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PHONON PROCESSES IN GRAPHENE AND SILICON-BASED NANOSTRUCTURES

131.04 - COMPUTATIONAL PHYSICS AND MODELING OF PROCESSES

Authoreferat of the doctor thesis in physics

CHISINAU, 2015

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One can become acquainted with the Thesis and Authoreferat in the library of the Moldova State University (A. Mateevici str. 60, Chisinau, MD-2009, Moldova) and on the web page of the National Council for Accreditation and Attestation (www.cnaa.md).

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GENERAL CHARACTERISTIC OF THE WORK

Relevance and importance of the subject of the Thesis is determined by a huge interest from both scientific and engineering community toward the nanoscale structures and materials with enhanced electron and phonon properties. The investigation of electron and phonon processes in nanostructures, as well as the search for novel nanoscale geometries and materials with properly engineered electron and phonon properties represents one of the most important problems of modern nanoscience. The technological progress in dimensional scaling of different material structures in the past few decades determined numerous advancements in various areas: electronics, phononics, thermal management, thermoelectricity, photovoltaics, energy storage, etc. Further development of these fields requires a thorough understanding of the electron and phonon processes at nanoscale.

Electrons and phonons manifest themselves in all properties of materials: mechanical, optical, thermal, etc. Spatial confinement of electrons and phonons in nanostructures strongly affects their energy spectra, density of states and electron-phonon interaction. Thus, nanostructures offer a new way of controlling electron and phonon processes together with electron-phonon interaction via tuning electron and phonon dispersion relations, i.e. electron and phonon engineering. One of the areas where phonon engineering is playing an extremely important role is heat management at nanoscale, since phonons are the main heat carriers in many nanostructures such as semiconductor and carbon nanostructures. Aggressive miniaturization of electronic devices and increasing their operation speed makes the problem of heat removal from the electronic circuits particularly important. Therefore the scientific search of materials with high thermal conductivity becomes extremely crucial for the future development of nanoelectronics. Another area where electron and phonon engineering has given a significant performance boost is thermoelectricity. Thermoelectricity provides unique opportunity since it can be used as a generator deriving power out of waste heat from different sources: integrated chips, cars, buildings, etc. This opens up the exciting area of waste heat recovery. One- and two-dimensional nanostructures are one of the most promising thermoelectric materials that allow separate engineering of electron and thermal properties. The ability to manipulate material properties at the atomic scale using nanostructures such as nanowires, nanolayers and superlattices plays a key role in enhancing the thermoelectric efficiency.

The goal of this Thesis is the investigation of phonon processes in graphene and silicon-based nanostructures, as well as determination of novel nanostructures for effective electron and phonon engineering.

In order to achieve this goal, the following *objectives* are formulated:

1. Determination of novel one-dimensional and two-dimensional nanostructures with specific geometrical and material parameters, as perspective candidates for electron and phonon engineering.
2. Development of theoretical models to describe phonon and electron states in novel one-dimensional and two-dimensional nanostructures.
3. Investigation of electron, phonon and thermal properties of novel as well as generic one-dimensional and two-dimensional nanostructured materials.

The following theoretical *methods and models* are used to accomplish the objectives:

1. Lattice dynamics theory for theoretical modeling the phonon states in novel one-dimensional and two-dimensional nanostructures.
2. Extension and application of the effective mass approach in order to investigate electron states in novel nanostructures.
3. Extension and application of the Boltzmann transport equation approach for modeling the thermal properties of novel one-dimensional and two-dimensional nanoscale structures.

Theoretical importance and scientific novelty of the results consists in the following:

1. A Born - von Karman lattice dynamics model for cross-section modulated nanowires and multilayer graphene with different atomic stacking was developed.
2. The influence of cross-section modulation on phonon and electron processes in Si-based nanowires was studied for the first time.
3. A theoretical approach for calculation of scattering time of phonons on interfaces of Si/Ge superlattices was developed and the influence of Si/Ge interface quality on phonon and thermal properties of these superlattices was analyzed.
4. The influence of different atomic stacking on phonon and thermal processes in multilayer graphene was elucidated for the first time.

An *important scientific problem* was solved in the Thesis namely it was demonstrated and investigated theoretically the possibility to control the phonon processes in two-layer graphene by rotation of graphene layers one against another around the axis perpendicular to the graphene plane.

Main items to be defended:

1. An up to 5 times drop of the phonon heat flux at room temperature is predicted in Si cross-section modulated nanowires in comparison with generic uniform Si nanowires.
2. It was demonstrated theoretically that in Si/Ge core/shell cross-section modulated nanowires the combination of cross-section modulation and acoustic mismatch between Si and Ge materials can lead to a three orders of magnitude drop of room temperature phonon thermal conductivity as compared to bulk Si.

3. A new type of hybrid folded rotationally-dependent phonon modes in twisted bilayer graphene were predicted.
4. It was theoretically demonstrated that in single-layer, bilayer and twisted bilayer graphene the phonon specific heat at temperatures less than 15 K varies as T^n, where n = 1 for graphene, n = 1.6 for bilayer graphene and n = 1.3 for twisted bilayer graphene.

Practical significance of the Thesis consists in the following recommendations proposed on the basis of the obtained theoretical results:

1. Planar Si/Ge superlattices with atomic intermixing at interfaces are perspective for phonon filtering aplications.
2. The Si-based modulated nanowires with Ge or SiO_2 covering shell are perspective for thermoisolant and thermoelectric applications owing to drastically reduced thermal transport.
3. Twisted bilayer graphene with different angles of rotation can be recommended for controllable heat removal applications from electronic devices due to enhanced thermal properties and rotaion angle-dependent specific heat.

Approbation of the results: the results obtained in the Thesis were presented at following international scientific conferences: International Conference of Young Researchers „*ICYR*" (Chisinau, Moldova, editions 2009-2012); 9th European Conference on Thermoelectrics „*ECT-2011*" (Thessaloniki, Greece, 2011); DPG Spring Meeting – 2012 (Berlin, Germany, 2012); International Conference on Modern Information and Electronic Technologies „*MIET*" (Odessa, Ukraine, editions 2012-2014); I-st All-Russian Congress of Young Scientists (Saint-Petersburg, Russia, 2012); International Scientific Conference for Undergraduate and Postgraduate Students and Young Scientists „*Lomonosov*" (Moscow, Russia, editions 2012-2013); CECAM-Workshop: Nanophononics (Bremen, Germany, 2013); DPG Spring Meeting – 2014 (Dresden, Germany, 2014).

Publications: based on the results presented in the Thesis 33 scientific works were published, including 6 articles in ISI journals and 15 abstracts in proceedings of international conferences. 2 articles and 2 abstracts were published without coauthors.

Structure of the Thesis: the Thesis consists of Introduction, 4 Chapters and Conclusions. The Thesis contains 200 references, 140 pages, 66 figures and 7 tables.

Key-words: phonons, electrons, nanolayer, superlattice, nanowire, graphene, lattice dynamics, modulation, thermal properties.

CONTENTS OF THE THESIS

In the **Introduction** the relevance, scientific importance and novelty of the results presented in the Thesis are outlined.

In **Chapter 1** is presented a detailed review of recent theoretical and experimental investigations of electron and phonon processes in one-dimensional and two-dimensional nanostructures.

In **Chapter 2** a Born-von Karman (BvK) model of lattice dynamics for nanolayers and planar superlattices with diamond crystal lattice is developed. The schematic view of the considered structures is shown in Figure 1.

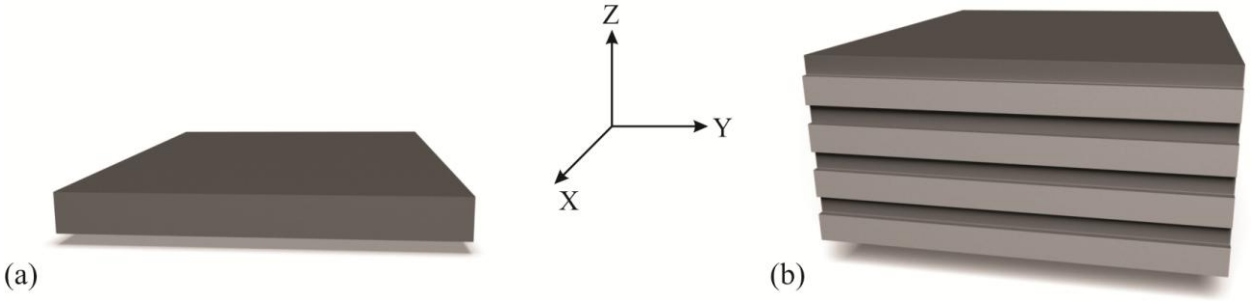

Fig. 1. Schematic view of a freestanding homogeneous layer (a) and planar superlattice (b).

