## Phase transformations and P-T diagram of carbon at pressures up to 130 GPa

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Studies of the behavior of carbon at high pressures are most popular, this is associated not only with the conversion of graphite-diamond [1,2], but also with the discovery of fullerenes  $C_{60}$  and  $C_{70}$  [3], as well as with the synthesis of new structural forms. However, the equilibrium P-T-diagram has not changed in the last 50 years despite numerous theoretical and experimental works in this area. Moreover, practically none of the proposed phases obtained in various calculations did not find serious experimental confirmation.

This paper presents experimental data from studies of various forms of carbon at high pressures up to 130 GPa under conditions of shear and laser heating, including for <sup>12</sup>C and <sup>13</sup>C isotopes. The studies were carried out in diamond anvil cells for shear under pressure using the Raman spectroscopy method. After removal of the load, samples were also studied using HREM, EELS and other methods.

It was shown that under shear conditions, a direct transition to diamond is observed at pressures of p = 20-40 GPa and p = 100 GPa (T = 300 K), regardless of the initial structural form of carbon and isotopic composition. In the pressure range from 40 to 100 GPa, the initial graphite (nanotubes) are transformed into onions ("fullerene-like type"). During laser heating, single-crystal diamond (particle size 25 nm) under a pressure of 50–70 GPa [T> 3000 K] also turns into onions. As the pressure increases above 100 GPa, diamond becomes stable again.

This situation does not contradict thermodynamics, and under pressure (T = 0), a state with a lower specific volume and, as a result, less enthalpy should become stable. In our case, it may be onion carbon. Calculations using computer simulation confirmed this situation. However, is it possible to call it a bulbous carbon phase? This is an open question, if only because they themselves have a variable density at the nano level. In the case of macrovolumes, this material becomes isotropic. However, in the phase diagram of carbon, an instability region of diamond appears in the pressure range from 40 to 100 GPa (T = 300 K) and from 50 to 70 GPa (T = 3000 K). This situation is of interest for many reasons, in particular, it allows us to explain some of the problems of diamond synthesis in shock waves.

On the other hand, this indicates the parameters of the region of diamond synthesis in the earth's crust, and can also explain the behavior of carbon under such conditions and its interaction with other elements.

- 1. Bundy F.P.-J.Chem.Phys.,1963,v.38.p.618.
- 2. TonkovE.V.-Ponyatovsky, Phase transformations of elements under high pressure, 2005, CRC Press, LLC, p. 357
- 3. Kroto H.W., Heath J.R., O'Brien S.C., Curl R.E., Smalley R.E., 1985, Nature, 318,162.