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Anharmonic coupling, thermal transport and acoustic wave attenuation in cubic semiconductors and bismuth.

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Abstract. In this work we present our recent results of the *ab initio* calculations of anharmonic coupling in cubic semiconductors and bismuth. Our results allow us to explain the anomalous behavior of the attenuation of the longitudinal acoustic phonon in GaAs as a function of the phonon energy in the subterahertz domain, which shows a plateau between 0.6 and 1 THz at low temperatures. The plateau is explained by the competition between different phonon-phonon scattering processes such as Herring's mechanism, which dominates at low frequencies, saturates, and disappears at higher frequencies. We found an excellent agreement between measurements performed by some of us, and new *ab initio* calculations of third-order anharmonic processes. We predict that the same phenomenon should occur in other cubic semiconductors. In the case of bismuth, we discuss the occurrence of the hydrodynamic heat transport regime at low temperatures, in consistency with the experimental observations. Bismuth is one of the rare materials in which second sound has been experimentally observed. Our calculations predict the occurrence of the Poiseuille phonon flow in Bi between 1.5 K and 3.5 K for sample size of 3.86 mm and 9.06 mm, in consistency with the experimental observations. We will also discuss a Gedanken experiment allowing to assess the occurrence of the hydrodynamic regime in any bulk material.

1. Introduction

Phonon-phonon interaction manifests itself in a wealth of temperature-induced physical phenomena like melting, thermal transport, and in the increase with temperature of phonon linewidths observed in Raman spectroscopy. Indeed, as temperature increases, anharmonic coupling between phonons also increases and gives rise to scattering processes that limit the mean free paths of phonons in general, and of heat-carrying phonons in particular. Precise knowledge about phonon lifetimes is directly useful to understand and predict the thermal conductivity of materials, and design specific materials with new thermal properties. Phonon lifetimes and phonon-phonon interactions have been the subject of theoretical studies since a long time [1,2]. Nowadays, high frequency phonon lifetimes are actively



studied in relation to thermal and thermoelectric transports, both experimentally [3,4] and by computer simulations [5-7]. Here, we present some of our recent theoretical results on the thermal transport regimes in bismuth, and show which are the conditions necessary for the occurrence of the hydrodynamic regime [8].

Another physical phenomenon which is governed by the anharmonic coupling is the attenuation of acoustic waves. In the subterahertz range, attenuation can be studied for example by the so-called “picosecond ultrasonic technique” [9,10]. The discussion of other experimental methods which allow the detection and generation of acoustic waves can be found in a recent review [11]. Above 10 GHz and up to a few tens of K, the damping of acoustic waves in pure crystals is mainly due to three-phonon interactions. Under such conditions, one can get access to accurate experimental information about lifetimes of individual longitudinal acoustic (LA) phonons. Recent experimental measurements on the absorption of subterahertz longitudinal waves made by some of us in gallium arsenide [10] showed that after a steep increase, the attenuation exhibits an unexpected plateau as a function of the excitation frequency in the 700 GHz to 1 THz range. It must be noted that in the experimental method of Ref. 10, the measured quantity is in fact the difference between the acoustic wave attenuation at a given temperature and the one at 10 K. Thus, only temperature-dependent part of attenuation is studied, while other contributions, such as impurity or isotopic scattering [12], are eliminated. Here, we report on our recent *ab initio* calculations of third-order anharmonic processes which have shown that the formation of the plateau can be explained by the competition between different phonon-phonon scattering processes such as Herring’s mechanism, which dominates at low frequencies, saturates, and disappears [13].

2. Thermal transport regimes in bismuth: a theoretical viewpoint.

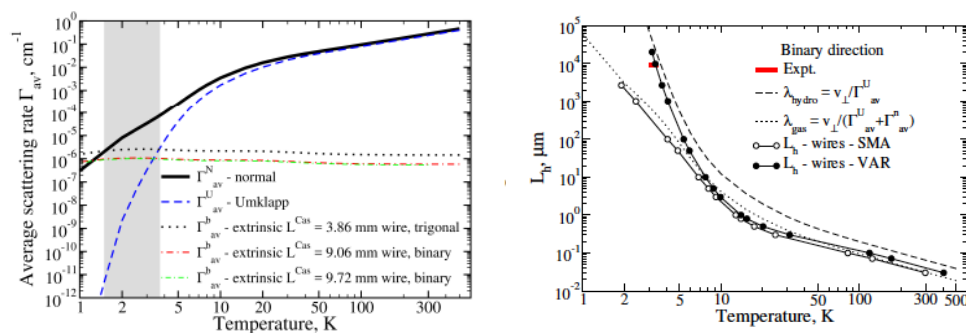


Fig. 1 From our Ref. [8]. Bismuth. Left panel: Temperature dependence of the thermodynamic average of the anharmonic scattering rates for normal and umklapp processes (respectively, black solid and blue dashed line) and of the (boundary) extrinsic scattering rates (dashed black, dot-dashed red and green lines). The shaded region corresponds to the temperature interval in which a second sound peak has been reported, $1.5 < T < 3.5$ K, for a length of 3.86 mm in the trigonal propagation direction [17]. Right panel: Phonon propagation lengths of individual phonons (black dotted line) compared with the heat wave propagation length extracted from the lattice thermal conductivity calculations which take into account the phonon repopulation (solid line with black filled disks). In hydrodynamic regime, the two quantities differ.