In the framework of BvK lattice dynamics theory for nanolayers and planar superlattices, the system of equations of motion for atoms from monolayer *s* can be represented, in a harmonic approximation, as:

$$m_s\omega^2 U_i(s,\vec{q}) = \sum_{j=x,y,z}\sum_{s'=1}^{N} D_{ij}\left(s,s',\vec{q}\right)U_j(s',\vec{q}) \qquad i=x,y,z\,, \tag{1}$$

where s, s' – numerate monolayers and take values between 1 and N, m_s – mass of the atom from monolayer s, ω – phonon frequency, $\vec{q}$ – phonon wavevector, $U_i(s)$ – i-th component of the atomic displacement amplitude vector of the s-th monolayer, D_{ij} – dynamic matrix element, given by expression:

$$D_{ij}\left(s,s',\vec{q}\right) = \sum_{n'_{s'}} \Phi_{ij}(n_s,n'_{s'}) \exp\left(\mathbf{i}\vec{q}\times\left(\vec{r}(n'_{s'})-\vec{r}(n_s)\right)\right), \tag{2}$$

where $\vec{r}(n_s)$ – radius-vector of the atom n_s and $\Phi(n_s,n'_{s'})$ – matrix of the force constants describing interaction between a pair of atoms $(n_s,n'_{s'})$. It is taken into account the interaction within two nearest neighbor coordination spheres, therefore the summation in Equation (2) is

performed over all atoms n' from two nearest spheres of atom *n*. The index *n* here denotes atom lying in the center of the coordination sphere for which the equations of motion are written. The lattice dynamics is described by two force constant matrices:

$$\Phi(n_s, n'_{s'}) = -\begin{pmatrix} \alpha(n_s, n'_{s'}) & \beta(n_s, n'_{s'}) & \beta(n_s, n'_{s'}) \\ \beta(n_s, n'_{s'}) & \alpha(n_s, n'_{s'}) & \beta(n_s, n'_{s'}) \\ \beta(n_s, n'_{s'}) & \beta(n_s, n'_{s'}) & \alpha(n_s, n'_{s'}) \end{pmatrix}$$ for the nearest sphere and

$$\Phi(n_s, n'_{s'}) = -\begin{pmatrix} \gamma(n_s, n'_{s'}) & \gamma(n_s, n'_{s'}) & 0 \\ \gamma(n_s, n'_{s'}) & \gamma(n_s, n'_{s'}) & 0 \\ 0 & 0 & 0 \end{pmatrix}$$ for the second nearest sphere.

In order to obtain the phonon energy spectra the system of equations of motion (1) with dynamic matrix (2) was solved numerically. In Figure 2 are shown phonon energy spectra in [100] crystallographic direction in bulk silicon (panel (a)) and silicon nanolayer with 10 nm thickness (panel (b)).

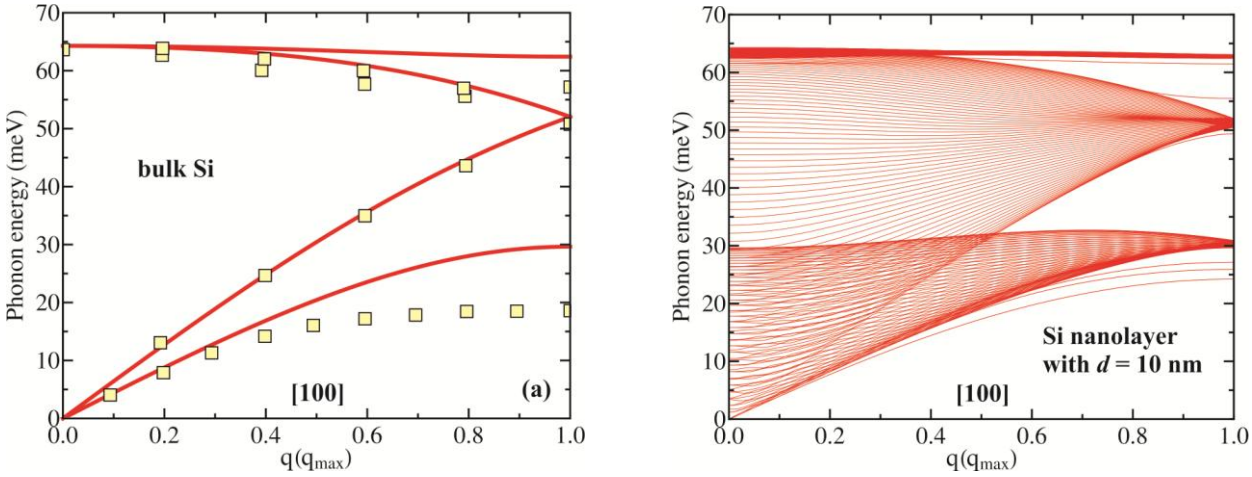

Fig. 2. Phonon energy spectra of bulk Si (a) and Si nanolayer with 10 nm thickness (b). Squares denote experimental points from Ref. [1].

It is seen from Figure 2(a) that the developed three-parameter BvK model reproduces reasonably well all the features of the bulk silicon phonon spectra, except for the overestimation of TA and TO phonon energies for $q > 0.5 \cdot q_{\max}$, where $q_{\max} = 11.57\ nm^{-1}$. This overestimation is explained by the fact that the short-range interatomic interactions are only considered in this model. The behavior of phonon dispersion curves in the [110] and [111] directions is analogous. In Figure 2(b) we present the phonon energy spectra for a Si nanolayer with $d = 10\ nm$ in the [100] crystallographic direction. The strong dimensional confinement along the *Z*-axis results in a quantification of the phonon energy spectra, i.e. the appearance of a large number of size-quantized energy branches. Analogously to the bulk silicon phonon spectrum in nanolayer's

spectrum one can distinguish three bunches of phonon branches: TA-like, LA-like and TO(LO)-like branches. However, unlike in the bulk case, where all atomic vibrations are exactly distinguished on transversal/longitudinal and acoustic/optic, in nanolayers appear essentially new transverse-longitudinal acousto-optical mixed vibrations. As a result, a numerous phonon modes in the nanolayers possess low phonon group velocity.

In Figure 3 the phonon energy spectra in Si(23ML)/Ge(5ML) planar superlattice are shown for two different directions in the Brillouin zone (BZ).

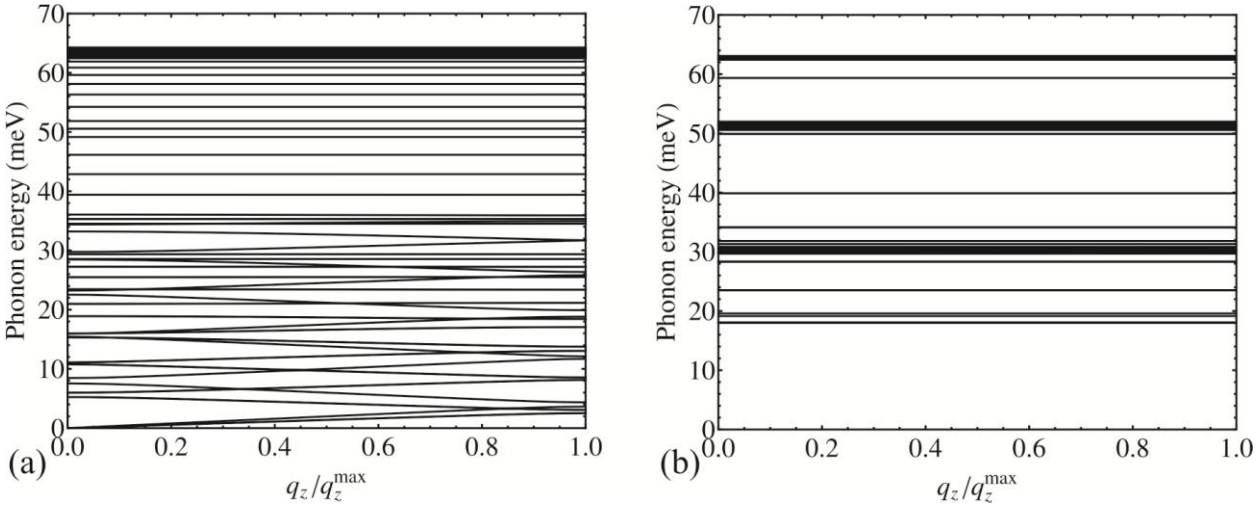

Fig. 3. Phonon energy spectra of Si(23ML)/Ge(5ML) planar superlattice in $(0,0,0) \to (0,0,q_z^{\max})$ direction (a) and $(0,q_y^{\max},0) \to (0,q_y^{\max},q_z^{\max})$ direction (b).

One can see from Figure 3 that phonon energy spectra in Si/Ge planar superlattices is strongly modified compared to bulk silicon or silicon nanolayers (see Figure 2). Due to the superlattice nature of the considered planar Si/Ge nanostructure i.e. the existence of a set of consecutive Si/Ge interfaces and due to the acoustic mismatch between Si and Ge materials, there appear a large number of phonons trapped (localized) in different segments of the superlattice: Si layers, Ge layers or Si/Ge boundary. A clear manifestation of the trapping effect one can found considering the high-energy phonons from Figure 3(a). The maximal phonon energy in germanium is ~ 40 meV, therefore all phonon modes in a Si/Ge superlattice with energy more than this value should be localized in Si segments. It is clearly seen from Figure 3(a) that phonons with energy more than 40 meV are dispersionless i.e. they posses group velocity close to zero and therefore they are localized in silicon segments of Si/Ge superlattice. Moreover, one can see from Figure 3(b) that in directions close to BZ edge the short-wavelength phonons are also dispersionless and posses a very low group velocity.

