Monte Carlo studies of B-C-N graphene-like alloys: ordering phenomena in the presence of defects and lattice vibrations

Presenting Author: A. Jamroz
Co-Authors: J. A. Majewski
Faculty of Physics, University of Warsaw
ul. L. Pasteura 5, 02-093 Warsaw, Poland
agnieszka.jamroz@fuw.edu.pl

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 and combining advantages. There are already many reports on boron and nitrogen doped graphene layers and more generally B-GL, N-GL, graphene-like B-C-N (or h-BN-GL) alloys. It has become important class of materials, mostly because B and N constitute natural dopants for carbon systems (*p*- and *n*-type, respectively). 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).

In our previous studies [1], it has been shown that binary B_xC_{1-x} and N_xC_{1-x} alloys in honeycomb structure exhibit rather pronounced short range order and deviate strongly from the random alloys. For ternary $B_xC_{1-x-y}N_y$ alloys, we have observed formation of boron nitride domains surrounded by pristine graphene domains, which also indicates presence of short range ordering phenomena. Presence of defects (edges, vacancies, 5-7 defects) changes slightly 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, see e.g. Figure 1.

In the present communication, we report further, more detailed studies of short-range order in B_xC_{1-x}, N_xC_{1-x}, and $B_xN_yC_{1-x-y}$ layered graphene based alloy structures containing defects. Through the studies of energetics, we aim to determine equilibrium configurations and positions of atoms substituting carbon in graphene-like lattice. This comprehensive analysis covers relevant temperature range and is based on Monte Carlo (MC) calculations within the NVT ensemble (Metropolis algorithm). Valence Force Field (VFF) approach allows for calculation of energies of big systems containing up to 20 000 atoms. We use Tersoff bond-order potential [2] for C, N, and B atoms as parameterized by Matsunaga [3]. We develop algorithm to perform a number of swaps of atoms of different species, which leads to optimized configurations. Recently we involved also small simultaneous movements of atomic positions within the lattice to mimic the entropy effects, which lead either to lowering or increasing energy. Alternating both types of change within Monte Carlo simulations allows for better convergence to local (global) minimum of energy i.e. determination (meta-) stable state of the system.

References

[1] A.Jamroz, J. A. Majewski,, arXiv:1606.05548
[2] J. Tersoff, Phys. Rev. B, **37** (1988) 6991.
[3] N. Matsunaga *et al.*, *Jpn. J. Appl. Phys.*, **39** (2000) 48

Figures

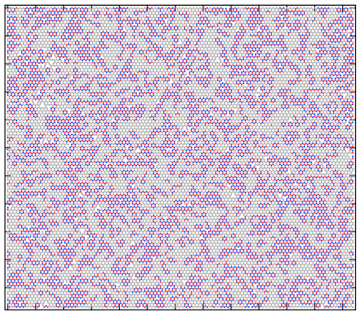

Figure 1: B-C-N system with 15%B, 15%N and 0.05% vacancies, after MC simulation in T = 500K.