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to be suitable for atomistic simulation to find the elastic moduli of grapheme structures on a wide scale ranges.

It is shown that in the frame of lattice statics approach to finding elastic moduli the homogeneous deformation of graphene monolayer transfers it into the non-equilibrium state. It is necessary to shift part of graphene atoms which form one of its "triangular" sublattices with respect to atoms of another sublattice in order to provide the sample minimum potential energy in a deformed state, while each sublattice is deformed homogeneously. Taking into account these inner displacements of graphene lattice allows obtaining more precise estimations of its elastic moduli. The exact expression for the vector of inner displacements depending on applied deformations is found.

Finding the values of parameters for the simplest Mie's family potentials is performed in order to find elastic moduli of graphene monolayers using lattice statics approach. The coincidence criterion of the experimentally determined Poisson's ratio with the estimated value is taken in order to select dimensionless power parameters of the Mie-type potential. It allowed obtaining more precise estimation of elastic properties in compare with variety of other potentials for carbon atoms.

For the aim of the crystal temperature control the computational-statistical approach to studying thermo-mechanical properties for finite sized crystals is presented. The approach is based on the combination of the high-performance computational techniques and statistical analysis of the crystal response on external thermo-mechanical actions for specimens with the statistically small amount of atoms (for instance, nanoparticles). The heat motion of atoms is imitated in the statics approach by including the independent degrees of freedom for atoms connected with their oscillations. Under non-zero temperature all elastic moduli of graphene monolayer are found to be closely coincided with the experimental values. These theoretical estimations are the most precise in compare with all other known computational results. Also we obtained that under heating graphene material response is nonsymmetric.

MAGNETISM AND DYNAMIC STABILITY OF CO, FE AND CR MONONITRIDES FROM FIRST PRINCIPLE CALCULATIONS

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Novel materials based on the transition metal mononitrides are of great interest for research from technological and scientific points of view due to their exceptional properties, ranging from superconductivity to hardness, high melting temperature and stability against corrosion. Most of transition metal nitrides

known up to day are formed by nonmagnetic metals and mostly tends to crystallize in the rocksalt (NaCl) structure, however the crystalline structure of equiatomic magnetic *3d* metal mononitrides is still under debates. For example, in earlier publications [1-3] it has been reported that CoN adopts either zinc-blend (ZnS) or NaCl-type crystalline structure depending on a method used to synthesize CoN. There is little published data on Fe and Cr mononitrides crystal and magnetic structure as well. The experimental data are rather controversial, and there is no general agreement between theory and experiment regarding compound ground state structure [4-6].

In this work we study structural, electronic, magnetic and dynamical properties of CoN, FeN and CrN phases in the framework of density functional theory and pseudopotential plane-wave method, as it is implemented in the Quantum Espresso code [8]. Exchange-correlation effects were treated by means of the generalized gradient approximation [9]. Phonon dispersion modes for different phases are obtained using the density functional perturbation method [10]. Our spin-polarized total energy calculations allow us to conclude that NaCl- and ZnS-type CoN phases are nonmagnetic. An influence of external pressure in ZnS-type CoN phase is found to be significant for dynamic stability. The results obtained from the lattice vibration analysis suggest that different FeN phases obtained experimentally for thin films can be explained as a substrate effect, as a results of the stress which occurs during the growth process, depending on the experimental conditions. Anti-ferromagnetic nature and lattice dynamic of CrN discussed as well.

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