CARBON UNDER PRESSURE AND RADIATION

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Structure behavior of different carbon modifications due to the specific volume change under high pressure ($\Delta V<0$) and reactor radiation ($\Delta V>0$) was investigated by means of the neutron and X-ray scattering. It was observed that at density decreasing the polyamorphic transition from the diamond-like amorphous structure to the graphite-like structure takes place. In the process the coordination number decreases and the electrical resistivity and hardness fall off. Stability of the graphite-like phase under pressure and temperature increasing was studied and a appearance of new crystal modifications was found as result of annealing. The modifications are different from the diamond and graphite structures [1].

Structural behavior of graphite after the reactor irradiation with big fluence was studied by neutron diffraction. Information on variation of the lattice spacings in dependence on the irradiation conditions was obtained. As a result of the data analysis the dependence of the lattice spacings ratio *c/a* on fluence and temperature was established. The *c/a* ratio appeared to grow with the value of fluence and descends with the growth of temperature. At the temperature above 500 ^{o}C the c/a ratio does not depend on fluence and corresponds to the initial value indicating the radiation annealing of defects.

As a result of comparison of the structural data after irradiation and under high pressure the dependence of c/a ratio on volume change was deduced. I was found that at the 3% volume change an amorphous phase appears in the structure of graphite. Graphite becomes completely amorphous at the relative volume change of 8%. Under high pressure the phase transition to lonsdeylite takes place at the relative volume change of 15%. Critical values of *c/a*, which indicate the structural instability of graphite, are determined. Under the irradiation the critical value of *c/a*=3.10 (increase by 13%), under pressure *c/a*=2.37 (decrease by 14%). So the graphite lattice looses stability at similar values of c/a regardless the sign of volume change.

An assumption on the conditioning of the radiation amorphization of graphite by softening (or zeroization) of the phonon frequencies at the volume increase during irradiation was made on the basis of phonon frequencies and elastic modules behavior at volume decrease (at high pressure) [2].

The equations of state of fullerenes and their hydrides under high pressure were studied and their connection with intermolecular potential parameters was recognized. The radiation amorphization of crystalline fullerenes C_{60} and structure changes at annealing were detected [3]. A appearance of amorphous fullerenes at ball-milling and increasing of their sorption properties at interaction with hydrocarbons and hydrogen was also observed.

So the combined study of structural behavior under pressure, irradiation and high temperature enables to make conclusions about structural stability in the wider range of thermodynamical parameters.

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References

1. S.S.Agafonov, V.P.Glazkov, V.A.Nikolaenko, and V.A.Somenkov. Short-Range Order in Irradiated Diamonds. JETP Letters 2005;81(3):122–124.
2. Ivanov A.S., Goncharenko I.N., Somenkov V.A. Changes of phonon dispersion in graphite at high pressure. High Pressure Research 1995; 14:145-154.
3. V.I. Voronin, V.P. Glazkov, B. N. Goshchitskiy et al. In: Abstracts of XVII Meeting on Use of Neutron Scattering in Studies of Condensed State (Gatchina, Russia, 2002), p.169.