In nanolayers it was taken into account two basic mechanisms of phonon scattering: Umklapp phonon-phonon scattering and phonon-boundary scattering. Total scattering time of a phonon with wavevector $\vec{q}$ from *s*-th energy level was calculated according to Matthiessen's rule: $\tau_{tot,s}(q) = \left(\tau_{U,s}^{-1}(q) + \tau_{b,s}^{-1}(q)\right)^{-1}$, where $\tau_{U,s}(q)$ and $\tau_{b,s}(q)$ are phonon lifetimes in Umklapp and boundary scattering process, respectively. In order to evaluate the scattering time of the phonons in three-particle U-processes the following model formula from Ref. [2] was used:

$$\tau_{U,s}^{-1}(q) = B\left(\omega_s(q)\right)^2 T \exp\left(-C/T\right), \tag{3}$$

According to [2] this form of the Umklapp scattering rate ensures an adequate temperature dependence of the thermal conductivity both at high as well as low temperatures. Parameters *B* and *C* are fitted to reproduce the experimental thermal conductivity of bulk silicon.

For calculation of the phonon-boundary scattering time a phenomenological formula first introduced by Ziman [3] was used:

$$\tau_{b,s}^{-1}(q) = \frac{1-p(q)}{1+p(q)}\frac{\left|\upsilon_s(q)\right|}{d}, \tag{4}$$

In this approach the *p*-th part of the phonons is reflected specularly from the boundary, while all the other phonons are scattered diffusively, i.e. uniformly in all directions independently on the initial direction of the phonon wave before impact with the boundary. In this context, the parameter *p* characterizes the degree of boundary roughness, namely, the values of *p* close to 0 correspond to a very smooth boundary, while *p* close to 1 correspond to a very rough boundary. According to authors of Refs. [3] the parameter *p* can be determined from the following expression: $p(q) = \exp\left(-2\pi q^2 \delta^2\right)$, where δ – average height of the surface roughness. This form of the parameter *p* takes into account that when the average height of the surface roughness is much higher than the wavelength of the incident phonon, then the scattering is very strong and phonon "feels" even the smallest surface imperfections. In this case the parameter *p* is close to 0. In the case when phonon wavelength is much larger than δ then surface details are hardly distinguishable for such waves and the scattering will take place almost specularly with *p* close to 1.

To model the phonon scattering processes in real planar Si/Ge superlattices it was taken into account three basic mechanisms of phonon scattering: Umklapp phonon-phonon scattering, scattering on external boundaries (on the bottom and top segments) and scattering on Si/Ge interface. Total scattering time of a phonon with wavevector $\vec{q}$ from *s*-th energy branch was calculated according to Matthiessen's rule: $\tau_{tot,s}(q) = \left(\tau_{U,s}^{-1}(q) + \tau_{B,s}^{-1}(q) + \tau_{I,s}^{-1}(q)\right)^{-1}$, where $\tau_{U,s}(q)$,

$\tau_{B,s}(q)$ and $\tau_{I,s}(q)$ are phonon lifetimes in Umklapp, boundary and interface scattering processes, respectively. The perturbation theory and second quantization formalism were used in order to model the scattering of phonons on Si/Ge interfaces due to mass mixing, and the equation for phonon lifetime in interface scattering was obtained.

The Boltzmann transport equation approach was used for the investigation of the phonon and thermal processes in Si nanolayers and Si/Ge planar superlattices. An analytical expression for phonon thermal conductivity coefficient for nanolayers and planar superlattices is obtained from Boltzmann transport equation in relaxation time approximation:

$$\kappa_{ph} = \frac{1}{4\pi k_B T^2 d} \sum_s \int_0^{q_{\max}} (\mathrm{h}\omega_s(q))^2 (\upsilon_s(q))^2 \tau_{tot,s}(q) \frac{\exp(\frac{\mathrm{h}\omega_s(q)}{k_B T})}{(\exp(\frac{\mathrm{h}\omega_s(q)}{k_B T}) - 1)^2} q dq, \qquad (5)$$

in case of nanolayers, and:

$$\kappa_{ph} = \frac{1}{4\pi^2 k_B T^2} \sum_s \int_0^{\frac{\pi}{L_z}} \left\{ \int_0^{\frac{2\pi}{a}} (\hbar\omega_s(\vec{q}))^2 (\upsilon_{z,s}(\vec{q}))^2 \tau_{tot,s}(\vec{q}) \frac{\exp(\frac{\hbar\omega_s(\vec{q})}{k_B T})}{(\exp(\frac{\hbar\omega_s(\vec{q})}{k_B T}) - 1)^2} q_\perp dq_\perp \right\} dq_z, \qquad (6)$$

in case if superlattices.

In Figure 4 is plotted the temperature dependence of the phonon thermal conductivity in silicon nanolayers with d = 5, 10, 20 and 30 nm.

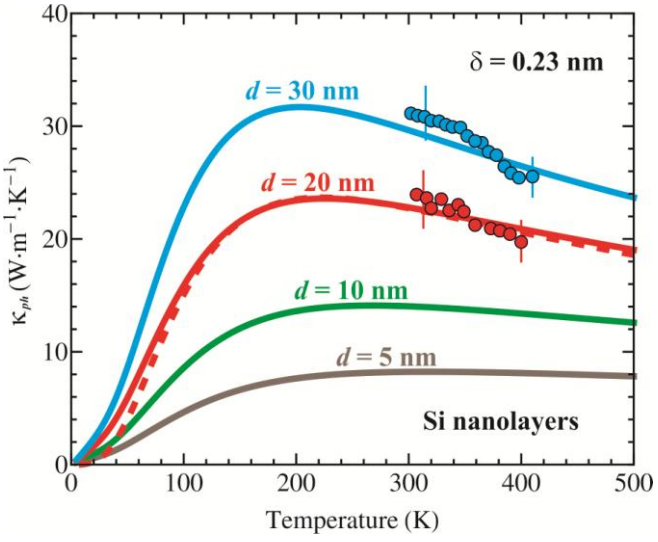

Fig. 2.4. Calculated temperature dependence of the phonon thermal conductivity of silicon nanolayers with d = 5, 10, 20 and 30 nm for average roughness height $\delta = 0.23$ nm. The experimental data points from Ref. [4] are also shown for comparison.

One should note a sharp drop of thermal conductivity in comparison with bulk case, which is explained by quantification of phonon energy spectrum, decrease of the phonon group velocity and additional scattering of phonons on nanolayer's external boundaries. A drop by a factor of 5 – 20 is found at the room temperature (RT) depending on nanolayer thickness. The experimental data points for nanolayers with d = 20 and 30 nm from Ref. [4] are also shown in Figure 4 for comparison. A good agreement is achieved for the average roughness height δ = 0.23 nm. As one can see from the figure, the maximum thermal conductivity shifts to higher temperatures with decrease of d, from T ~ 130 K for 30-nm-thick layer to T ~ 320 K for 5-nm-thick layer. This behavior can be explained as follows: the position of the thermal conductivity maximum separates the low-temperature region, where phonon scattering is mainly due to the boundary, from the high-temperature region, where Umklapp scattering is dominant. In a thinner nanolayer the boundary scattering is stronger in a comparison with a thicker one and dominates up to higher temperatures, therefore the position of the thermal conductivity maximum on the temperature dependence curves shifts to the right.

In Figure 5 is presented the calculated phonon thermal conductivity of planar Si(35ML)/Ge(9ML) superlattice as a function of temperature.

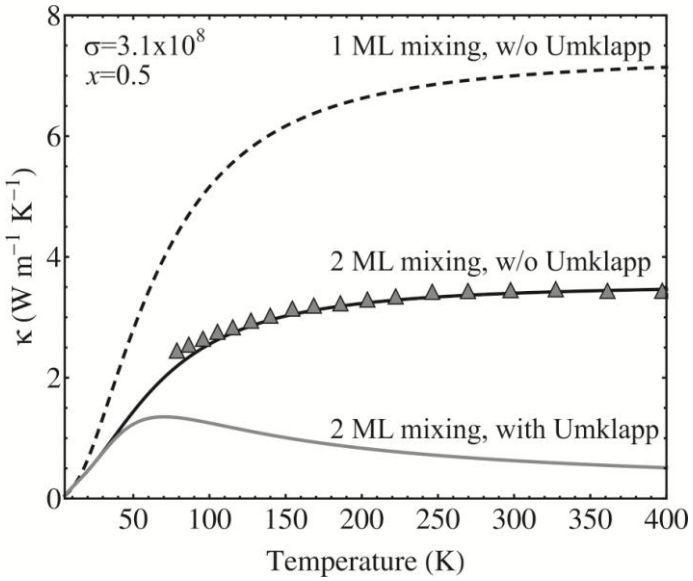

Fig. 5. Temperature dependence of the phonon thermal conductivity in Si(35ML)/Ge(9ML) planar superlattice. Gray triangles denote experimental points from Ref. [5].

The black dashed and solid lines correspond to calculations for 1 ML and 2 ML interface mixing without taking into account Umklapp scattering, while solid gray line represents calculation with 2 ML mixing and all three basic mechanisms of phonon scattering. A good agreement between theoretical and experimental data was obtained only in the case when Umklapp scattering was not accounted in calculations, indicating that in a real

Si(35ML)/Ge(9ML) planar superlattice from Ref. [5] the interface mass-mixing scattering is the dominant mechanism of phonon scattering. Indeed, if Umklapp scattering was dominating over interface scattering, then one should find a slow decrease of thermal conductivity at high temperatures, since Umklapp scattering time scales with temperature as $\tau_U \sim T^{-1}$, which is clearly seen from the solid gray curve. However, the experimental data demonstrated no such behavior (follow gray triangles on the figure) and thermal conductivity remained almost independent on temperature. Another important conclusion can be made if one compares black solid and dashed curves i.e. calculations with different number of mixed monolayers at interface. The thermal conductivity of planar Si(35ML)/Ge(9ML) superlattice with 1 ML interface mixing is almost 2 times larger than with 2 ML mixing for a wide range of temperatures, which demonstrates the strongest influence of interface mass-mixing phonon scattering on thermal conductivity of planar Si/Ge superlattices.

