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A phonon depletion effect in ultrathin heterostructures with acoustically mismatched layers

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We demonstrate theoretically that modification of the acoustic phonon spectrum in semiconductor heterostructures with large acoustic impedance mismatch between the core and cladding layers may lead to strong phonon depletion in the core layer. The latter is achieved if the heterostructure parameters are properly tuned, i.e., the structure thickness is in nanometer scale to ensure phonon quantization and the cladding layers are acoustically "softer" than the core layer. Using a numerical solution of the elasticity equation, we show that one can achieve conditions when almost all acoustic phonon modes are squeezed in the cladding layers with the exception of a small fraction of phonons with very small wave vectors ($q \leqslant 0.3$ nm^{-1}). The predicted phonon depletion effect in the core layer of the acoustically mismatched heterostructures may lead to increased carrier mobility in certain regions of the heterostructure as well as improved thermal management of heterostructure-based devices. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1775033]

Acoustic phonons manifest themselves practically in all electronic, thermal, and optical phenomena in semiconductors. In nanoscale structures the acoustic phonon spectrum undergoes modification due to spatial confinement resulting in emergence of many quantized phonon dispersion branches, change in the phonon density of states, and hybridization of phonon modes.[1–3] Strong modification of the acoustic phonon spectrum is expected when the structure sizes are much smaller than the phonon mean free path Λ and approaches the dominant phonon wavelength λ_d at given temperature. By tuning the size, shape, interface, and mass density of nanostructures one can change the phonon spectrum in a desired way, thus accomplishing what has been termed as *phonon engineering*.[2] Practical realization of the phonon engineering concept in nanostructures may lead to a progress in electronic and optoelectronic devices.

Recently, several research groups demonstrated free-standing nanostructures, such as ultrathin slabs, nanowires and quantum dots.[4–6] Li *et al.*[7] reported on fabrication and measurement of thermal conductivity K in a single crystalline free-surface Si nanowires with diameters as small as 22 nm. The experimentally observed strong decrease of K in such nanowires ($K \sim 9$ W/cmK at $T=300$ K) was in excellent agreement with the earlier theoretical prediction ($K \sim 13$ W/cmK at $T=300$ K) of Zou and Balandin,[3] which explained the decrease by the acoustic phonon confinement in nanowires.

Practical examples of a structure, where phonon spectrum modification takes place, are nanostructures or ultrathin films embedded into material of distinctively different elastic properties. Invoking the concept of acoustic impedance $\eta = \rho V_s$ (ρ is the mass density and V_s is the sound velocity in the given material), we term such heterostructures as *acoustically mismatched*. In this letter we show that modification of acoustic phonon spectrum in heterostructures with large acoustic impedance mismatch $\eta_{\mathrm{core}}/\eta_{\mathrm{cladding}}$ at the interface between the core and cladding layers may lead to the strong *phonon depletion* in the core layer. The latter is achieved if the heterostructure parameters (thickness and mass density) are properly tuned and the cladding layers are acoustically "softer" than the core layer, i.e., $\eta_{\mathrm{core}} > \eta_{\mathrm{cladding}}$.

Vibrational spectrum in different structures has been theoretically studied over an extended period of time.[8–11] It has been shown[12] that in the freestanding three-layer heterostructures hybridization of the dilatational (DL) and flexural (FL) slab modes from different layers leads to formation of symmetrical (SA) and antisymmetrical (AS) normal modes that extend through the whole three-layer heterostructure. The notation SA and AS, used in this letter, is related to the symmetry of the components of displacement vector $\mathbf{U}$ (U_1, U_3), where U_1 is a component parallel to the layers while the component U_3 is perpendicular to them (see inset to Fig. 1). As an example material system we select GaN acoustically "hard" core layer embedded into acoustically "soft" plastic layer. Axis X_3 is perpendicular to the layer surfaces and parallel to the hexagonal reference axis c in wurtzite GaN lattice. Axes X_1 and X_2 of the Cartesian coordinate system are in the plane of the layers. The layers thicknesses are denoted by $d_i (i=1, 2, \text{ and } 3)$. The structure is symmetric, $d_2 = d_3$, with total thickness $d = d_1 + 2d_2$.

