Short-range ordering effects in binary and ternary B-C-N two-dimensional hexagonal structures in the presence of defects

A. Jamroz[1] J. A. Majewski[1]
[1]Faculty of Physics, University of Warsaw, ul. L. Pasteura 5, 02-093 Warsaw, Poland

Boron and Nitrogen doped graphene layers constitute very important class of materials, mostly because B and N are natural dopants for carbon systems (p- and n-type, respectively). At higher concentration of dopants, one should actually consider such systems as binary or ternary alloys. A fundamental issue for any alloy is the degree of ordering among its constituent atoms and to quantify the alloy position between its extreme phases (completely random alloy or perfectly ordered crystal). In our previous studies, it has been shown that binary B_xC_{1-x} and N_xC_{1-x} layered alloys constituting ideal honeycomb lattice exhibit (at least for the dopant concentration x ranging from 0 to 0.5, and temperatures up to 1500 K) rather pronounced short range order and deviate strongly from the random alloys. For ternary $B_xC_{1-x-y}N_y$ alloys, we observed formation of boron nitride domains surrounded by pristine graphene areas, which also indicates presence of short range ordering phenomena. Furthermore, we started investigating behavior of abovementioned structures containing typical for graphene internal defects, such as single and multiple vacancies, 5-7 Stone-Wales defects, grain boundaries. We extent our studies also to the systems with reduced periodicity just considering the alloyed nano-ribbons and platelets. In the present communication, we report the detailed studies of short range order in binary B_xC_{1-x}, and N_xC_{1-x} alloys, and of ternary $B_xC_{1-x-y}N_y$ layered graphene based alloys containing defects and having full or reduced periodicity. Through the studies of energetics of the system, we determine first the thermodynamic equilibrium morphology of the studied systems and then we analyze short-range ordering, as quantified by the Warren-Cowley short-range order parameters. We focus on parameters corresponding to first, second, third and fourth coordination shell for each atom, that allow us to draw conclusions on the trends not only for nearest neighbors but also further relations within the lattice. This comprehensive analysis covers relevant range temperatures and is based on Monte Carlo (MC) calculations within the NVT ensemble employing Metropolis algorithm and Valence Force Field (VFF) approach to calculate the total energies of the of the system. We use Te rsoff like potentials for C, N, and B atoms with Matsunaga's parameterization [1]. We have also implemented into the computational algorithm the conjugate-gradient method to determine the equilibrium geometry. This turns out to be essential for systems containing edges and defects. To get reasonable statistics, we perform few dozen of Monte Carlo runs for each concentration of elements and temperature (with

up to $2 \cdot 10^5$ MC steps per run), and perform simulations for temperatures up to 1500 K. Generally, the simulations for defected structures confirm the existence of the short range order in alloys (at least up to 1500 K) and the finding that the mixed C-N and B-N bonds are favorable for all dopant concentrations up to 50 %. A number of noteworthy effects in the defects' area is observed, and suggests that breaking the lattice symmetry disturbs locally distribution of species, and additionally this may impact concentrations of atoms in the whole alloy structure.

[1] N. Matsunaga et al., *Jpn. J. Appl. Phys.* **39**, 48 (2000).