The results of the investigation of the thermal properties of silicon nanolayers presented in the Thesis were published in the research article [1] from the *List of published articles on the subject of the thesis*.

In **Chapter 3** the effective mass approximation is extended and applied for calculation and investigation of electron energy spectra and electron wave functions in core/shell Si/SiO_2 nanowires with constant (denoted as NW) and periodically modulated cross-section (denoted as MNW). In Figure 6 is shown the schematic view of considered core/shell nanowires. Nanowires consist of two periodically repeated Si segments with dimensions $d_x^1 \times d_y^1 \times l_z^1$ and $d_x^2 \times d_y^2 \times l_z^2$ covered by SiO_2 shell.

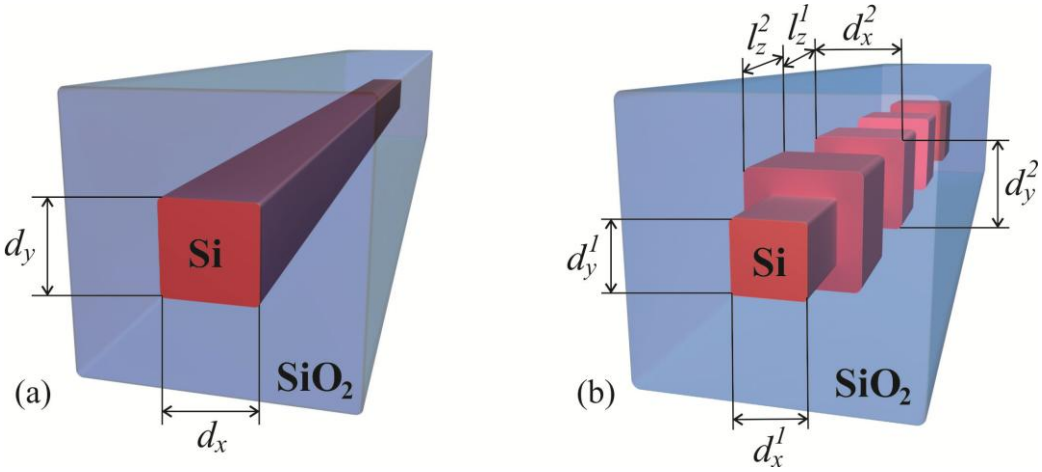

Fig. 6. Schematics of a Si nanowire with constant cross section (a) and periodically cross-section modulated Si nanowire (b). Both wires are covered with a SiO_2 shell.

Electron states in these structures were described with time-independent Schrodinger equation, which was solved numerically using finite-difference technique. In Figure 7 are shown ten lowest electron energy branches in Si NW with constant cross-section $d_x \times d_y$ = 9x9 nm^2 and Si MNW $d_x^1 \times d_y^1 \times l_z^1$=5x5x1 nm^3; $d_x^2 \times d_y^2 \times l_z^2$=9x9x1 nm^3. Both wires are covered with SiO_2 shell in such a way that total cross-sectional dimensions are equal to 15x15 nm^2.

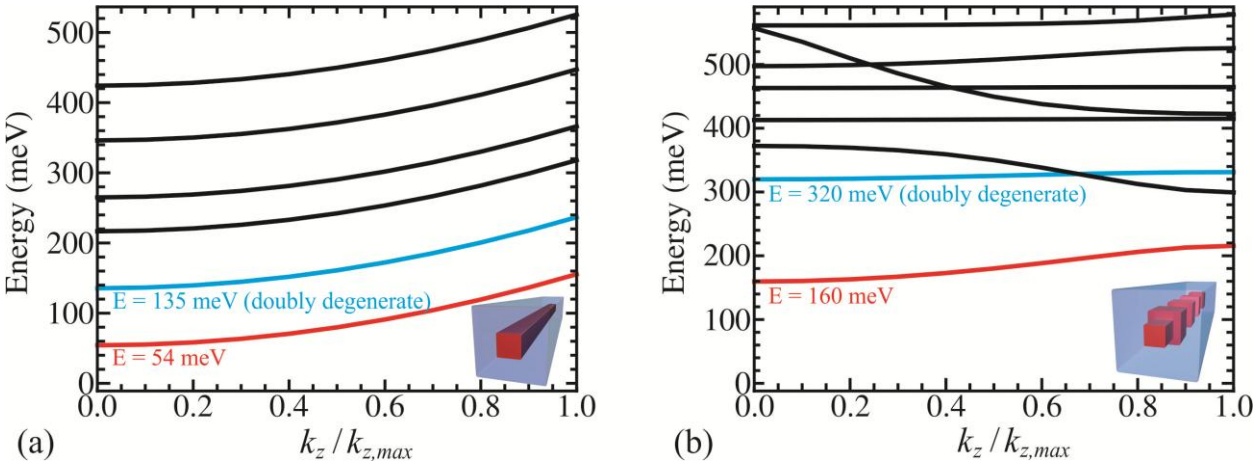

Fig. 7. Electron energy dispersion in Si nanowire with constant (a) and periodically modulated (b) cross-section, covered with SiO_2 shell.

Due to the nanometric cross-sectional dimensions of the considered wires, electron motion in *XY* plane is quantified and its energy can have only discrete values. In case of Si NW with constant cross-section the electron motion along the NW axis remains free and is described by a parabolic energy dispersion (see panel (a) in Figure 7). In case of a Si NW with modulated cross-section (panel (b) in Figure 7) there is a significant deviation from parabolic law, which indicates that electron motion along the *Z* axis is not free and a part of electron wave function being localized in wide segments of the modulated wire. One can observe also that lowest energy levels in MNW possess higher energy compared to generic NW, suggesting that electron confinement in nanowires with modulation manifests itself more strongly. Analyzing the electron wave functions an inhomogeneity in the ground state wave function distribution along the wire's axis was found.

The lattice dynamics Born – von Karman model and the Boltzmann transport equation were applied for the investigation of phonon and thermal processes in Si nanowires, Si cross-section modulated nanowires and novel Si/Ge core/shell cross-section modulated nanowires. The phonon energy spectra of Si NW with cross-section 14 ML x 14 ML and Si MNW with dimensions 14 ML x 14 ML x 6 ML – 22 ML x 22 ML x 6 ML are shown in Figure 8(a) and (b), correspondingly. In the figure, were shown 20 lowest branches $\hbar\omega_s(q_z)$ (s=1,2,…,20) in both

structures as well as several higher branches with s=20,25,30,35,…, 285,290,294 for the NW and with s=35,50,65,80,…,1515,1530 for the MNW.

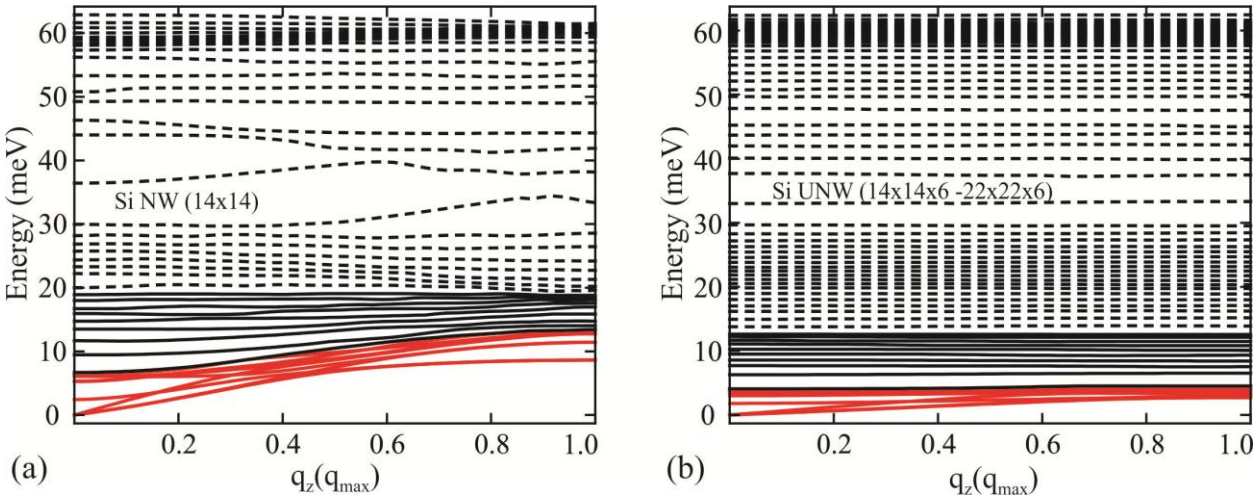

Fig. 8. Phonon energies as a function of the phonon wave vector q (a) in Si NW (the phonon branches with s=1 to 20, 25, 30, 35…290, 294 are shown) and (b) in Si MNW (the phonon branches with s=1 to 20, 35, 50, 65, …, 1515, 1530 are depicted).

The NW cross section is chosen the same as the cross section of narrow segments of the MNW. The volume of a translational period in the MNW is larger than that in the NW, therefore the number of quantized phonon branches in the MNW is substantially larger as compared to the NW. In the MNW, there are 1530 branches, while only 294 branches exist in the NW. As follows from Figure 8, a great number of phonon modes in the MNW with energy $\hbar\omega > 5$ meV are dispersionless and possess group velocities close to zero due to the trapping into the MNW segments.