In order to solve the elasticity equation we follow the standard approach[8] and choose the free-surface boundary (FSB) conditions at the outside boundaries of the heterostructure. We begin by writing the expansion of the phonon displacement vector over the normal modes in the standard form

$$\boldsymbol{U}(x_1, x_2, x_3) = \sum_{\alpha, s, \vec{q}} \boldsymbol{U}_s^{(\alpha)}(\boldsymbol{r}, x_3, \boldsymbol{q}), \quad (1)$$

where index $\alpha = (\mathrm{SA}, \mathrm{AS})$ indicates the polarization type, index $s = 0, 1, 2, \ldots n$, is the quantum number of a normal pho-

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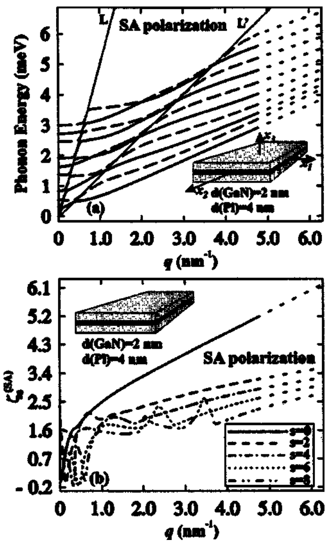

FIG. 1. (a) Phonon dispersion $\hbar\omega_s^{SA}(q)$ for symmetric (SA) hybrid acoustic phonon modes in the acoustically mismatched heterostructure. Solid and dashed curves correspond to even and odd phonon modes, respectively. (b) Phonon depletion coefficient for even SA phonon modes in the core layer of the acoustically mismatched heterostructure. Positive values of $\zeta_s^{(SA)}$ indicate ranges of the phonon wave vector q, for which the lattice vibrations in the core layer of the heterostructure are suppressed.

non mode, the position vector $\boldsymbol{r}(x_1,x_2)$ and wave vector of normal vibrations $\boldsymbol{q}(q_1,q_2)$ have two components. The displacement vector for the $(\alpha,s,\boldsymbol{q})$ normal mode can be written as

$$\boldsymbol{U}_s^{(\alpha)}(\boldsymbol{r},x_3,\boldsymbol{q}) = \frac{1}{\sqrt{L_1L_2}}A_s^{(\alpha)}(q,t)\boldsymbol{w}_s^{\alpha}(q,x_3)e^{\mathbf{iqr}}, \qquad (2)$$

where L_1, L_2 are the sizes of heterostructure along the X_1 and X_2 axes, respectively $(L_1,L_2 \gg d)$, $A_s^{(\alpha)}$is the amplitude and $\boldsymbol{w}_s^{\alpha}(q,x_3)$is the polarization vector for the $(\alpha,s,\boldsymbol{q})$ normal mode. The phonon polarization vector $\boldsymbol{w}_s^{\alpha}(q,x_3)$, in its turn, satisfies the following orthonormal conditions

$$\int_{-d/2}^{d/2}\boldsymbol{w}_s^{(\alpha)}(q,x_3)\rho(x_3)\boldsymbol{w}_{s'}^{(\alpha')*}(q,x_3)dx_3 = \tilde{\rho}_s^{(\alpha)}(q)\,\delta_{ss'}\,\delta_{\alpha\alpha'},$$

$$\times\int_{-d/2}^{d/2}|\boldsymbol{w}_s^{(\alpha)}|^2\,dx_3 = 1, \qquad (3)$$

where $\rho(x_3)$ is the coordinate dependent mass density of the constituent material such that $\rho(x_3)=\rho_1$(constant mass density in core layer) when $|x_3| \leqslant d_1/2$ and $\rho(x_3)=\rho_2$ (constant mass density in cladding layers) when $d_1/2 < |x_3| \leqslant d/2$ and the heterostructure mass densities are given as $\tilde{\rho}_s^{(\alpha)}(q) = \int_{-d/2}^{d/2}\rho(x_3)|\boldsymbol{w}_s^{(\alpha)}(q,x_3)|^2dx_3$. Polarization vector $\boldsymbol{w}_s^{(\alpha)}$ defined this way, determines not only the direction of the displacement, but also the spatial distribution of the displacement vector amplitude. We find the coordinate dependence of $w_{1,s}^{(\alpha)}$ and $w_{3,s}^{(\alpha)}$ components by solving the elasticity equation.[12] Material constants and deformation potentials for wurzite GaN were taken from Ref. 13. As an acoustically "soft" material we used plastic (Pl) with the value of the longitudinal velocity of sound $v_l=2$ km/s, transversal velocity $v_t=1$ km/s, and density $\rho=1$ g/cm^3.[14]

