ACOUSTIC PROPERTIES OF CYLINDRICAL NANOWIRES WITH THE ELASTICALLY DISSIMILAR BARRIERS

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Abstract. We have theoretically investigated the effect of the coating made of the elastically dissimilar material on the acoustic phonon properties of semiconductor nanowires. It is shown that the acoustic impedance mismatch at the interface between the nanowire and the barrier coating affects dramatically the phonon spectra and group velocities in the nanowires. Coatings made of the materials with a small sound velocity ("acoustically slow") lead to compression of the phonon energy spectrum and strong reduction of the phonon group velocities. The coatings made of the materials with a high sound velocity ("acoustically fast") have an opposite effect. Our calculations reveal substantial re-distribution of the elastic deformations in coated nanowires, which results in modification of the phonon transport properties, and corresponding changes in thermal and electrical conduction.

Key words: nanowire, acoustical phonons, coating, nanodevices.

INTRODUCTION

Acoustic phonon spectrum modification in semiconductor nanostructures continues to attract significant attention [1-4]. The interest to the confinement-induced changes in the acoustic phonon dispersion in thin films and nanowires has been increased after Balandin *et al.* [5-6] pointed out that the phonon confinement leads to a strong reduction of the thermal conductivity. Indeed, the thermal conductivity coefficient K_T can be written, in Debye model, as $K_T \sim C_V V \Lambda$, where C_V is the specific heat per unit volume, Λ is the average phonon mean free path and V is the phonon group velocity, averaged over all phonon polarizations. The acoustic phonon spectrum modification in free-standing films and nanowires results in decreased group velocity V and Λ.

We have previously shown that the barrier layer made of elastically dissimilar material can strongly affect the acoustic phonon spectrum in planar three-layered heterostructures [7-9]. In this paper, we demonstrate that the phonon spectrum modification is even more pronounced in coated

nanowires. Moreover, the acoustic phonon spectrum can be tuned, i.e. engineered, by a proper selection of the acoustically mismatched coating layer parameters.

RESULTS AND DISCUSSION

As the material system of choice for our calculations we have chosen wurtzite GaN due to its technological importance. The high quality coated GaN nanowires with radius as small as 5 nm and length up to several hundreds micrometers have already been demonstrated [10]. A schematic view of the considered structure and basic designations is presented in the insets to Fig. 1. It is assumed that the axis *c* in wurtzite crystal is directed along the nanowire axis. To fully use the advantage of the cylindrical symmetry of structure, we use the cylindrical coordinate system with the radius vector $\vec{r}$ and angle φ in the cross-sectional plane, and axis *Z* along the nanowire axis. The length of the nanowire is considered to be infinite.

In the cylindrical coordinate system the displacement vector $\vec{U}$ has the following components: $U_r(r,\varphi,z)$, $U_\varphi(r,\varphi,z)$, $U_z(r,\varphi,z)$. For the considered nanowire we have derived the system of three equations for these components, taking into account the nanowire homogeneity along Z-axis:

$$(c_{44}q^2-\rho\omega^2)u_r = c_{11}\frac{d^2u_r}{dr^2}+(\frac{c_{11}}{r}+\frac{dc_{11}}{dr})\frac{du_r}{dr}+(\frac{1}{r}\frac{dc_{12}}{dr}-\frac{c_{11}}{r^2}-\frac{m^2c_{66}}{r^2})u_r$$
$$+m(\frac{1}{r}\frac{dc_{12}}{dr}-\frac{c_{11}+c_{66}}{r^2})u_\varphi+\frac{m(c_{11}-c_{66})}{r}\frac{du_\varphi}{dr}+q(c_{13}+c_{44})\frac{du_z}{dr}+q\frac{dc_{13}}{dr}u_z \quad (1)$$

$$(c_{44}q^2-\rho\omega^2)u_\varphi = c_{66}\frac{d^2u_\varphi}{dr^2}+(\frac{c_{66}}{r}+\frac{dc_{66}}{dr})\frac{du_\varphi}{dr}-(\frac{c_{66}}{r^2}+\frac{1}{r}\frac{dc_{66}}{dr}+\frac{c_{11}m^2}{r^2})u_\varphi$$
$$-\frac{m(c_{11}-c_{66})}{r}\frac{du_r}{dr}-m(\frac{c_{11}+c_{66}}{r^2}+\frac{1}{r}\frac{dc_{66}}{dr})u_r-\frac{mq(c_{13}+c_{44})}{r}u_z \quad (2)$$

$$(c_{33}q^2-\rho\omega^2)u_z = c_{44}\frac{d^2u_z}{dr^2}+(\frac{c_{44}}{r}+\frac{dc_{44}}{dr})\frac{du_z}{dr}-\frac{c_{44}m^2}{r^2}u_z-q(\frac{c_{13}+c_{44}}{r}+\frac{dc_{44}}{dr})u_r$$
$$-q(c_{13}+c_{44})\frac{du_r}{dr}-\frac{qm(c_{13}+c_{44})}{r}u_\varphi, \quad (3)$$

where ρ is the mass density of the material, c_{mikj} are the elastic modulus, ω is the phonon frequency, $m=0,\pm1,\pm2,\pm3,\ldots$, and q is the phonon wave vector. The system of Eqs. (1-3) has been solved numerically, using the finite difference method [7-8] with free boundary condition (all components of the stress tensor $\sigma_{rr}=0$, $\sigma_{r\varphi}=0$ and $\sigma_{rz}=0$ on the outer surfaces of the nanowire).