The thermal properties of Si MNWs and Si/Ge core/shell MNWs were investigated in the framework of Boltzmann transport equation. The phonon flux per unit temperature gradient in the Si NWs and the Si MNWs was modeled by equation:

$$\Theta = \frac{1}{2\pi k_B T^2} \sum_{s=1,\ldots,3N} \int_0^{q_{z,\max}} \left(\mathrm{h}\omega_s(q_z)\upsilon_{z,s}(q_z)\right)^2 \tau_{tot,s}(q_z) \frac{\exp\left(\frac{\mathrm{h}\omega_s(q_z)}{k_B T}\right)}{\left(\exp\left(\frac{\mathrm{h}\omega_s(q_z)}{k_B T}\right)-1\right)^2} dq_z \,. \qquad (7)$$

The dependence of the ratio $\eta = \Theta(\text{Si NW})/\Theta(\text{Si MNW})$ of the thermal fluxes in Si NW 14 ML x 14 ML and Si MNW 14 ML x 14 ML x N_z ML – 22 ML x 22 ML x N_z on N_z for the temperatures T = 100 K, T = 200 K, T = 300 K and T = 400 K and p = 0.85 is presented in Figure 9. The calculated points for N_z = 2,4,6,…,18 are joined by the smooth curves as guides for an eye.

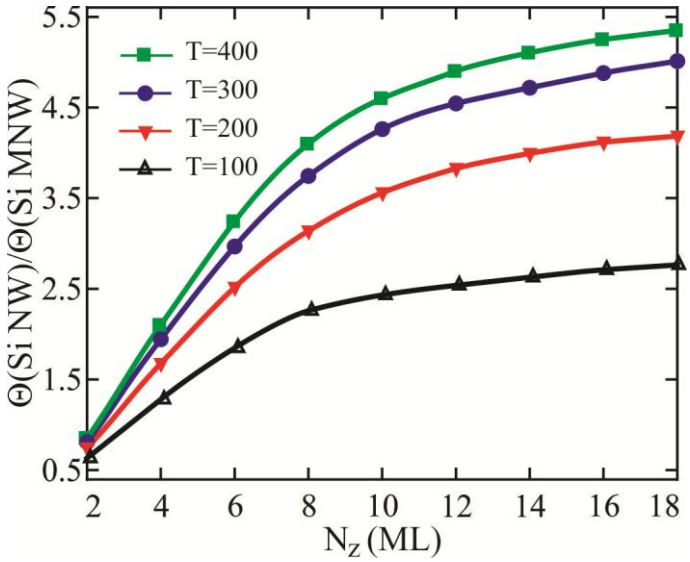

Fig. 9. Ratio of thermal fluxes in Si NW and Si MNWs as a function of N_z. The results are shown for different temperatures T = 100 K, 200 K, 300 K and 400 K.

The overall trend of these curves is determined by the interplay of two effects: (i) the phonon modes trapping, which suppresses the heat flux and (ii) augmentation of the MNW average cross-section, which enhances the heat flux due to the emergence of additional phonon modes for heat propagation and attenuation of the phonon-boundary scattering. In Si MNW with the ultra-narrow segments N_z = 2 ML, the trapping of phonon modes is weak and the thermal flux is larger than that in Si NW (η <1) due to the weakening of the phonon-boundary scattering in MNW in comparison with NWs. The rise of N_z enhances the trapping, and for all temperatures under consideration the flux ratios rapidly increase with N_z rising up to the values 8 ML to 12 ML, and reach their maximum values at around N_z = 16 ML to 18 ML. It is expected that a subsequent rise of N_z should decrease η due to augmentation of the MNW average cross-section. Thus, the possibility of a significant suppression of the phonon heat flux in Si cross-section modulated nanowires in comparison with the generic uniform cross-section Si nanowires was theoretically demonstrated. A strong decrease of the average phonon group velocities together with a corresponding suppression of the phonon thermal flux was found and the mechanisms behind this suppression were elucidated.

For Si/Ge core/shell cross-section modulated nanowires it was found theoretically that a combination of cross-section modulation and acoustic mismatch between Si and Ge materials can lead to an even more drastic reduction of the thermal conductivity. The performed calculations indicate that the RT thermal conductivity of Si/Ge core/shell cross-section modulated nanowires is almost three orders of magnitude lower than that of bulk Si. Thermal flux in the modulated nanowires is suppressed by an order of magnitude in comparison with

generic Si nanowires. The effect is explained by modification of the phonon spectra in modulated nanowires leading to decrease of the phonon group velocities and localization of certain phonon modes in narrow or wide nanowire segments.

The analytical expression for the electron-phonon scattering rate with emission and absorption of a phonon in Si/SiO_2 core/shell modulated nanowires was derived in the deformation potential approach. It was shown that cross-section modulation of the Si core results in a substantial modification of the RT electron-phonon scattering rate with phonon absorption.

The obtained theoretical results demonstrate that geometry modulation is an efficient instrument in engineering electrons and phonons in Si-based nanowires, which proved to be excellent candidates for thermoelectric and thermal insulator applications due to extremely low values of thermal conductivity.

The results of the investigation of the phonon processes in modulated nanowires presented in the Thesis were published in the research articles [2, 3] from the *List of published articles on the subject of the thesis*.

The **Chapter 4** is devoted to the investigation of phonon and thermal properties of single-, two- and three-layer graphene as well as of twisted bilayer graphene structure with different angles of rotation between the graphene planes. The schematic view of the single-layer, AB two-layer, ABA (Bernal) three-layer and ABC (rhombohedral) three-layer graphene is shown in Figure 10.

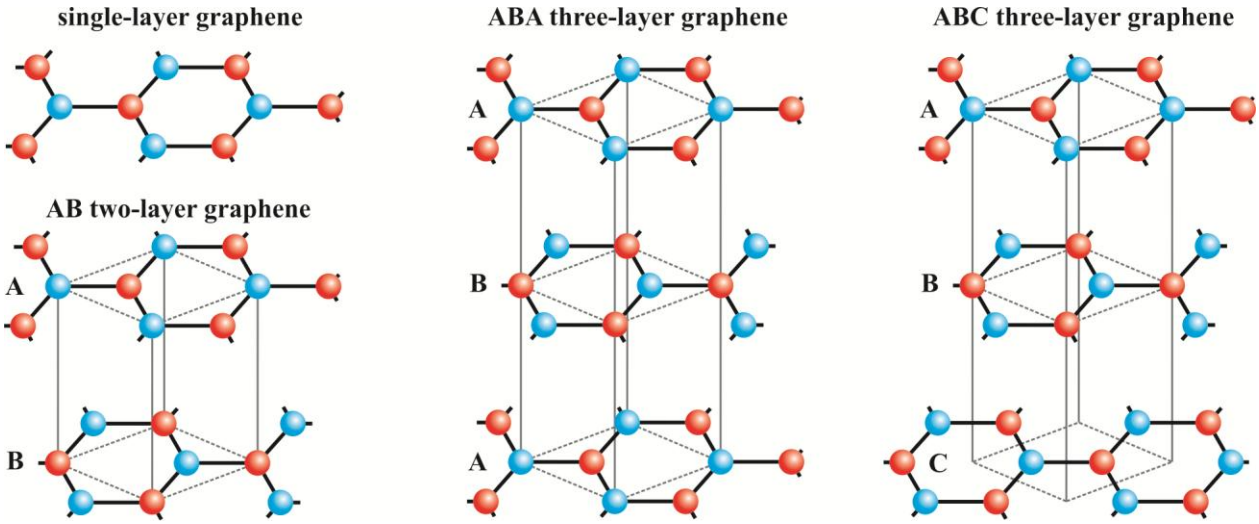

Fig. 10. Schematics of single-, two- and three-layer graphene.

A Born – von Karman model of lattice dynamics for these structures was developed. In Figure 11 is presented the phonon energy spectrum for single-layer graphene, obtained within BvK model. As can be seen from the figure, our calculated results are in a good agreement with

experimental data from Refs. [6, 7] for all phonon branches: in-plane acoustic branches (LA and TA), in-plane optic branches (LO and TO), out-of-plane acoustic (ZA) and optic (ZO) branches.

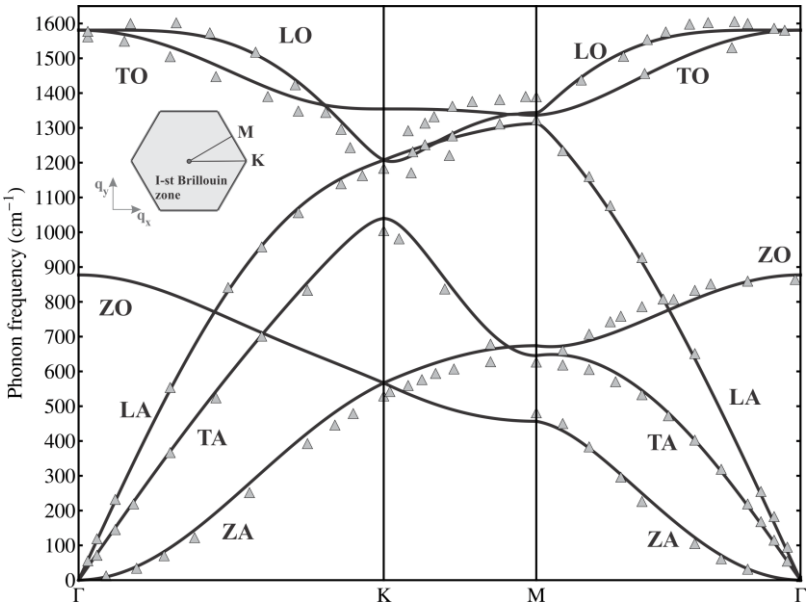

Fig. 11. Vibrational spectrum of the monolayer graphene. Symbols Γ, K and M denote high symmetry points of the first BZ. Experimental data points (gray triangles) for graphite from Refs. [6, 7] are also shown for comparison

An interesting behavior demonstrates out-of-plane acoustic ZA branch, in contrast to the linear dispersion near the Γ point for the in-plane TA and LA branches, it shows a q^2 dispersion, which is a characteristic feature for layered crystals [8].

