NANOPHONONICS: FINE-TUNING PHONON DISPERSION IN SEMICONDUCTOR NANOSTRUCTURES

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Abstract

Phonons manifest themselves in all electrical, thermal, optical and noise phenomena in semiconductors. Reduction of the feature size of electronic devices below the acoustic phonon mean free path creates a new situation for the phonon transport. On the one hand, the phonon–rough boundary scattering complicates heat removal from the downscaled devices. On the other hand, spatial confinement of the acoustic phonons creates an opportunity for intelligent tuning of the phonon dispersion in semiconductor nanostructures and achieving enhanced operation of devices based on these nanostructures. This paper presents a brief review of the recent developments in the field of *nanophononics*. Specifically, it focuses on methods of tuning the phonon spectrum in acoustically mismatched nano- and heterostructures in order to change the electron mobility and phonon thermal conductivity.

1. Introduction

Phonons are quantized modes of vibrations, which occur in the rigid crystal lattices, such as the atomic lattices of solid materials. One can speak of the gas of phonons, which consists of the quasi-particles of the energy $\hbar\omega$ and quasi-momentum $p=\hbar q$ obeying Bose-Einstein statistics. Phonons manifest themselves practically in all electrical, thermal, optical and noise phenomena in semiconductors. For example, acoustic and optical phonons limit electrical conductivity. Optical phonons strongly influence optical response of semiconductor bulk materials and nanostructures, while acoustic phonons are the dominant heat carriers in semiconductors and insulators. The long-wavelength phonons give rise to sound waves in solids, which explains the name *phonon*.

Similar to electrons, the properties of phonons are characterized by their dispersion $\omega(q)$, i.e. dependence of the phonon frequency ω on its wave vector q. In bulk semiconductors with g atoms per unit cell, there are $3g$ phonon dispersion modes for every value of q. In the limit of long waves, three modes describe the motion of the unit cell and form the three acoustic phonon branches. The other $3(g\text{-}1)$ modes describe the relative motion of atoms in a unit cell and form the optical phonon branches. Acoustic phonons have nearly linear dispersion, which can be written as $\omega=V_S q$ (where V_S is the sound velocity). Optical phonons, in general, are nearly dispersion-less for small q values (long-wavelength approximation) and have a small group velocity $V_G=d\omega/dq$.

The spatial confinement of phonons in nanostructures and heterostructures can strongly influence the phonon dispersion and modify phonon properties such as phonon group velocity, polarization, density of states, as well as affect the phonon interaction with electrons, point defects, other phonons, etc. Figures 1 and 2, based on the calculations reported by Po-

katilov *et al.* [1], illustrate the phonon spectrum modification in nanoscale heterostructures. Figure 1 shows the phonon energy dispersion in a thin film, while Figure 2 presents the phonon dispersion in the three-layered heterostructure for the symmetric and antisymmetric modes. The results are shown for the 6 nm-wide AlN slab and the three-layer heterostructure with the core layer thickness d_2=4 nm. One can see that the phonon dispersion in these structures strongly differs from the bulk phonon modes. Modification of the acoustic phonon dispersion is particularly strong in freestanding thin films or in nanostructures embedded into elastically dissimilar materials. Such modification may turn out to be desirable for some applications while detrimental for others.
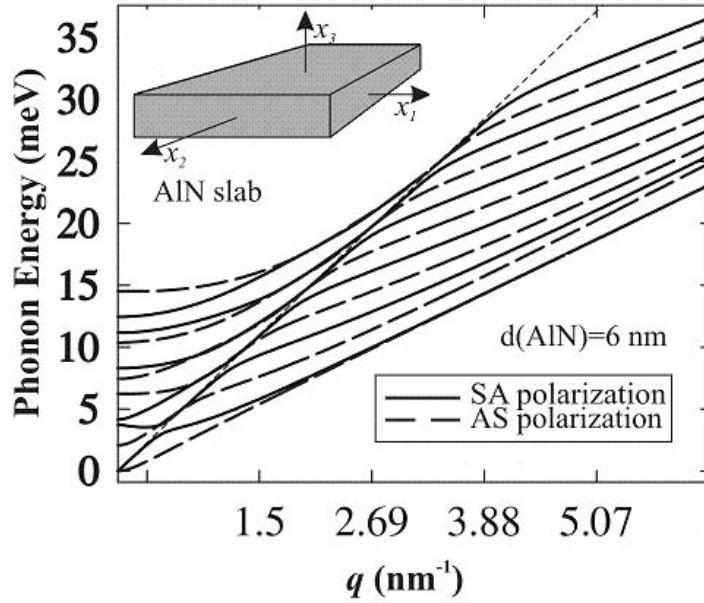