Currently, a lot of attention is devoted to the study of phonon-based heat transport regimes in nanostructures [14-16]. Of particular interest is the hydrodynamic regime, in which a number of fascinating phenomena such as Poiseuille’s phonon flow and second sound occur and where temperature fluctuations are predicted to propagate as a true temperature wave. Bismuth is a semimetal with relatively low carrier concentrations so that the dominant mechanism for heat conduction at low

temperatures is via phonons. It is one of the rare materials that is sufficiently isotopically pure so that second sound could be observed [17].

Recently, we have studied thermal transport in Bi using Boltzmann transport equation beyond single mode approximation, coupled to the ab initio description of anharmonicity [8]. We found that three-phonon collisions turn out to be particularly strong at low temperatures and lead to the creation of new phonons in the direction of the heat flow (normal processes), which enhance the heat transport. This induces time and length scales over which heat carriers behave collectively and form a hydrodynamic flow that cannot be described by independent phonons with their own energy and lifetime. Indeed, the thermodynamic averages of phonon-scattering rates for normal, resistive (Umklapp), and boundary collisional processes are compared on the left panel of Fig. 1. As one can see, normal scattering processes dominate at low temperatures, in the interval of temperatures which corresponds to the one where the second sound was observed experimentally [17].

Moreover, we have extracted from the lattice thermal conductivity a characteristic length, heat wave propagation length, whose behavior as a function of temperature, when compared to the phonon mean free path, is a fingerprint of the hydrodynamic-to-kinetic transition regime (right panel of Fig. 1).

3. Breakdown of Herring's processes in cubic semiconductors for subterahertz longitudinal acoustic phonons

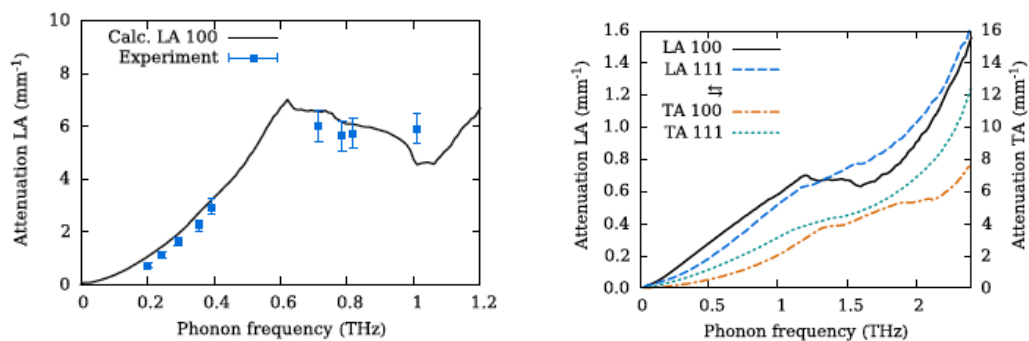


FIG. 2 From our Ref. 13. Left panel: Phonon attenuation in GaAs: comparison of calculations with experiments at fixed temperature (50 K) as a function of phonon frequency along the [100] direction. Right panel: Silicon. Attenuation of the longitudinal and transverse acoustic phonons along the [100] and [111] directions at 50 K.

In the Landau Rumer regime, the interaction of three phonons is the main mechanism of the phonon decay [1]. For a longitudinal acoustic wave propagating in an anisotropic crystal, Herring has pointed out a dominant three-phonon coalescence mechanism involving the scattering of the excited longitudinal acoustic wave by a slow transverse phonon into a fast transverse phonon. Herring's processes are dominant because they allow the coupling of low-energy longitudinal phonons with transverse phonons with large wavevectors, and, thus, a large density of states [2].

We have computed within density functional perturbation theory the intrinsic phonon-phonon scattering processes for the very low frequency region of crystalline gallium arsenide and silicon phonons [13]. For GaAs we have compared the calculations of the phonon attenuation along the [100] direction with experiments, finding the agreement to be excellent, both as a function of the phonon frequency, at constant temperature (left panel of Fig.2), and as a function of temperature, for a given phonon frequency. The attenuation plateau is caused by the three-phonon coalescence Herring processes, which

dominate at low frequency, progressively saturate and then rapidly decrease as the states involved in the scattering move up in energy, over the limit of the acoustic part of the transverse phonon dispersion curves. The saturation is caused by the acoustic phonon dispersion changing from linear to constant at low energy, which is a common feature of cubic semiconductors. Indeed, our theoretical results predict a similar plateau for the attenuation of the LA [100] phonons in silicon, between 1.2 and 1.7 THz (right panel of Fig. 2)

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