When two graphene layers are placed on top of each other they can form a Moiré pattern [9]. In this case, one layer is rotated relative to another layer by a specific angle ("twisting"). Although twisting only weakly affects the interlayer interaction, it breaks symmetry of the Bernal stacking resulting in an intriguing dependence of the electronic and phonon properties on the rotation angle θ. The rotation scheme for obtaining the twisted bilayer graphene (T-BLG) is shown in Figure 12(a).

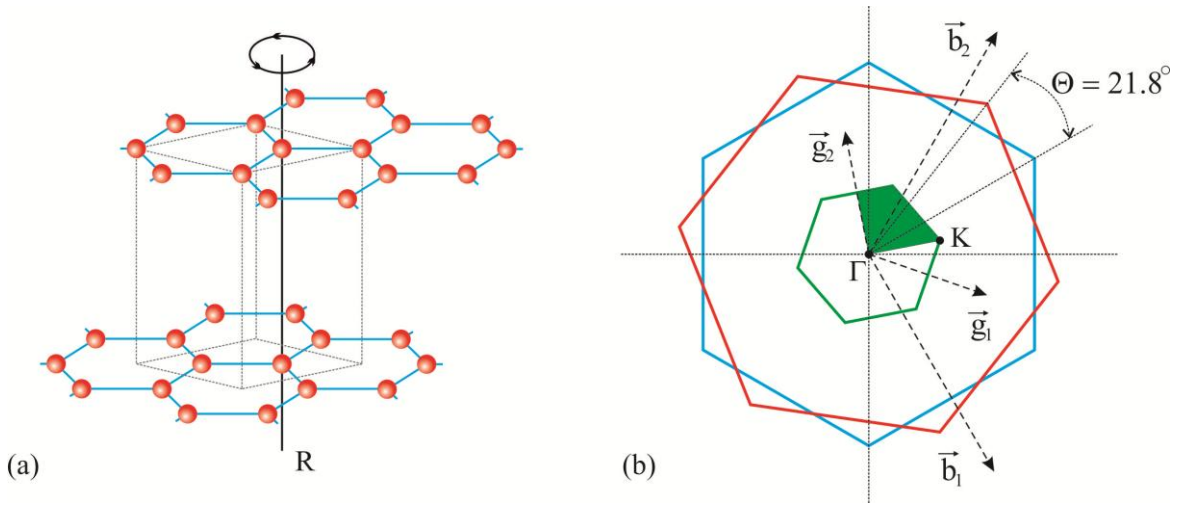

Fig. 12. (a) Rotational scheme. R denotes rotation axis. (b) BZ of T-BLG with $\theta = 21.8°$. Γ and K denote two high-symmetry points of T-BLG BZ.

Commensurate structures, i.e. structures with translation symmetry, exist for a certain rotational angles only, determined by the following condition: $\cos\theta(p,n) = (3p^2 + 3pn + n^2/2)/(3p^2 + 3pn + n^2)$, where p and n are coprime positive integer numbers. The number of atoms in the commensurate cell is equal to $N = 4\left((p+n)^2 + p(2p+n)\right)$. The unit cells of T-BLG with larger indices (p,n) contain larger number of carbon atoms. For instance, the unit cell of T-BLG with $\theta(1,1) = 21.8°$ contains the smallest possible number of atoms N = 28, while a rotation by $\theta(2,1) = 13.2°$ increases this number to N = 76. In order to construct the BZ of the T-BLG with the angle of rotation $\theta(p,n)$ one should determine the corresponding reciprocal space. The reciprocal vectors of T-BLG $\vec{g}_1$ and $\vec{g}_2$ are given by relations:

$$\begin{pmatrix} \vec{g}_1 \\ \vec{g}_2 \end{pmatrix} = \frac{1}{(p+n)^2 + p(2p+n)} \times \begin{pmatrix} 2p+n & p+n \\ -(p+n) & p \end{pmatrix} \begin{pmatrix} \vec{b}_1 \\ \vec{b}_2 \end{pmatrix}, \tag{8}$$

where $\vec{b}_1 = (2\pi/3a, -2\pi/\sqrt{3}a)$ and $\vec{b}_2 = (2\pi/3a, 2\pi/\sqrt{3}a)$ are the basis vectors of the reciprocal lattice of the single layer graphene. The BZ of the T-BLG with $\theta(1,1) = 21.8°$ is shown in Figure 12(b) as a dark hexagon.

The phonon dispersions in T-BLG with the rotation angles $\theta = 21.8°$ and $\theta = 13.2°$ are shown in Figure 13(a-b) along *Γ-K* direction in BZ. The phonon frequencies were calculated for each phonon wave number q from the interval 0 to $q_{\max}(\theta)$, where $q_{\max}(\theta) = 2q_{\max}(\theta = 0)\sin(\theta/2) = 8\pi\sin(\theta/2)/(3\sqrt{3}a)$.

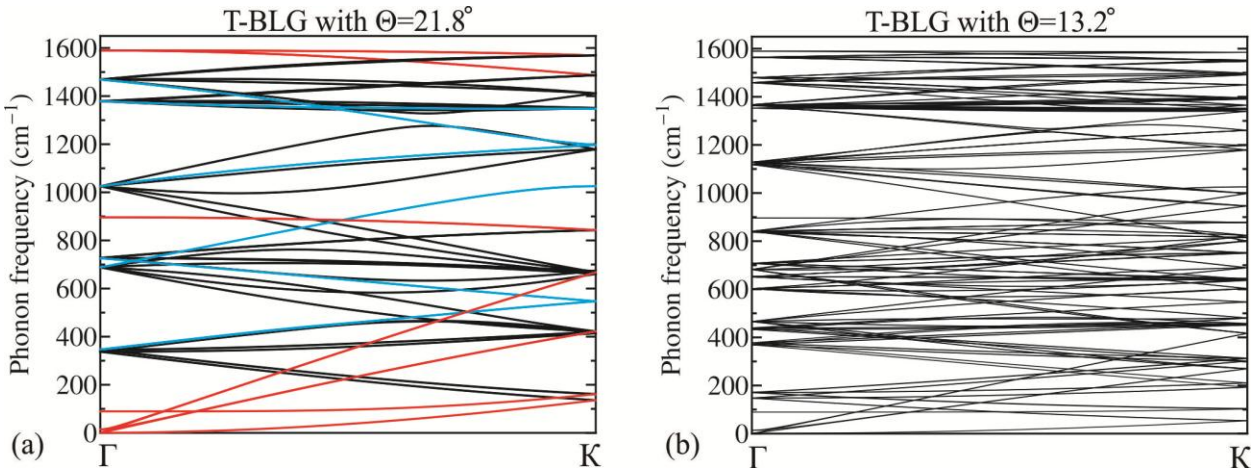

Fig. 13. Phonon dispersions in twisted bilayer graphene with $\theta = 21.8°$ (a) and $\theta = 13.2°$ (b).

The directions in BZ of T-BLG depend strongly on the rotational angle and do not coincide with the directions in BZ of bilayer graphene without a twist. As shown in Figure 12(b), the *Γ*-*K* direction in BZ of T-BLG is rotated relative to that in BZ of BLG. Therefore, the phonon curves in Figure 13(a-b) are shown for different directions in BZ of BLG. However, the *Γ*- and *K*-points in BZ of T-BLG correspond to those in BZ of BLG and the change of the phonon modes in these points is a direct effect of the twisting. The number of atoms in the unit cell of T-BLG with $\theta = 21.8°$ ($\theta = 13.2°$) increases by a factor of 7 (19) as compared with BLG. The number of phonon branches increases to 84 for T-BLG with $\theta = 21.8°$ and to 228 for T-BLG with $\theta = 13.2°$. The number of phonon modes at *Γ*- and *K*-points in BZ of T-BLG increases correspondingly. In addition to the degenerate TO/LO phonon modes of BLG at *Γ*-point with the frequency $\omega \sim 1589.5$ cm^{-1}, the new in-plane phonon modes appear in T-BLG. The frequencies of these modes depend strongly on the rotational angle and their number increases with decreasing θ.

The frequencies of the shear (LA_2, TA_2) and flexural (ZA_2) phonons are affected stronger by the twisting. The specific properties of these modes in T-BLG with $\theta = 21.8°$ (red curves) and T-BLG with $\theta = 13.2°$ (blue curves) as well as in AA-BLG (black curves) are presented in Figure 14.