Figure 1. Phonon energy dispersion in the AlN thin film (slab) with the thickness of 6 nm. Inset shows the geometry of the slab and the coordinate system.
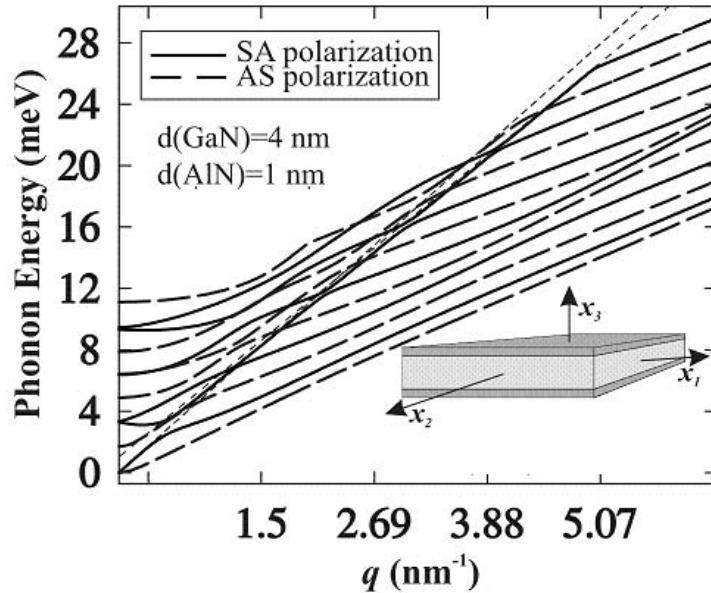

Figure 2. Phonon energy dispersion in the heterostructure with the cladding (barrier) layer thickness d_1=d_3=1 nm and the core layer thickness d_2=4 nm. Inset shows the geometry of the slab and three-layered structure.

Thus, nanostructures offer a new way of controlling the phonon transport via fine-tuning its dispersion relation, i.e. *phonon engineering* [2]. The concept of engineering the phonon dispersion in nanostructures has the potential to be as powerful as the concept of the band-gap engineering for electrons, which revolutionized the electronic industry.

2. The phonon engineering concept

The idea of looking at the changes that acoustic phonon spectrum experiences in heterostructures has a rather long history. More than half a century ago, Rytov [3] published a series of theoretical papers, where he analyzed acoustic vibrations in "artificial thinly-laminated media" and described folded acoustic phonons in such media. The folded phonons were later observed in quantum well superlattices using Raman spectroscopy [4]. In 1980-1990 there was a body of work done focused on calculating the confined acoustic phonon – electron scattering rates in free-standing thin films and nanowires [5-8]. Most papers on the subject used the elastic continuum approach for calculating phonon dispersion and adopted solution techniques developed in acoustics and mechanics. The prime motivation was to see if the spatial confinement and quantization of the acoustic phonon modes in freestanding thin films or nanowires produce noticeable effect on the deformation potential scattering of electrons. The opinions were split about importance of the acoustic phonon confinement in the description of electron transport in low-dimensional structures [6-9].

