ACOUSTICAL PROPERTIES OF RECTANGULAR QUANTUM HETEROWIRES WITH CLAMPED OUTER SURFACES

Nadejda D. Zincenco[1*], Denis L. Nika[1] and Moayad Al-Sabayleh[2]

[1]Department of Theoretical Physics, State University of Moldova,

A. Mateevich str., 60, Kishinev, MD-2009, Moldova

[2]Department of Physics, Mutan University, Iordan

Abstract. We had been theoretically studied the acoustic phonon spectra and group velocities of the phonons in the rectangular GaN nanowire with clamped outer surfaces, covered with elastically dissimilar barriers. The elastic properties of acoustically mismatched barrier influence dramatically on the phonon spectrum. The barriers with lower sound velocity ("acoustically slow" barriers) are "compressing" the phonon energy spectrum and reducing strongly the group velocities of the phonons. The barriers with higher sound velocity ("acoustically fast barriers") are demonstrated the opposite influence. The reason for such strong influence of barrier had been established. It is consisted of the re-distribution of the elastic deformations in heterowire. It is concluded that these effects can be used in phonon engineering.

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

INTRODUCTION

In the last decade the electronic and phonon properties of low-dimensional structures (quantum wells, quantum wires, quantum dots) attract the attention of researchers. The features of the acoustic phonon energy spectrum, stipulated by the dimensions and shape of sample [1-5], are manifested themselves in kinetic and optic phenomena.

The important properties of the acoustic phonons in the slabs, quantum wires and quantum dots were established in the works [1-2]. Dispersion of the phonons in quantum dot superlattices was recently calculated with account of the elastic properties of both quantum dot (QD) and barrier material in Ref. [3]. The phonon spectra in the rectangular nanowires with an aspect ratio of 2 or greater were considered in Ref. [4]. The complete solution of this problem with the description of all types of the polarization of the acoustic modes was given in Ref. [5]. In Refs. [6-8] acoustic phonons spectra and electron-phonon phenomena in the planar three-layered heterostructures with free and clamped surfaces were investigated in details. Our purpose is to investigate the acoustic properties of rectangular wires covered by acoustically dissimilar barrier (heterowires) with clamped external boundaries. Due to the lateral confinement in the quantum wires we can expect more pronounced manifestations of the quantum phonon effects than in the planar heterostructures.

We have calculated phonon dispersion spectra, phonon group velocities and distributions of the deformations in the rectangular quantum heterowire with GaN core wire and different cladding barriers.

RESULTS AND DISCUSSION

We consider the structure consisting of rectangular GaN wire (forming quantum well) confined in the rectangular barrier. As an example of the well material, there was used GaN, possessing wide perspectives of application in quantum electronics and optics. Generic view of the considered structure is presented in Fig. 1. It is assumed that the axis *c* in wurtzite crystal is directed along the nanowire axis. The length of the nanowire is considered to be infinite. For the considered nanowire we have derived three equations for components of the displacement vector $\vec{U}=(U_1,U_2,U_3)$:

$$\begin{aligned}(-\omega^2\rho+c_{44}q^2)u_1 &= c_{11}\frac{\partial^2 u_1}{\partial x_1{}^2}+c_{12}\frac{\partial^2 u_2}{\partial x_1\partial x_2}+c_{13}q\frac{\partial u_3}{\partial x_1}+c_{66}[\frac{\partial^2 u_1}{\partial x_2{}^2}+\frac{\partial^2 u_2}{\partial x_1\partial x_2}]\\ &+c_{44}q\frac{\partial u_3}{\partial x_1}+\frac{\partial c_{11}}{\partial x_1}\frac{\partial u_1}{\partial x_1}+\frac{\partial c_{12}}{\partial x_1}\frac{\partial u_2}{\partial x_2}+\frac{\partial c_{13}}{\partial x_1}qu_3+\frac{\partial c_{66}}{\partial x_2}[\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}]\end{aligned} \tag{1}$$

$$\begin{aligned}(-\omega^2\rho+c_{44}q^2)u_2 &= c_{11}\frac{\partial^2 u_2}{\partial x_2{}^2}+c_{12}\frac{\partial^2 u_1}{\partial x_1\partial x_2}+c_{13}q\frac{\partial u_3}{\partial x_2}+c_{66}[\frac{\partial^2 u_2}{\partial x_1{}^2}+\frac{\partial^2 u_1}{\partial x_1\partial x_2}]\\ &+c_{44}q\frac{\partial u_3}{\partial x_2}+\frac{\partial c_{11}}{\partial x_2}\frac{\partial u_2}{\partial x_2}+\frac{\partial c_{12}}{\partial x_2}\frac{\partial u_1}{\partial x_1}+\frac{\partial c_{13}}{\partial x_2}qu_3+\frac{\partial c_{66}}{\partial x_1}[\frac{\partial u_1}{\partial x_2}+\frac{\partial u_2}{\partial x_1}]\end{aligned} \tag{2}$$

$$\begin{aligned}&(-\rho\omega^2+q^2c_{33}-c_{44}(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}))u_3-(\frac{\partial c_{44}}{\partial x_1}\frac{\partial u_3}{\partial x_1}+\frac{\partial c_{44}}{\partial x_2}\frac{\partial u_3}{\partial x_2})=\\ &=-q(c_{13}+c_{44})(\frac{\partial u_1}{\partial x_1}+\frac{\partial u_2}{\partial x_2})-q(\frac{\partial c_{44}}{\partial x_1}u_1+\frac{\partial c_{44}}{\partial x_2}u_2)]\end{aligned} \tag{3}$$

where ρ is the mass density of the material, c_{mikj} are the elastic modulus, ω is the phonon frequency, u_i are the amplitudes of the displacement vector and q is the phonon wave vector. The system of equations (1-3) had been solved numerically with clamped boundary conditions $u_1=u_2=u_3=0$ on outer surfaces of the wire.