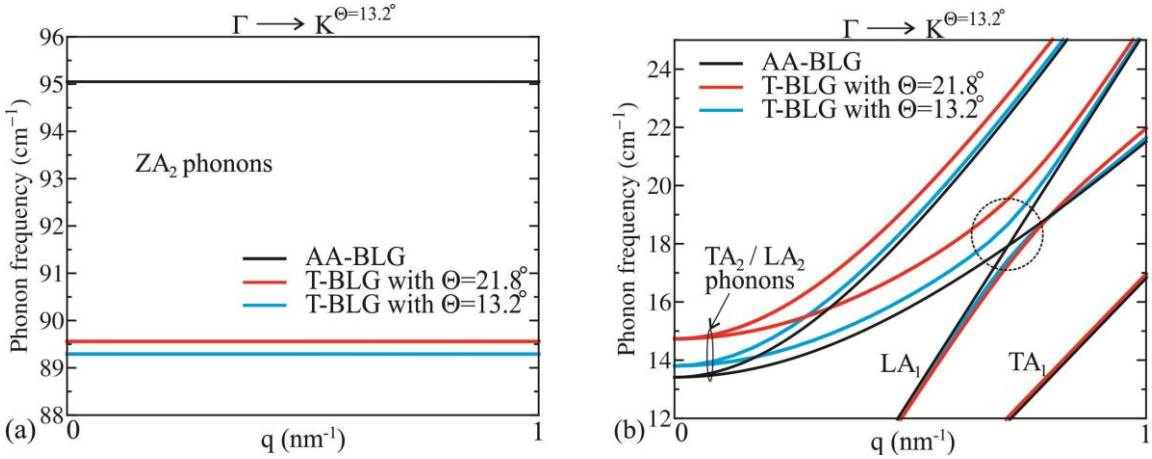

Fig. 14. Zone-center phonon dispersions of the out-of-plane (a) and in-plane (b) acoustic modes in AA-BLG (black curves), T-BLG with $\theta = 21.8°$ (red curves) and T-BLG with $\theta = 13.2°$ (blue curves). The region where anti-crossing of LA_1 and TA_2 hybrid folded phonon branches occurs are shown by dashed circle.

At Γ – point, the twisting increases the frequency of the shear modes by 1 – 2 cm^{-1} and decreases the frequency of ZA_2 modes by ~ 5 – 5.5 cm^{-1} depending on θ (see Figure 14(a)). In AA-BLG, the phonon branches LA_1 and TA_2 intersect at q ~ 0.7 nm^{-1}. Twisting changes the interaction between these phonons in T-BLG and leads to anti-crossing of LA_1 and TA_2 hybrid folded phonon branches (see Figure 14(b)).

Specific heat, C, is one of the key parameters that characterize the phonon and thermal properties of materials. It is defined as $C = \delta Q / \delta T$, where δQ is the change in energy density of a material when temperature changes by δT [3]. For calculation of the phonon specific heat in T-BLG was used the following formula [3]:

$$c_V(T) = \frac{3N_A}{k_B T^2} \int_0^{\omega_{max}} \frac{\exp(\frac{\hbar\omega}{k_B T})}{[\exp(\frac{\hbar\omega}{k_B T}) - 1]^2} (\hbar\omega)^2 \, f(\omega) d\omega, \qquad (9)$$

where ω is the phonon frequency, ω_{max} is the maximum phonon frequency, f is the 2D normalized phonon DOS, T is the temperature, N_A is the Avogadro constant, k_B is the Boltzmann constant and $\hbar$ is the Planck constant. The normalized phonon DOS is given by $f(\omega) = g(\omega) \Big/ \int_0^{\omega_{max}} g(\omega) d\omega$, where $g(\omega)$ is the 2D phonon DOS given by the relation $g(\omega) = \int_{q_x} \sum_{s(\omega,q_x)} \sum_{q_y(s,\omega,q_x)} \left| \frac{\partial \omega(q_x, q_y, s)}{\partial q_y} \right|^{-1} dq_x$. Here s numerates phonon branches. In order to calculate $g(\omega)$ a 200×200 2D grid was applied to a 1/4th part of BZ of T-BLG (shown as a dark

segment in Figure 12(b)), and then phonon frequencies for every (q_x,q_y) point was calculated in this grid.

In Figure 15 is plotted the difference between the specific heat in AB-BLG and T-BLG as a function of temperature: $\Delta c_v(\theta) = c_v(AB) - c_v(\theta)$ for $\theta = 21.8°$, $\theta = 13.2°$ and $\theta = 9.4°$.

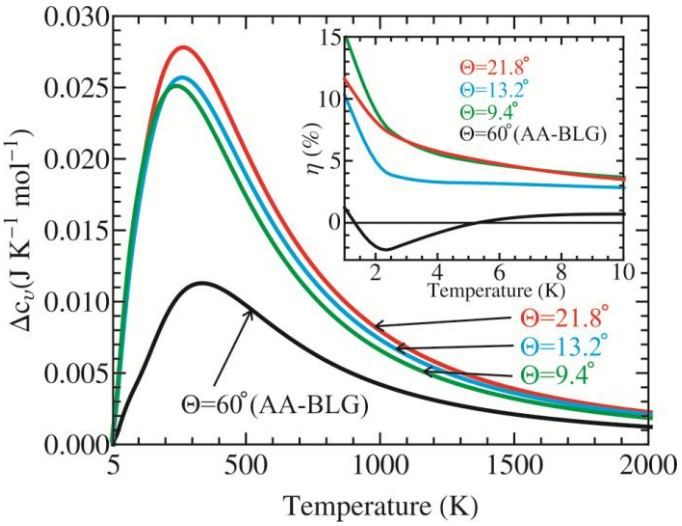

Fig. 15. Dependence of the deviation $\Delta c_v(\theta)$ of the specific heat in T-BLG from that in AB-BLG on the temperature. The inset shows the relative deviation η between AB-BLG and T-BLG specific heats as a function of temperature.

The change in the specific heat due to twisting is relatively weak in a wide temperature range 20 K - 2000 K. It attains its maximum value ~ 0.028 J K^{-1} mol^{-1} at T ~ 250 K. At the same time, at low temperatures the relative difference between specific heat in AB-BLG and T-BLG $\eta = (1 - c_V(\theta)/c_V(AB)) \times 100\%$ constitutes substantial 10-15% at T = 1 K and ~ 3-6% at T = 5 K in dependence on θ (see blue, red and green curves from the inset to Figure 15). The low temperatures specific heat depends stronger on the twist angle because twisting affects the low-frequency ZA phonon modes the most. The temperature dependence of low-temperature specific heat in T-BLG with $\theta = 21.8°$ differs from single-layer or bilayer graphene: $c_V \sim T^{1.3}$ for T < 10 K and $\sim T^{1.6}$ for 10 K $\leq T \leq$ 100 K. One should expect that twisting can produce stronger effects on the specific heat of the T-FLG with the larger number of the atomic planes rotated with respect to each other as well as in van der Waals materials with stronger interlayer coupling. The results suggest a possibility of phonon engineering of phonon and thermal properties of layered materials by twisting the atomic planes.

The results of the investigation of the phonon processes in single-layer and twisted bilayer graphene presented in the Thesis were published in the research articles [4-7] from the *List of published articles on the subject of the thesis*.

GENERAL CONCLUSIONS AND RECOMMENDATIONS

Below the summary of the results obtained in the Thesis is given.

1. A three-parameter Born-von Karman type model of lattice dynamics for nanolayers and planar superlattices with diamond crystal lattice was developed. The Boltzmann transport equation approach was used for investigation of the phonon and thermal processes in Si nanolayers and Si/Ge planar superlattices. For nanometer-wide silicon nanolayers was obtained a good agreement between theoretical calculations and the experimental data for 20-nm-thick and 30-nm-thick silicon nanolayers. It was demonstrated that optical phonons contribution to the thermal conductivity of silicon nanolayers under consideration constitutes only a few percent.

2. The perturbation theory and second quantization formalism were used in order to model the scattering of phonons on interfaces in Si/Ge planar superlattices. It was concluded that interface mass-mixing scattering of phonons plays an extremely important role in limiting the total phonon lifetime in Si/Ge planar superlattices and can lead to a peculiar behavior of phonon thermal conductivity of these structures owing to the non-trivial dependence of interface scattering rate on the amplitudes of the atomic displacements. For a wide temperature range from 50 K to 400 K a good agreement between theoretical and experimental phonon thermal conductivity was obtained for Si(35ML)/Ge(9ML) planar superlattice when phonon-phonon scattering was not taken into account, indicating that the interface mass-mixing scattering can be the dominant mechanism of phonon scattering in real Si/Ge planar superlattices.

3. The effective mass approximation was applied for investigation of electron energy spectra and electron wave functions in core/shell Si/SiO_2 nanowires with constant and periodically modulated cross-section. It was shown, that cross-section modulation strongly influences the electron energy spectra and electron wave functions in Si nanowires. For ground state there appear an inhomogeneity in the wave function distribution along the wire's axis, namely, the main part of the wave function modulus being localized in the wide segments of the modulated wire.

4. The lattice dynamics Born – von Karman model and the Boltzmann transport equation were applied for investigation of phonon and thermal processes in Si nanowires, Si cross-section modulated nanowires and Si/Ge core/shell cross-section modulated nanowires. For Si cross-section modulated nanowires it was theoretically demonstrated that phonon heat flux can be significantly suppressed in comparison with the generic uniform cross-section Si nanowires. Redistribution of the phonon energy spectra in the cross-section modulated nanowires leads to a strong decrease of the average phonon group velocities and a corresponding suppression of the phonon thermal flux. An up to 5 times drop of the phonon heat flux at room temperature is

predicted for Si cross-section modulated nanowires in comparison with uniform Si nanowires. For Si/Ge core/shell cross-section modulated nanowires it was found theoretically that a combination of cross-section modulation and acoustic mismatch between Si and Ge materials can lead to an even more drastic reduction of the thermal conductivity. The performed calculations indicate that the room temperature thermal conductivity of Si/Ge core/shell cross-section modulated nanowires is almost three orders of magnitude lower than that of bulk Si.

