Effect of boron on the structure of graphite formed at high pressure

Filonenko V P, Bagramov R Kh, Zibrov I P, Lyapin S G and Enkovich P V[@]

Institute for High Pressure Physics of the Russian Academy of Sciences, Kaluzhskoe Shosse 14, Troitsk, Moscow 142190, Russia

[@] enkovich@hppi.troitsk.ru

It has been experimentally established that high parameters (15-21 GPa, 1800-2500 C) are required for the direct transition of graphite to diamond without the use of catalyst metals. However, if the synthesis of diamonds is carried out not from pure carbon, but, for example, from hydrocarbons, then the thermobaric conditions of such a transition decrease. Boron is one of the interesting and promising alloying additions to carbon. Despite a large number of studies on the mechanisms of the formation of graphite-like structures, many questions still remain unclear. In my report I will present the analysis of boron graphite microcrystals obtained under high pressure and temperature conditions. The experimentally obtained diffraction patterns of boron-doped graphite demonstrate a structure with a high degree of ordering, which improves with increasing boron concentration. At the same time, the substitution of boron for carbon atoms leads to significant local distortions in the graphene layers, and the intensity of D and D 'peaks in the Raman spectra increases, which was noted earlier in [1]. The observed contradiction between the X-ray data and the Raman spectra is due to the fact that with an increase in the amount of boron in the graphene layer, the scattering of phonons by impurity atoms increases, while X-ray analysis gives only a general picture of the order. The refinement of the structure using X-ray data showed that the number of vacancies in graphene is higher than the amount of boron. Nevertheless, the answer to the question about the configurations of defect complexes of boron with vacancies requires further theoretical analysis. This work was supported by a grant from the Russian Science Foundation (No. 19-12-00111).

[1] Hagio T Nakamizo M and Kobayashi K 1989 *Carbon* **27** 259–263