Figure 1(a) shows phonon dispersion branches $\hbar\omega_s^{\alpha}(x_3,q)$ for SA polarization in plastic/GaN/plastic heterostructure with dimensions 4 nm/2 nm/4 nm. As one can see, the dispersion for zero mode $(s=0)$ is similar to the transverse acoustic (TA) phonon mode in bulk plastic with sound velocity $v \approx 1$ km/s. Other dispersion branches $(s \neq 0)$ correspond to quantized quasioptical, i.e., $\omega(q=0)\neq 0$, phonon modes $(s=1,2-9)$. The number of all quasioptical branches is determined by the ratio $d/2c$ (for wurzite GaN $c=0.51$ nm). The quasioptical branches have parabolic type dispersion $(\omega \sim q^2)$ for phonon wave vectors close to the Brillouin zone center with characteristic sharp change of the slope indicated by the straight line L. The slope along L is close to the sound velocity of the bulk TO phonon in GaN (~4 km/s). This narrow region of q values with drastic change in the dispersion slope is dominated by the elastic properties of the acoustically "hard" core layer. For all other values of q, the slopes of the dispersion curves, are significantly smaller. It means that the average group velocity of phonon modes, which extend through the whole heterostructure, is between the bulk TA and longitudinal acoustic (LA) phonon velocities in the "soft" plastic (the region near the LA bulk mode velocity of 1.6−1.9 km/s is denoted by line L'). The width of the regions with the high velocity is relatively small (~0.1 nm^{-1}). Thus, vibrational properties of the considered heterostructure are dominated by the acoustically "soft" cladding materials.

To elucidate the phonon depletion effect, i.e., squeezing the lattice vibrations out from the core layer to the claddings, we introduce a new parameter, phonon depletion coefficient, through the energy considerations. The total lattice vibration energy in heterostructure is given by[15]

$$E = \frac{1}{2}\int_V \rho(x_3)\dot{\vec{U}}^2dV + \frac{1}{2}\int_V c_{iklm}(x_3)U_{ik}U_{lm}dV, \qquad (4)$$

where U_{ik} is the strain tensor, and $c_{iklm}(x_3)$ are modules of elasticity of heterostructure layers. Here, the first term represents kinetic energy and the second term is potential energy of the lattice oscillations. Substituting Eqs. (1) and (2) to Eq. (4), and using orthonormalization condition of Eq. (3), we can write the energy of the normal mode in the form

$$E_s^{(\alpha)}(q) = E_{s,1}^{(\alpha)}(q) + E_{s,2}^{(\alpha)}(q) = (\omega_s^{(\alpha)})^2|A_s^{(\alpha)}|^2(\rho_1\int_1|\boldsymbol{w}_s^{(\alpha)}|^2dx_3$$

$$+ \rho_2\int_2|\boldsymbol{w}_s^{(\alpha)}|^2dx_3), \qquad (5)$$

where indices 1 and 2 are related to the core and cladding layers of the heterostructure, respectively. The terms in Eq. (5) are structured in such a way that the first one corresponds to the energy $E_{s,1}(q)$ of elastic vibrations of the (α,s,q) normal mode in the core layer while the second one to the energy of vibrations $E_{s,2}(q)$ in the cladding (barrier) layers. We now define the phonon depletion coefficient $\xi_s^{(\alpha)}(q)$ as a ratio of the elastic energy inside the core layer to the elastic energy in the whole heterostructure (both energies are taken per unit volume):

$$\xi_s^{(\alpha)}(q) = \frac{E_{s,1}^{(\alpha)}(q)}{V_1}\frac{V}{E_s^{(\alpha)}(q)} = \frac{d}{d_1}\frac{\rho_1}{\tilde{\rho}_s^{(\alpha)}}\int_1|w_s^{(\alpha)}(q,x_3)|^2dx_3, \qquad (6)$$

where $V_1=L_1L_2d_1$ and $V=L_1L_2d$. According to this definition, $\xi_s^{(\alpha)}(q)$ shows the relative amount of lattice vibrational energy inside the core layer with the respect to the total

