Substitution solid solution from boron vapor saturated liquid carbon

Basharin A.Yu.[1,@] **and Dozhdikov V.S.**[1]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow, 125412, Russia

[@] a.basharin@jiht.ru

Liquid carbon saturated with dry boron vapor was experimentally obtained at laser induced process. It was established that vapor solution solidified as a graphite-like solid solution ($C\text{-}B_{SS}$) under conditions of diffusion inhibition at rapid quenching. However, at quasi-equilibrium process and absence of inhibition the vapor solution was solidified as B_4C. Atomic concentration of boron in $C\text{-}B_{SS}$ at rate 4.7% [1] enables recommending it as a precursor for boron-doped diamond at direct phase transition graphite to boron at HT-HP process. It is known that boron-doped diamond at $[B] > 1\%$ possesses superconducting properties under strong magnetic fields, but catalytic HT-HP process permitted only $[B] < 1\%$.

Atomistic modeling of the quenching was performed by molecular dynamics with a machine-learning potential and, therefore, identified $C\text{-}B_{SS}$ as a substitutional solution, where boron atoms replace carbon atoms in amorphized graphite. The explanation of the specific corrugated form of graphene layers was suggested. These are mechanical stresses caused by the pentagonal motif imposed by the introduction of a boron atom into the graphite lattice. The modeling of quenching was processed in the molecular dynamics package LAMMPS [2] with the GAP potential model [3], specifically developed for distinct molecular configurations involving B, N, C and they chemical species. The reliability of the potential was validated by comparing structural characteristics calculated using DFT-MD over a temperature range from 300 to 5000 K.

[1] Basharin A Y, Dozhdikov V S and Vasiliev A L 2024 *Vesnik Obedinennogo Instituta Vysokih Temperatur* **14** 36–39

[2] Plimpton S 1995 *Journal of computational physics* **117** 1–19

[3] Kaya O, Colombo L, Antidormi A, Lanza M and Roche S 2023 *Nanoscale horizons* **8** 361–367