A new dimension to the subject was added when Balandin and Wang [10] pointed out that the confinement-induced changes in the acoustic phonon dispersion may affect the lattice (phonon) thermal conductivity as well. Before that the acoustic phonon confinement was only considered in the context of its effect on the charge carrier mobility and electrical conductivity. Decreased averaged phonon group velocity in freestanding thin films or nanowires may lead to the increased acoustic phonon relaxation on point defects, dislocations, as well as changes in three-phonon Umklapp processes [11]. Thermal conductivity reduction, while bad news for thermal management of electronic devices, is good news for the thermoelectric devices, which require materials with low thermal conductivity and high electrical conductivity [12].

More recently, Pokatilov *et al.* [13-14] have shown that in the ultra-thin films or nanowires embedded in the "acoustically fast" or "acoustically hard" materials, the phonon group velocity and thermal conductivity can be enhanced along certain directions. The "acoustically fast" material is the one with a higher sound velocity V_S, while an "acoustically hard" material is the one with higher acoustic impedance $Z = \rho V_S$ (ρ is the mass density of the material). The phonon group velocities in Figure 3 are shown as the functions of the phonon wave vector for the shear polarization in AlN/GaN/AlN heterostructure. Notice that the presence of the barrier layers with higher sound velocity increases the phonon group velocity for the whole heterostructure. A possibility of forming the *phonon stop-bands* in quantum dot superlattices made of materials with periodic modulation of the acoustic impedance and inhibition of the thermal conductivity has been predicted by Lazarenkova and Balandin [15]. As a result, the concept of phonon engineering has been extended to include the fine-tuning of the acoustic phonon transport to achieve the desired thermal conductivity of the material. Due to the continuing reduction in the electronic device feature size the thermal management at nanoscale gains a particular importance.

The free-standing nanostructures are not very practical for applications. More interesting are nanoscale structures, which are embedded into other materials. Pokatilov *et al.* [17-18] have suggested that the strong phonon confinement could be achieved if one

considers a hetero- or nanostructure coated with elastically dissimilar material. In the case of embedded nanostructures, the phonon depletion with the corresponding scattering rate suppression can be achieved in acoustically harder materials, while the phonon accumulation occurs in the acoustically softer material [17].
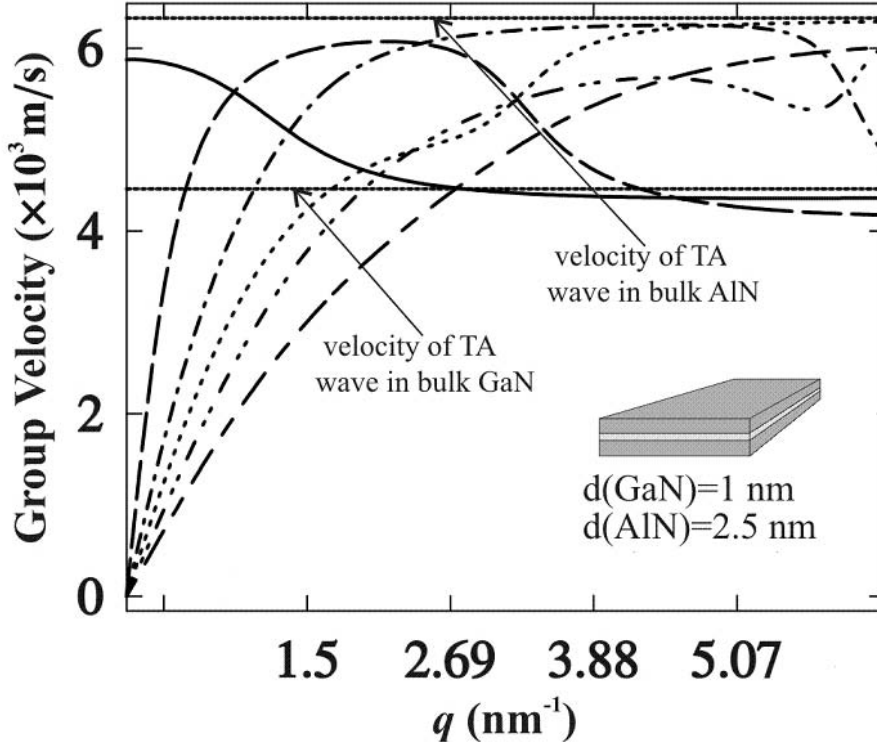

Figure 3: Phonon group velocities as the functions of the phonon wave vector for the shear polarization. Results are shown for the AlN/GaN/AlN three-layered heterostructure with dimensions 2.5 nm / 1 nm / 2.5 nm. Notice that the presence of the barrier layers with higher sound velocity increases the phonon group velocity for the whole heterostructure.