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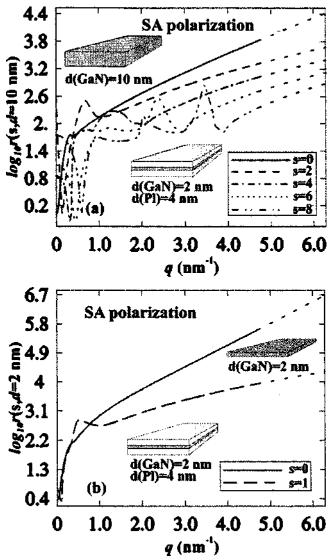

FIG. 2. Phonon damping coefficient for even SA phonon modes: (a) Comparison of the square mean displacements in the GaN slab and in the acoustically mismatched heterostructure of the same thickness. The positive value of log $r_s^{(\alpha)}$ indicates that lattice vibrations in the core layer of the heterostructure are suppressed compared to the generic slab; (b) the same as in (a) but the thickness of the slab is chosen the same as the thickness of the heterostructure core layer.

energy per unit thickness of the heterostructure. It is also illustrative to compare the mean square polarization vectors of the normal modes in the core layer of the heterostructure with the mean square polarization vectors in slabs. For this purpose, we introduce the phonon damping coefficient $r_s(q,d)$ defined as

$$r_s^{(\alpha)}(q,d)=\frac{d_1\int_{-d/2}^{d/2}|\boldsymbol{w}_{s,sl}^{(\alpha)}(q,x_3)|^2dx_3}{d\int_{-d_1/2}^{d/2}|\boldsymbol{w}_{s,h}^{(\alpha)}(q,x_3)|^2dx_3}, \quad (7)$$

where $\boldsymbol{w}_{s,sl}^{(\alpha)}(q,x_3)$ is the polarization vector $\boldsymbol{w}_s^{(\alpha)}(q,x_3)$ in the slab with thickness d and $\boldsymbol{w}_{s,h}^{(\alpha)}(q,x_3)$ is the polarization vector $\boldsymbol{w}_s^{(\alpha)}(q,x_3)$in the heterostructure.

In Fig. 1(b) we presented the logarithm of the phonon-depletion coefficient taken with negative sign as a function of q. The results are shown for even SA polarization modes of the plastic/GaN/plastic heterostructure with dimensions 4 nm/2 nm/4 nm. For almost all values of q the $\boldsymbol{\zeta}_s^{(\mathrm{SA})}(q)$ values are positive. For $q \geqslant 2$ nm^{-1}, the $\boldsymbol{\zeta}_s^{(\mathrm{SA})}$ value is 2, which means that phonon energy density in acoustically "soft" cladding layers of the heterostructure exceeds the phonon energy density in the acoustically "hard" core layer by the two orders of magnitude. Thus, a significant depletion of phonons, i.e., inhibition of lattice vibrations, in the core layer is observed.

In Fig. 2 we compare the mean square polarization vector $\boldsymbol{w}_s^{(\alpha)}(q,x_3)$ for the analogous phonon modes of the acoustically mismatched heterostructure and generic slab. Figure 2(a) shows the phonon-damping coefficient $\log_{10} r_s^{(\alpha)}(q,d=10\text{ nm})$. The thickness of the slab ($d=10$ nm) is chosen equal to the total thickness of the heterostructure. One can see from this figure that the mean square polarization vectors in GaN core layer is almost two orders of magnitude less than that in slab. Perhaps it is even more illustrative to compare the lattice vibrations in the core layer of the heterostructure with those in the GaN slab of the same thickness as the core layer, i.e. $d=2$ nm. It is interesting to note that there exist only two modes ($s=0$ and 1) in a 2-nm-thick slab. Figure 2(b) shows the damping coefficient $\log_{10} r_s^{(\alpha)}(q,d=2\text{ nm})$ for both modes. The mean square polarization vectors in the slab exceeds that one in the core layer of the acoustically mismatched heterostructure by many orders of magnitude for almost all q. The lattice vibrations are strongly damped in the heterostructure core.

