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Analytical Calculation of Frequency Spectrum and Group Velocities of Acoustic Phonons in Quasi-two-dimensional Nanostructures

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Low-dimensional crystal structures that are attractive materials for the fabrication of modern nanoelectronic devices due to their unique physical properties are considered. Type of nanostructure (quantum well, quantum wire or quantum dot) and its sizes with respect to quasiparticle confined movement are determining factors for the formation of its mechanical, kinetic, optical and electronic properties and, since, main physical parameters. The processes of interaction between quasiparticles (in particular, electron-phonon interaction) also play an important role. Renormalized energy spectra of electrons and phonons define the physical processes, which are produced by electron-phonon interaction in nanostructure. In order to understand these peculiarities, it is necessary to study how the energy spectra of both these systems of quasiparticles are transformed in nanostructures of different types and sizes, as well as mechanisms of their interaction. Therefore, one should know the analytical form of dispersion relation for the electron energy and frequencies of all types of phonons in a particular nanostructure. In this paper, we propose the method how to obtain the explicit dispersion relations for all modes of confined acoustic phonons in plane quasi-two-dimensional nanostructures with hexagonal crystal lattice. Using the dielectric continuum model, the formulas describing frequency as a function of the phonon wave vector are derived and phonon group velocity, in its turn. Computer simulations are performed for GaN nanofilm with wurtzite structure.

Keywords: Nanostructure, Nanofilm, Acoustic phonons, Frequency spectrum, Group velocity.

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1. INTRODUCTION

Nanosized crystal structures and materials have been studied for a long time [1], however, interest to their research is still not declining [2, 3]. Despite the great number of theoretical and experimental research works in this field, the theoretical description of electron-phonon interaction in nanoheterostructures remains an actual problem. This interaction is an important factor in the processes of electrical and thermal conductivity, optical absorption, radiation, luminescence and Raman scattering in such systems [4]. It is particularly difficult to describe consistently the influence of acoustic phonons on these processes. The reasons lay in the discrepancy of some integrals in the expressions for the electron-phonon binding functions and difficulties in calculating spectral dependences of the modes of the acoustic phonon spectrum in nanostructures. Therefore, the explicit expression for the function describing these dependences analytically is actual for the development of the theory of electron-phonon interaction in such structures.

In this paper, we propose a simple method to establish the analytical dependences of energies and velocities of acoustic phonons in a plane quasi-two-dimensional crystal nanostructure – nanofilm. It is based on the idea of expansion of components of the displacement vector of elastic vibrations of atoms in the crystal lattice into Fourier series. This gives an opportunity to find the analytical solution of equations of motion and the dispersion relation for frequency.

Computer simulations are performed for hexagonal structure of GaN type in order to compare the obtained results with the data presented by the authors of paper [5], who used the numerical methods.

2. MODEL FOR THE PROBLEM AND METHOD OF ITS SOLUTION

The processes of interaction between acoustic phonons and electrons in nanosized quasi-two-dimensional crystal structures can be described in the framework of an elastic continuum model using the method of deformation potential [6]. In this case, the Hamiltonian of the electron-phonon interaction is expressed within the functional dependences of frequency ω of elastic vibrations in a nanofilm on the magnitude of the wave vector q and amplitudes of the displacement vector u_m ($m = 1, 2, 3$) on the coordinate x_3 along the direction of its surface, Fig. 1. Such dependences are obtained in this paper for all modes of the acoustic phonon spectrum in such quasi-two-dimensional crystal structures.

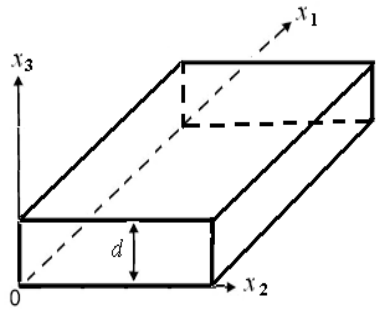

Fig. 1 – Geometrical scheme of a nanofilm

For the solution of the problem, like the authors of paper [5], we use the dielectric continuum model and equation of motion for the description of elastic vibrations in an anisotropic medium with mass density ρ

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