The phonon depletion effect can be used in the design of the nanoscale transistors, vertical field-effect transistors, alternative-gate dielectric transistors, etc. As the transistor feature size L reduces well below the acoustic phonon mean free path (MFP), the possibilities for fine-tuning the phonon dispersion to improve the carrier and heat transport increase.

3. Fine-tuning the phonons in semiconductor nanostructures

The feature size of the state-of-art transistor is already well below the room-temperature phonon MFP in Si, which is about 50 nm – 150 nm according to different estimates and measurements. In hetero- and nanostructures with feature size smaller than the phonon MFP, the acoustic phonon spectrum undergoes strong modification and appears quantized provided the structures are free standing or embedded within material of different elastic properties [14, 17]. This modification is particularly strong when the structure feature size becomes much smaller than the phonon meat free path, $L <<$ MFP, and approaches the scale of the dominant phonon wavelength $\lambda_0 \simeq 1.48 V_S \hbar / k_B T$. Here k_B is the Boltzmann constant, T is the absolute temperature, $\hbar$ is the Plank's constant and V_S is the sound velocity. For many crystalline materials λ_0 is on the order of 1.5 nm – 2 nm at room temperature, which is about the size of the transistor gate dielectric thickness.

Spatial confinement of acoustic phonons in nanoscale structures with the large mismatch of the acoustic impedances at the interfaces can strongly affect the phonon spectrum and substantially modify the electron - phonon interaction in comparison with bulk (see Table 1). In such structures, both confinement of electron states and acoustic phonons should be taken into account while calculating the scattering rates. Pokatilov *et al.* [17] have shown theoretically that the phonon population in thin films or nanowires embedded into acoustically softer materials can be depleted and the carrier – phonon scattering rate is suppressed. The latter is achieved if the nanostructure parameters (diameter, interface, mass density) are properly tuned and $Z_{inside} > Z_{matrix}$. This effect can be potentially used to suppress the inelastic scattering in nanowires and to increase electron carrier mobility. The physical origin of the described phonon depletion in the core layer of the acoustically mismatched heterostructure is redistribution of the displacement components, which leads to the situation when there are much less lattice vibrations in the core layer than in acoustically "soft" cladding layers.

Table 1. Phonon transport regimes.

Scale	Phonon Dispersion	Dominant Scattering Processes
$L >> MFP$	bulk dispersion	• three-phonon Umklapp • point defects
$\lambda_0 << L \leq MFP$	bulk dispersion	• three-phonon Umklapp • point defects • boundary scattering
$\lambda_o \leq L << MFP$	modified dispersion with many phonon branches populated	• three-phonon Umklapp • point defects • boundary scattering
$L < \lambda_0$	modified dispersion; only lowest phonon branches populated	• ballistic transport