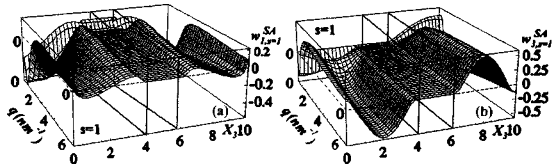

FIG. 3. Components $w_{1,s=1}^{\mathrm{SA}}(x_3,q)$ (a) and $w_{3,s=1}^{\mathrm{SA}}(x_3,q)$; (b) of the vibration amplitude vector $\boldsymbol{w}_{s=1}^{(\mathrm{SA})}(x_3)$ as the functions of the phonon wave vector q and coordinate x_3.

The physical origin of the described phonon depletion in the core layer of the acoustically mismatched heterostructure is redistribution of the displacement $\boldsymbol{U}_s^{(\alpha)} \sim A_s^{(\alpha)}\boldsymbol{w}_s^{(\alpha)}(x_3)$, which leads to the situation when there are much less lattice vibrations in the core layer than in acoustically "soft" cladding layers. The latter is illustrated in Fig. 3, which shows the components $w_{1,s=1}^{\mathrm{SA}}(x_3,q)$ (a) and $w_{3,s=1}^{\mathrm{SA}}(x_3,q)$ (b) of the vibration amplitude vector $\boldsymbol{w}_{s=1}^{(\mathrm{SA})}(x_3)$ as functions of q and x_3. Note that the displacement component surfaces are nearly flat for $w_{1,s=1}^{\mathrm{SA}}$ and $w_{3,s=1}^{\mathrm{SA}}$ and approximately equal to zero inside the core layer while the amplitudes of vibrations are high in the cladding layers. Similar dependence is observed for other SA and AS modes. In conclusion, we demonstrated that modification of the acoustic phonon spectrum in semiconductor heterostructures with large acoustic impedance mismatch ($\eta_{\mathrm{core}} > \eta_{\mathrm{cladding}}$) between the core and cladding layers results in the strong phonon depletion in the core layer.

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[1] N. Bannov, V. Aristov, V. Mitin, and M. A. Stroscio, Phys. Rev. B **51**, 9930 (1995).
[2] A. Balandin and K. L. Wang, Phys. Rev. B **58**, 1544 (1998).
[3] J. Zou and A. Balandin, J. Appl. Phys. **89**, 2932 (2001).
[4] C. S. Yung, D. R. Schmidt, and A. N. Cleland, Appl. Phys. Lett. **81**, 31 (2002).
[5] Y. Huang, X. F. Duan, Y. Cui, and C. M. Lieber, Nano Lett. **2**, 101 (2002).
[6] J. L. Liu, S. J. Cai, G. L. Jin, and K. L. Wang, Electrochem. Solid-State Lett. **1**, 188 (1998).
[7] D. Li, Y. Wu, P. Kim, L. Shi, P. Yang, and A. Majumdar, Appl. Phys. Lett. **83**, 2934 (2003).
[8] *Physical Acoustic* edited by W. P. Meson (Academic, New York, 1964), part A, Vol. I; A. N. Cleland, *Foundations of Nanomechanics* (Springer, New York, 2003).
[9] V. G. Grigoryan and D. G. Sedrakyan, Akust. Zh. **29**, 470 (1983).
[10] N. Nishiguchi, Y. Ando, and M. Wybourne, J. Phys.: Condens. Matter **9**, 5751 (1997).
[11] S. M. Rytov, Akust. Zh. **2**, 71 (1956); [Sov. Phys. Acoust. **2**, 67 (1956)].
[12] E. P. Pokatilov, D. L. Nika, and A. A. Balandin, Superlattices Microstruct. **33**, 155 (2003).
[13] I. Vurgaftman and J. R. Meyer, and L. R. Ram-Mohan, J. Appl. Phys. **89**, 5815 (2001).
[14] See, for example, <http://www.ondacorp.com/tables/plastics.htm>.
[15] L. D. Landau and E. M. Lifshits, *Theory of Elasticity* (Fizmatlit, Moscow, 2001).

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