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PROPERTIES OF DELOCALIZED NONLINEAR VIBRATIONAL MODES IN GRAPHENE

Semenova M.N.

Keywords: molecular dynamics modeling, graphene, nonlinear vibrations, crystal lattice, mode.
Abstract. The molecular dynamics method based on well-tested Savin interatomic potentials is used to analyze the properties of all possible one-, two-, and three-component delocalized nonlinear vibrational modes in graphene. The results of computer simulations are in full agreement with the predictions of the theory based on the analysis of lattice symmetry. It was confirmed that for graphene there are four one-component, twelve two-component, and a single three-component mode.

СВОЙСТВА ДЕЛОКАЛИЗОВАННЫХ НЕЛИНЕЙНЫХ КОЛЕБАТЕЛЬНЫХ МОД В ГРАФЕНЕ

Семёнова М.Н.

Ключевые слова: молекулярно-динамическое моделирование, графен, нелинейные колебания, кристаллическая решетка, мода.
Аннотация. Методом молекулярной динамики, основанным на хорошо апробированных межатомных потенциалах Савина, проанализированы свойства всех возможных одно-, двух- и трехкомпонентных делокализованных нелинейных колебательных мод в графене. Результаты компьютерного моделирования находятся в полном согласии с предсказаниями теории, основанной на анализе симметрии решеток. Подтверждено, что для графена существует четыре однокомпонентные, двенадцать двухкомпонентных и единственная трехкомпонентная мода.

One of the important branches of crystal physics is the study of crystal lattice vibrations, since they determine such important properties as thermal conductivity, heat capacity, thermal expansion and many others. Along with experimental methods for studying the nonlinear dynamics of a crystal lattice, effective methods of computer modeling are widely used, such as ab initio modeling and the method of molecular dynamics.

In this work, we investigated the properties of multicomponent delocalized nonlinear vibrational modes (DNVM) in graphene. Graphene was chosen because, due to the unique combination of its physical and mechanical properties (record high strength and rigidity, high thermal and electrical conductivity, chemical stability, etc.), it has a high potential for application in nanotechnology. For the hexagonal graphene lattice, we used the sp^2 interatomic potential of carbon, developed by Savin [1]. This is a many-body potential widely used to describe covalent chemical compounds.

The structure of a hexagonal graphene lattice with a zigzag (armchair) direction along the *x(y)* axis is shown in Fig. 1. Primitive rhombus-shaped translation cells with side *a* are shown with dashed lines. Translation vectors of both lattices: $(a, 0)$ and $(a/2, a\sqrt{3}/2)$.

One-, two-, and three-component modes were studied by the molecular dynamics method. An *NVE* ensemble was used, so that the number of atoms, *N*,

volume, *V*, and the total energy of the computational block *E* were conserved over time. Atoms have three degrees of freedom - two components of motion in the plane, as well as a component of displacement along the normal to the plane of the graphene sheet. To excite DNVM, the initial displacements were assigned to carbon atoms according to the schemes described in [2, 3], while the atoms had zero initial velocities.

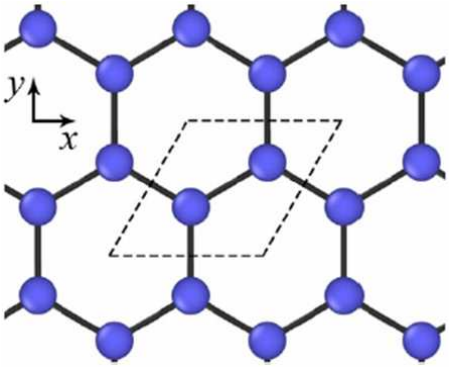

Fig. 1. The structure of the hexagonal lattice of graphene

It has been well established that for graphene, there are four single-component DNVMs, twelve two-component DNVMs, and a single three-component DNVM. Let us describe some physical parameters of three-component DNVM in the mode of periodic oscillations in time. In Fig. 2, as a function of the amplitude of the root mode, shows (a) frequency, (b) energy per atom, and (c) average stress σ_{xx} and σ_{yy} over the oscillation period, which appear in the graphene sheet after DNA initiation. Note that in calculating the stresses, it was assumed that the graphene sheet has a thickness of *3.3 Å*, equal to the distance between atomic planes in graphite.

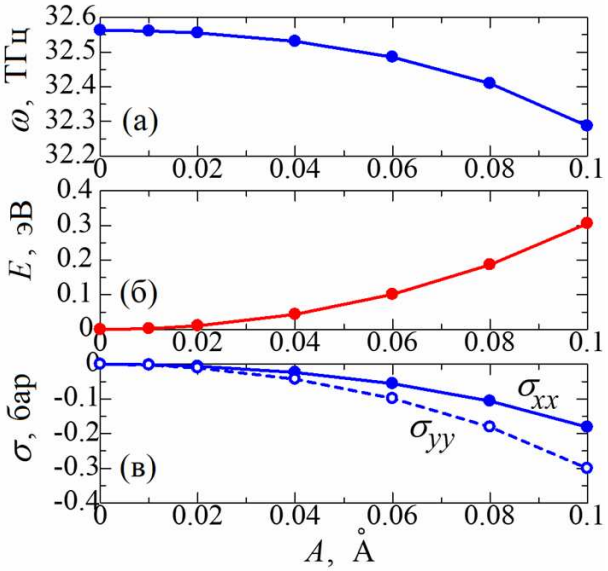

Fig. 2. Functions of the amplitude of the root mode of the ternary DNAM

As follows from the results obtained, the frequency of three-component DNVM decreases with increasing amplitude, that is, this mode has a soft type of nonlinearity. The DNVM energy is proportional to the square of the amplitude of the root mode. An increase in the amplitude of the root mode leads to an increase in the difference between the stress components σ_{xx} and σ_{yy}. Hence, it follows that the excitation of three-component DNVM destroys the isotropy of the elastic properties of graphene, which in the ordinary state is elastically isotropic. Anomalies in the form of the appearance of negative pressure upon excitation of three-component DNVM are not observed, since the pressure, defined as $p=-(\sigma_{xx}+\sigma_{yy})/2$, turns out to be positive at negative values of normal stresses. The results indicate that vibrations with an amplitude of $A<0.02$ Å can be considered small, since in this range of amplitudes, the effect of three-component DNVM on the properties of graphene is negligible, but becomes noticeable at large amplitudes.

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Семёнова Мария Николаевна – кандидат физико-математических наук, старший преподаватель, Северо-Восточный федеральный университет им. М.К. Аммосова, Якутск, Россия, mariya_semyonova86@mail.ru	**Semenova Maria Nikolaevna** – candidate of physical and mathematical sciences, senior lecturer, Ammosov North-Eastern Federal University, Yakutsk, Russia, mariya_semyonova86@mail.ru

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