Stability and electronic structure of C-B-N hexagonal 2D structures

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Two-dimensional materials such as graphene and hexagonal boron nitride continue to be under interest of scientist due to their very appealing properties. Putting them together in the form of an alloy opens new perspectives for materials engineering. B and N are natural dopants for carbon systems (*p*- and *n*-type respectively) and there are already many reports on doped graphene layers and more generally B-GL, N-GL, graphene-like B-C-N (or h-BN-GL) alloys. A fundamental issue for any alloy is to provide quantitative measure of ordering among constituent atoms and to quantify the alloy position between its extreme phases (completely random alloy or perfectly ordered crystal). Another important point is dependence of the alloy's electronic structure on the concentration of constituting elements.

In our previous studies, it has been shown that B_xC_{1-x}, N_xC_{1-x}, and $B_xC_{1-x-y}N_y$ alloys in honeycomb structure exhibit short-range order and deviate strongly from the random alloys. Presence of defects (edges, vacancies, 5-7 defects) changes locally abovementioned picture, mostly due to the higher possible local concentrations of B(N) atoms in the direct neighborhood of defects. However, overall picture of atomic correlations remains valid.

In the present communication, we report further, more detailed studies of the B-C-N structures. Through the studies of energetics, we aim to determine equilibrium configurations and positions of atoms substituting carbon in the lattice. This analysis is based on Monte Carlo (MC) calculations within the NVT ensemble (Metropolis algorithm) and the Valence Force Field (VFF) approach that allows for calculation of energies of big systems containing up thousands of atoms. We use Tersoff bond-order potential [1] for C, N, and B atoms as parameterized by Matsunaga [2]. Next we calculate the electronic structure of the studied alloys employing the tight-binding method. Recently, we have considered also small random displacements of atoms within the lattice to mimic the thermal vibrations, and therefore, the entropy effects. Taking into account random shifts of atoms in the MC simulations leads to very interesting results, especially in the structures with reduced periodicity (nanoribbons and nanoflakes) where one observes stabilization of the B-C-N systems with areas of slightly waved h-BN and graphene areas remaining flat. The behavior of binary alloys (graphene doped with B and N) becomes also more dynamic when atomic vibrations are considered. Specifically, B atoms tend to move out of GL plane as they have bigger dimensions than carbon atoms, and this behavior is even more pronounced near the structure edges and vacancies.

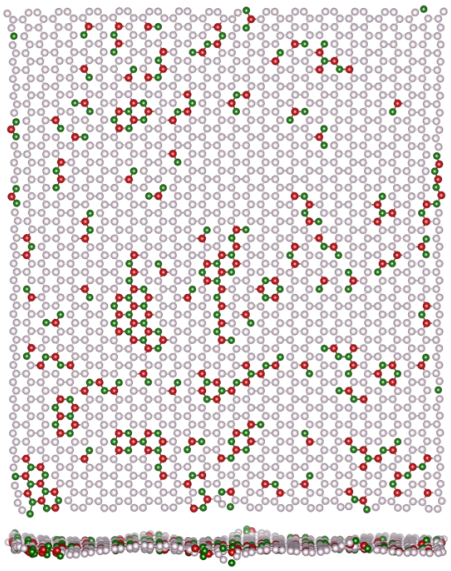

Fig. 1. Positions of C (grey), B (green), and N (red) atoms after simulations of nanoflake containing 1800 atoms with 10% B and 10% N, at 300K. Thermal vibrations of atoms were included in the MC simulations.

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[1] J. Tersoff, *Phys. Rev. B*, **37**, 6991 (1988).
[2] N. Matsunaga *et al*., *Jpn. J. Appl. Phys*. **39**, 48 (2000).