Another interesting effect, within the phonon-engineering concept, is the predicted formation of the phonon stop-bands in nanostructures with periodic modulation of the elastic constant values. Drawing on the analogy with the photon band gap materials, Balandin *et al.* [19] have shown using the elastic continuum approximation that the acoustic phonon propagation can be inhibited along certain directions in three-dimensionally (3D) regimented QDS with the appropriately chosen parameters. It has been also demonstrated that for realistic quantum dot parameters it is possible to achieve a stop band in the phonon energy range that affects the value of the thermal conductivity tensor. The latter may lead to a novel way for thermal conductivity reduction and for increasing the thermoelectric figure of merit of nano-structured materials. Imamura and Tamura [20] theoretically studied the effect for the acoustic phonon lensing in anisotropic crystalline slabs. Lacharmoise *et al.* [21] have experimentally demonstrated that the low energy phonons can be strongly confined in semiconductor acoustic microcavities. The conclusion was based on Raman scattering study of acoustic phonons confined in planar GaAs/AlAs phonon cavities. The authors observed a huge increase in Raman signal in phonon cavities when the maxima of the acoustic and optical fields were tuned exactly at the same location [21]. The proposed phonon lenses and phonon reflectors together with the acoustically mismatched heterostructures [12, 17] significantly extend the phonon engineering concept and can be incorporated to the building blocks of future phonon-engineered nanodevices.

One of the recent nanophononics developments includes a result obtained by Fonoberov and Balandin [22], which indicates a possibility of enhancing the low-field electron drift mobility in silicon nanowires embedded into the "acoustically hard" material such as diamond. The reported electron mobility in the cylindrical silicon nanowires with 4-nm diameter, which are coated with diamond, is two orders of magnitude higher at 10 K and a factor of two higher at room temperature than the mobility in a free-standing silicon nanowire. The importance of this result for downscaled architectures and possible silicon-carbon nanoelectronic devices is augmented by extra benefit of diamond, a superior heat conductor, for thermal management.

4. Nanophonics in hybrid bio-inorganic nanostructures

Properties of phonons in biological or hybrid bio-inorganic systems are significantly different from those in conventional semiconductor materials. Hybrid systems are particularly interesting from the phonon-engineering point of view due to strong mismatch of the acoustic impedance at the interface between bio and inorganic materials. The specifics of phonon spectrum and phonon transport in hybrid bio-inorganic nanostructures can provide valuable information about the properties of bio-inorganic interfaces. Hybrid bio-inorganic nanostructures may also offer some properties beneficial for the carrier transport. In addition, the knowledge of phonon modes in such hybrid structures can be used to monitor the synthesis of these structures.

The examples of the bio-inorganic nanostructures are functionalized plant viruses. Recently, tobacco mosaic viruses (TMV) have been utilized as biological templates in the synthesis of semiconductor and metallic nanowires [23]. They were also proposed as elements in the hybrid nanoelectronic circuits. TMV viruses have cylindrical shape and suitable dimensions: they are 300 nm long, 18 nm in diameter and they have a 4-nm-diameter axial channel. Since these viruses have the diameters of the same order of magnitude as diameters of semiconductor nanocrystals and nanowires, elastic vibrations of TMV manifest themselves in low-frequency Raman scattering spectra. The knowledge of the low-frequency vibrational modes of the viruses is important for interpretation of Raman spectra and monitoring the template-based chemical assembly processes [24-25].

Fonoberov and Balandin [26] have theoretically studied the low-frequency vibrational modes of TMV and M13 viruses. The radial breathing modes of TMV and M13 viruses in air are found to be 1.85 cm^{-1} and 6.42 cm^{-1}, respectively. If the viruses are in water, the above frequencies become 2.10 cm^{-1} and 6.12 cm^{-1}, respectively. They have also shown theoretically that in addition to their role as nano-templates for assembly, the soft virus enclosures inside the inorganic nanotubes affect the phonon spectrum, which can be beneficial for nanoelectronic applications of such hybrid nanotubes at low temperature [27]. Liu *et al.* [24] demonstrated experimentally that the change of the vibration modes of TMV due to attachment of the participles to the TMV surface, clearly observed in Raman spectra, can be used for monitoring of the TMV coating, i.e. assembly using biological templates.

5. Conclusions

The paper gives a brief review of the development of nanophononics, a new sub-field of nanoscale science. The review focuses on the approaches for fine-tuning the phonon spectrum in acoustically mismatched nano- and heterostructures in order to change the electrical and thermal conductivity. The specifics of phonon spectra in biological and hybrid bio-inorganic nanostructures are also addressed.

Acknowledgement

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