Phonon spectrum of graphene bilayer and monolayer graphene

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In this work numerical calculation of the phonon spectrum of double carbon nanoribbons is hold. The phonon spectrum was calculated by methods of classical mechanics in the framework of the Hamilton. The mutual arrangement of layers of graphene corresponds ABAB packing. Hamiltonian system is written in the harmonic approximation, taking into account the nearest-neighbor interactions. The quantum-chemical semi-empirical MNDO method is used to calculate the coupling constants in the framework of a molecular cluster.

The homogeneous system of linear algebraic equations for the amplitudes of the oscillations was obtained by writing the equations of motion of atoms and substituting the solution in the form of plane waves. From this we obtain the dispersion equation for the phonon spectrum of double graphene layer [1]. The boundary conditions for the two types of carbon nanoribbons "arm-chair" and "zig-zag" are used in solving the dispersion equation. The varying the width of the tapes is also carried out.

The results of the calculations shows that the phonon spectrum of double-wall carbon nanoribbons has a doublet character, that in turn is associated with the interaction of layers with each other. The effect of the configuration relative position of layers of double-wall carbon nanoribbons on the phonon spectrum is also studied. Because of the weak interaction of atoms at different layers, changes in the phonon spectrum were several orders of magnitude smaller compared with the values of characteristic frequencies. Thus we can say that the phonon spectrum calculated in the harmonic approximation, and the neareSt neighbor approximation with sufficient accuracy remains unchanged at a bias layers.

The gap is present between the acoustic and optical vibration modes in contraSt to graphene in the phonon spectrum of graphene nanoribbons of any type and width. Features of the vibration spectrum of graphene may serve as an indicator to identify this structure.

The calculated phonon spectra allow us to determine the Debye temperature for the bilayer graphene and graphene 1832 to 6052 K, as well as sound velocity 22390 m / s and 50,334 m / s, respectively.

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[1] G.S. Ivanchenko, N.G. Lebedev, *Solid State Physics* **48**(12), 2354 (2006).