In Fig.1 are presented dispersion curves of the dilatational polarization for GaN/plastic-heterowire of 4nm x 6nm cross-section with GaN core of 2nm x 3nm cross-section. The carried out calculations have shown that in the GaN wire of 4nm x 6nm cross-section the first ten phonon branches are concentrated in the energy interval of 9.8 meV. In the GaN/plastic heterowire the same number of lower branches is concentrated in the considerably less energy interval of 3 meV. So, “slow” covering is “compressed” phonon energy spectrum. Analogous results are also obtained for other phonon polarizations (Flexural1, Flexural 2 and Shear).

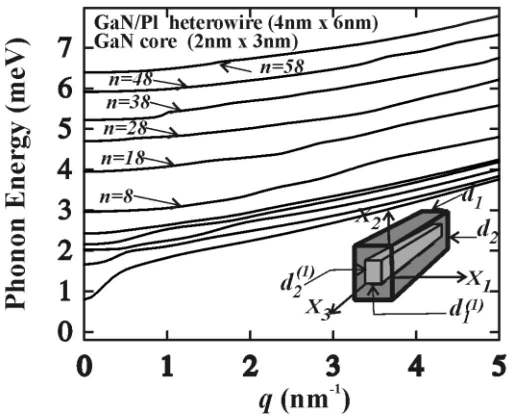

Fig.1. Phonon energy spectrum as the function of the phonon wave number for dilatation polarization for GaN/Pl heterowire 4nm x 6nm, core GaN 2nm x 3nm.

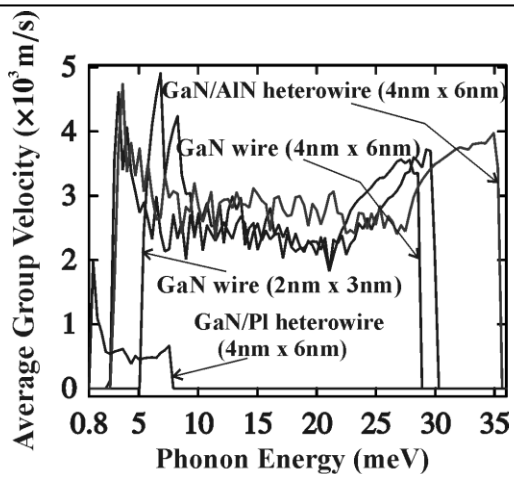

Fig.2. Averaged phonon group velocities as the function of the phonon frequencies for different GaN wires and different heterowires.

In Fig.2 are presented group velocities averaged over all quantum branches from $n=0$ to $n_{\max}$ and over all polarizations types. From the Fig.2 one can see that plastic barriers in the heterowire of 4nm x 6nm cross-section with GaN core of 2nm x 3nm decreases sound velocity in comparison with GaN wires without barriers. This effect is further reinforced if the barrier thickness increases. Using of the “fast” AlN barriers increases the group velocities of phonons in the heterowire.

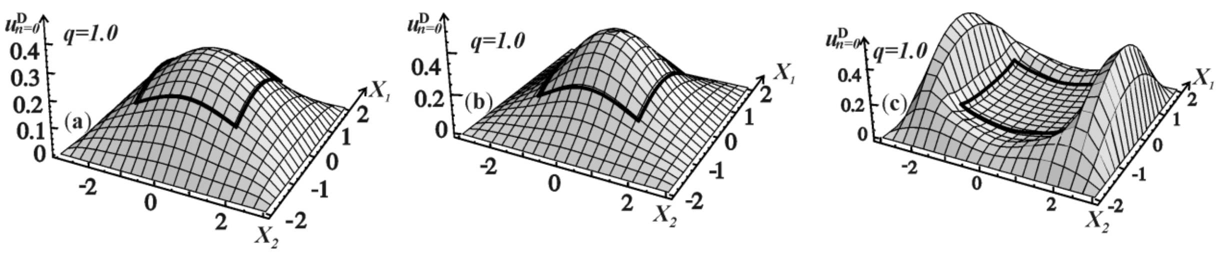

Fig.3. Distribution of the displacement vector amplitude $u=\sqrt{u_1^2+u_2^2+u_3^2}$ for the normal dilatation mode ($n=0, q=1$) in 4nm x 6nm wires: (a) GaN wire; (b) GaN/AlN heterowire; (c) GaN/Pl heterowire.

The reason for strong influence of the barriers we can find considering the distribution of the displacements $\vec{u}(x_1, x_2, q)$ in the cross-sectional plain of the heterowire. From the comparison of the graphs in Fig.3 one can see that in GaN/Pl heterowire the displacements are concentrated in Pl barrier and practically absent in GaN core. The decrease of the u function takes place in the GaN/AlN heterowire in the external AlN region in comparison with its values in GaN wire.

CONCLUSIONS

The acoustic properties of rectangular wires covered by elastically dissimilar barriers had been considered. Boundary conditions with clamped outer surfaces were accepted. It was established that “slow” barriers “compress” the phonon energy spectrum but “fast” ones “widen” it. Acoustically dissimilar barriers strongly influence on the phonon group velocities, increasing or decreasing the last ones, depending on material of facings. The reason for given barriers influence had been also established and it is consisted in the pushing out of the elastic wave, in the case of “slow” barriers, from the “fast” core wire to the barrier region. The opposite situation takes place in the case of the “fast” barriers (depletion and accumulation of phonons in core wires). The established effects should have important manifestations in the thermal processes and electron-phonon phenomena in the nanodimensional heterowires.

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