5. The analytical expression for the electron-phonon scattering rate with emission and absorption of a phonon in Si/SiO_2 core/shell modulated nanowires was derived in the deformation potential approach. It was shown that cross-section modulation of the Si core results in a substantial modification of the room temperature electron-phonon scattering rate with phonon absorption.

6. A Born – von Karman model of lattice dynamics for single-, two-layer and three-layer graphene as well as for twisted bilayer graphene with different angles of rotation was developed. Phonon energy spectra of these structures in all high-symmetry crystallographic directions were calculated. The obtained results for phonon frequencies of single-layer and non-rotated few-layer graphene are in a very good agreement with experimental data of bulk graphite. It was found that, since many of the zone-center acoustic and optical vibrational modes of non-rotated few-layer graphene are Raman or infrared active, they can provide important information on layer number and stacking configuration of graphene multilayers. It was found that middle- and high-frequency phonons in twisted bilayer graphene are practically independent on the twisting angle, while the low-frequency phonons strongly depend on it. Thus, *an important scientific problem was solved* in the Thesis namely it was demonstrated the possibility to control the phonon processes in two-layer graphene by rotation of graphene layers one against another around the axis perpendicular to the graphene plane.

7. A new type of hybrid folded rotationally-dependent phonon modes appear in the twisted bilayer graphene due to reduction of the BZ size and changes in the interaction between graphene layers. These modes can manifest themselves in Raman or infrared measurements and, thus, can be used for the non-contact characterization of twisted bilayer graphene. The phonon specific heat in single-layer, bilayer and twisted bilayer graphene was studied. It was found that at temperature $T<15$ K, specific heat varies with temperature as T^n, where $n = 1$ for graphene, $n = 1.6$ for bilayer graphene and $n = 1.3$ for the twisted bilayer graphene.

Based on the conclusions presented above, the following recommendations can be made:

1. The Si/Ge planar superlattices with atomic intermixing at interfaces are perspective candidates for phonon filtering applications.

2. The acoustically-mismatched Si-based core/shell modulated nanowires with suppressed phonon heat transport are perspective for thermoelectric and thermal insulator applications.
3. The twisted bilayer graphene with different angles of rotation can be recommended for heat spreading and heat management applications owing to their unusual angle-dependent phonon processes.

The obtained theoretical results contribute to a better understanding the phonon and electron processes in graphene and silicon-based nanostructures and are important for the design and practical realization of novel nanomaterials with optimized and properly engineered electron and phonon properties.

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LIST OF PUBLISHED ARTICLES ON THE SUBJECT OF THE THESIS

[1] Cocemasov A. and Nika D. Phonons and phonon thermal conductivity in silicon nanolayers. In: J. Nanoelectron. Optoelectron., 2012, vol. 7, p. 370-375.

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SUMMARY

Cocemasov Alexandr, „Phonon processes in graphene and silicon-based nanostructures", doctor thesis in physics, Chisinau, 2015. Introduction, 4 Chapters, General conclusions and recommendations, 200 References, 140 Pages, 66 Figures, 7 Tables. The results presented in the thesis are published in 33 scientific works.

Key words: phonons, electrons, nanolayer, superlattice, nanowire, graphene, lattice dynamics, modulation, thermal properties.

Domain of study: physics of nanosystems.

Goal and objectives: investigation of phonon processes in graphene (single-, two-, three-layer graphene and twisted graphene) and silicon-based nanostructures (Si nanolayers, Si/Ge superlattices and Si-based modulated nanowires), and search of the methods for targeted control of their phonon properties.

Scientific novelty and originality: a Born – von Karman lattice dynamics model for nanolayers, planar superlattices, cross-section modulated nanowires and multilayer graphene with different atomic stacking was developed; the influence of shell material and cross-section modulation on phonon and electron processes in Si-based nanowires was studied; a theoretical approach for calculation of scattering time of phonons on interfaces of Si/Ge superlattices was developed and the influence of Si/Ge interface quality on phonon and thermal properties of these superlattices was investigated; the influence of different atomic stacking on phonon and thermal processes in multilayer graphene was studied.

Important scientific problem solved: it was demonstrated and investigated theoretically the possibility to control the phonon processes in two-layer graphene by rotation of graphene layers one against another around the axis perpendicular to the graphene plane. Theoretical model of lattice dynamics in rotated ("twisted") two-layer graphene was developed.

Theoretical importance: were developed theoretical approaches for targeted control of phonon processes in graphene and silicon-based nanostructures.

Practical significance: the practical implementation of the obtained theoretical results can lead to fabrication of new classes of nanostructures with specifically desired phonon properties.

ADNOTARE

Cocemasov Alexandr, „Procesele fononice în grafen și nanostructuri pe baza de siliciu”, teză de doctor în științe fizice, Chișinău, 2015. Introducere, 4 Capitole, Concluzii generale și recomandări, 200 Titluri bibliografice, 140 Pagini, 66 Figuri, 7 Tabele. Rezultatele prezentate în teză sunt publicate în 33 de lucrări științifice.

Cuvintele-cheie: fononi, electroni, nanostrat, suprarețea, nanofir, grafen, dinamica rețelei, modulație, proprietăți termice.

Domeniul de studiu: fizica nanosistemelor.

Scopul și obiectivele: investigarea proceselor fononice în grafen (cu un singur, două, trei straturi și grafen ”twisted”) și nanostructuri pe baza de siliciu (nanostraturi din Si, suprarețele Si/Ge și nanofire modulated pe baza de Si), și căutarea metodelor de control precondiționat a proprietăților lor fononice.

Noutatea și originalitatea științifică: a fost dezvoltat modelul Born – von Karman a dinamicii rețelei cristaline pentru nanostraturi, suprarețele planare, nanofire cu secțiunea transversală modulată și grafen multistrat cu aranjarea cristalină diferită; a fost studiată influența materialului de înveliș și modulației secțiunii transversale asupra proceselor fononice și electronice în nanofirele pe baza de Si; a fost dezvoltată o metodă teoretică pentru calcularea timpului de relaxare în procesele de împrăștiere a fononilor pe interfețele suprarețelelor Si/Ge și a fost studiată influența calității interfețelor Si/Ge asupra proprietăților fononice și termice al acestor suprarețele; a fost studiată influența aranjării cristaline asupra proceselor fononice și termice în grafenul multistrat.

Problema științifică importantă soluționată: a fost demonstrată și investigată teoretic posibilitatea de control a proceselor fononice în grafenul bistrat prin rotația straturilor de grafen unul împotriva altuia în jurul axei perpendiculare către planul straturilor. A fost dezvoltat modelul teoretic a dinamicii rețelei cristaline în grafenul bistrat cu rotația dintre straturi (”twisted”).

Semnificația teoretică: au fost dezvoltate metode teoretice de control precondiționat a proceselor fononice în grafen și nanostructuri pe baza de siliciu.

Valoarea aplicativă: implementarea practică a rezultatelor teoretice obținute poate contribui la fabricarea a nanostructurilor cu proprietăți fononice precondiționate.

АННОТАЦИЯ

Кочемасов Александр, „Фононные процессы в графене и наноструктурах на базе кремния”, диссертация на соискание ученой степени доктора физических наук, Кишинев, 2015. Введение, 4 Главы, Общие выводы и рекомендации, 200 Ссылок, 140 Страниц, 66 Рисунков, 7 Таблиц. Результаты, представленные в диссертации, опубликованы в 33 научных работах.

Ключевые слова: фононы, электроны, нанослой, сверхрешетка, нанонить, графен, динамика решетки, модуляция, тепловые свойства.

Область исследований: физика наносистем.

Цель и задачи: исследование фононных процессов в графене (одно-, двух-, трех-слойном и “twisted” графене) и наноструктурах на базе кремния (Si нанослоях, Si/Ge сверхрешетках, модулированных нанонитях на базе Si), и поиск методов целенаправленного управления их фононными свойствами.

Научная новизна и оригинальность: развита модель динамики решетки Борна – фон Кармана для нанослоев, плоских сверхрешеток, нанонитей с модуляцией поперечного сечения и многослойного графена с различной упаковкой графеновых слоев; исследовано влияние материала обкладки и модуляции поперечного сечения на фононные и электронные процессы в нанонитях на базе Si; развит теоретический подход для расчета времени рассеяния фононов на интерфейсах Si/Ge сверхрешеток и исследовано влияние качества Si/Ge интерфейса на фононные и тепловые свойства этих сверхрешеток; изучено влияние способа упаковки графеновых слоев на фононные и тепловые процессы в многослойном графене.

Решенная важная научная задача: теоретически продемонстрирована и исследована возможность управления фононными процессами в двухслойном графене путем поворота графеновых слоев друг относительно друга вокруг оси перпендикулярной к плоскости слоев. Развита теоретическая модель динамики решетки в двухслойном графене с поворотом (“twisted”).

Теоретическая значимость: разработаны теоретические подходы для управления фононными процессами в графене и наноструктурах на базе кремния.

Прикладная ценность: практическая реализация полученных теоретических результатов может способствовать появлению новых классов наноструктур с определенно заданными фононными свойствами.

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