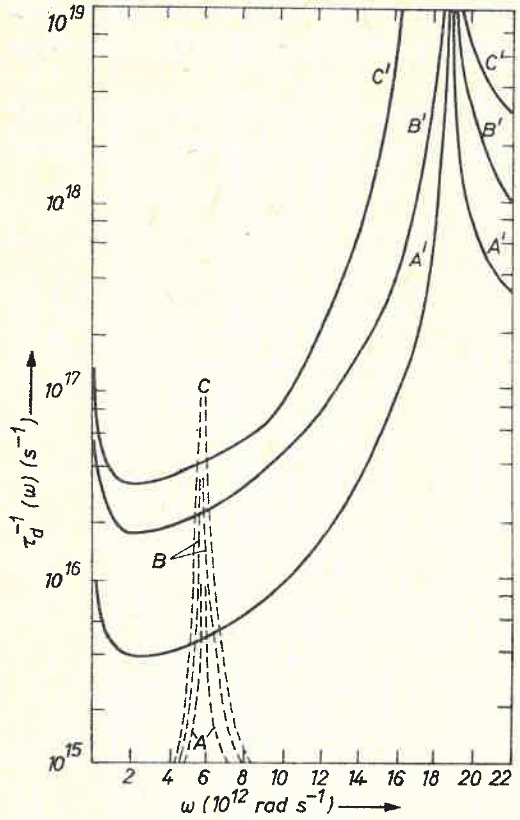

Fig. 2

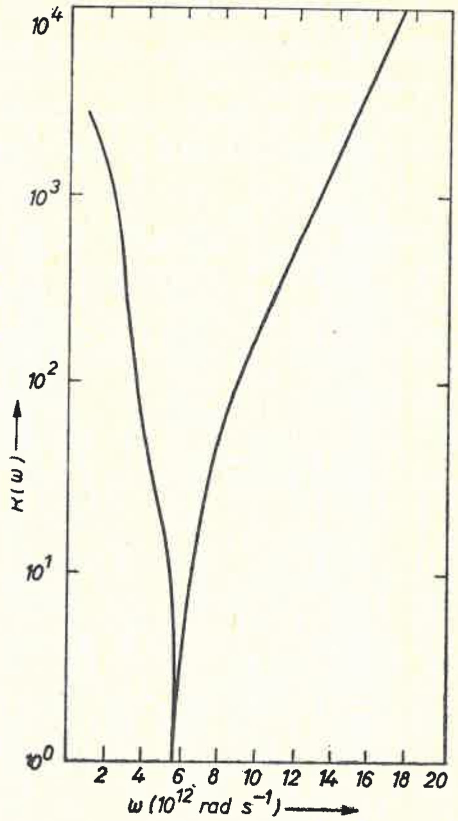

Fig. 3

Fig. 2. Curves for $\tau_d^{-1}(\omega)|_{Ni}$ and $\tau_d^{-1}(\omega)|_{NG}$ versus ω. A,A' — InSb-Ga0.0 PPM, B,B' — IbSb-Ga500 PPM, C,C' — InSb-Ga2000 PPM. Primes denote curves for Nabarro and Granato expressions

Fig. 3. Curves for $R(\omega)$ versus ω

This discrepancy of relaxation times may be studied easily. The ratio of the two relaxation rates is given by

$$R(\omega) = \frac{\tau_d^{-1}(\omega)|_{NG}}{\tau_d^{-1}(\omega)|_{Ni}},$$

$$= \frac{8(\omega_0^2-\omega^2)^2+\omega^4/16\pi^2}{(\omega^4/2\pi^2)\,[\ln(4v/b\omega)-1.077]^2}. \tag{8}$$

The plot between $R(\omega)$ and ω is shown in Fig. 3, which shows the relative variation of the two expressions of relaxation rates presented by Nabarro, Granato and Ninomiya. At the resonant frequency the curve approaches zero while at $\omega = 0$ and $3.25\omega_0$ it goes to infinity.

Fig. 4 shows the variation of the resonant scattering relaxation rate with frequency at various temperatures. $\tau_R^{-1}(\omega)$ increases with increasing temperature. At the resonant frequency the phonon resonant relaxation rate goes to infinity. This rate shows a T^2 dependence at each frequency but a ω^4 dependence at each temperature. The increase of the dislocation concentration increases the relaxation rate considerably. Since $\tau_R^{-1}(\omega)$

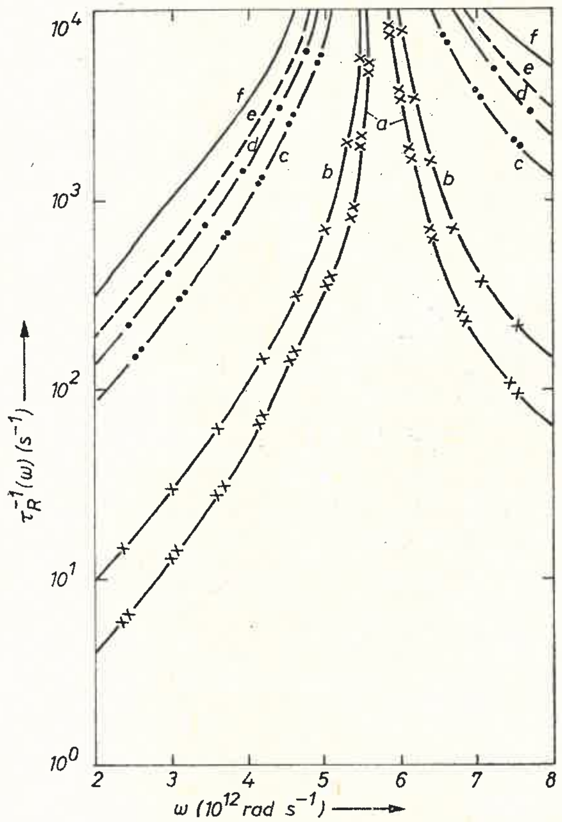

Fig. 4. Variation of $\tau_R^{-1}(\omega)$ with ω for InSb-Ga. At $T = 10$K, a — InSb-Ga0.0 PPM, c — InSb-Ga500 PPM, d — InSb-Ga2000 PPM. At $T = 15$K, b — InSb-Ga0.0 PPM, e — InSb-Ga-500 PPM, f — InSb-Ga-2000 PPM

also appears in the phonon conductivity relation in the form $\tau_R(\omega)$, at the resonant frequency it will offer a very high thermal resistance and thus explains the characteristic depression in the conductivity curve.

The entire discussion of the relaxation rate spectrum explains well that the plastic deformations (dislocations) play a prominant role in contributions to thermal resistance at lower temperatures. At the temperatures where phonon scattering from the point defects remains insignificant, the scattering of phonons from the vibrating dislocations becomes important and offers the expected thermal resistance remarkably. Phonon resonance scattering proportional to $\omega^2(\omega^2 \sim \omega_0^2)^{-2}$ is capable of explaining the occurrence of dips in the lattice thermal conductivity curves.

Editorial note. This article was proofread by the editors only, not by the áuthors.

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