In Fig.1 (a) we present the breathing modes for GaN nanowire with the core radius R_1=6 nm embedded into the "acoustically slow" plastic shell with the thickness ΔR =4 nm. The number S of the dispersion branches presented in Fig. 1 (a) has been estimated from the relationship $S=R/2a$ (where a is the lattice constant, a(GaN)=0.31 nm).

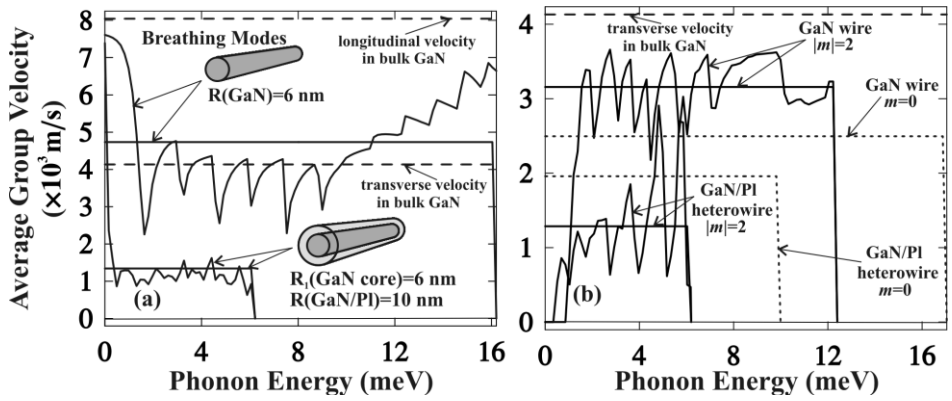

Fig. 2. Averaged phonon group velocity as a function of the phonon frequency for (a) breathing modes in the GaN nanowire with the "acoustically slow" barrier layer (R_1(GaN)= 6 nm, R=10 nm) and the uncoated GaN nanowire (R=6 nm); (b) torsional modes (m=0 and $|m|$=2) in the GaN nanowire with the "acoustically slow" barrier layer (R_1(GaN)= 6 nm, R=8 nm) and the uncoated GaN nanowire.

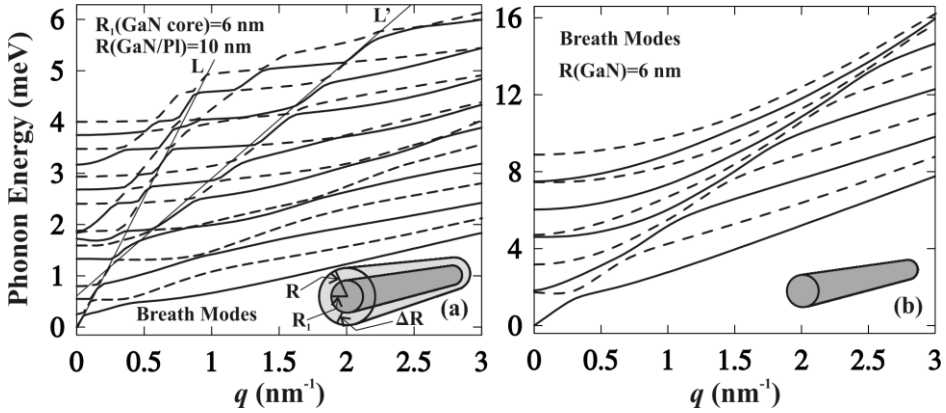

Fig. 1. Phonon energy as a function of the phonon wave vector q for the breathing modes (m=0). The results are shown for (a) GaN nanowire with the "acoustically soft" barrier layer (R_1(GaN)= 6 nm and R=10 nm); and (b) GaN nanowire without the barrier layer (R=6 nm). The insets show the geometry of the nanostructures.

Each of the dispersion curves in the coated nanowire has narrow regions with distinctively different slopes. The steep segments of the dispersion curves reflect the properties of the "acoustically fast" material (GaN in this case). These segments can be approximated by a straight line, which is indicated in Fig. 1 (a) by the symbol L. The slope of the straight line L is close to the sound velocity of the bulk transverse acoustic (TA) phonons in GaN. The slope of the straight line L' is close to the sound velocity of the bulk longitudinal acoustic (LA) phonons in plastic material. Another effect produced by the acoustically mismatched barrier layer is the compression of the confined phonon branches. The latter can be seen from the comparison of the spectrum in Fig. 1 (a) with that of the nanowire without coating shown in Fig. 1 (b). The breathing modes in uncoated

GaN nanowire are calculated for the radius R=6 nm, which equals to the radius of the coated nanowire core in Fig. 1 (a). In Fig. 1 (a), there are 16 dispersion branches confined in the energy interval of 4.0 meV, while in Fig. 1 (b) there are 10 branches in the wider energy interval of 9 meV.

The phonon group velocity dependence on frequency for breathing modes in the coated and uncoated nanowires is presented in Fig. 2. For the convenience of comparison, the average values of the velocities are shown in all figures by the straight horizontal lines. It is follows from Fig. 2 that the average phonon group velocity for the breathing and torsional waves in the GaN nanowire with the "acoustically slow" plastic coating are 3-4 times smaller than that in the uncoated nanowire of the same radius. Analogous results have been obtained for other phonon polarization with $m = \pm 1, \pm 3$.

CONCLUSIONS

We have theoretically shown that the acoustic phonon properties in semiconductor nanowires can be engineered via proper selection of the elastically dissimilar barrier (coating) parameters. We argue that tuning of the coated nanowire material parameters and the coating thickness can be used for engineering the thermal and electrical properties of such nanostructures.

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