NEW STRUCTURE AND HARDNESS OF CUBIC GRAPHITE

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In the last decade the new phases of carbon attract interest in the same level, as fullerenes and nanotubes. Among these new phases it is possible to mark C8, carbynes, cube graphite. Structure of cube graphite was proposed only recently, although this phase was synthesized about fifty years ago. A similar problem of determination of structures of new phases is ordinary for the new forms of carbon from their small mass yields, unlike, for example, nanotubes, the mass yield of which is relatively higher.

Aust and Drickamer [1] found the new phase in 1963 during transformation of graphite at high pressure. In 2004 we offered the structure of this phase on the basis of available data. The phase was indexed in the cubic system with the period of ~5.55 Å with the structure of LTA of zeolite [2].

In this report we propose the new structure of cubic graphite, namely as carbon KFI zeolite, by simulation and analysis of characteristic peaks of diffraction patterns. Optimized structure of the unit cell of KFI zeolite is represented on Fig.1, as calculated with the quantum chemistry method at the rhf/6-31g level of theory. A nanocluster represents the unit cell of this phase with sp^3-bonds.

The calculated unit cell equal to ~9.1 Å, density is 2.3 g/cm^3. The calculated diffraction patterns of KFI structure well correlates with the experimental one [1], if we replace reflexes 111 on 220, 200 on 310, 210 on 320, 211 on 400, 220 on 421, 221 on 422, 222 on 440, and 321 on 600. Thus, the new unit cell of cubic graphite equals to ~9 Å. Bond lengths equal to 1.54 and 1.58 Å in connecting squares, 1.53, 1.56, and 1.57 Å in prisms, angles equal to 90 and 135 degrees.

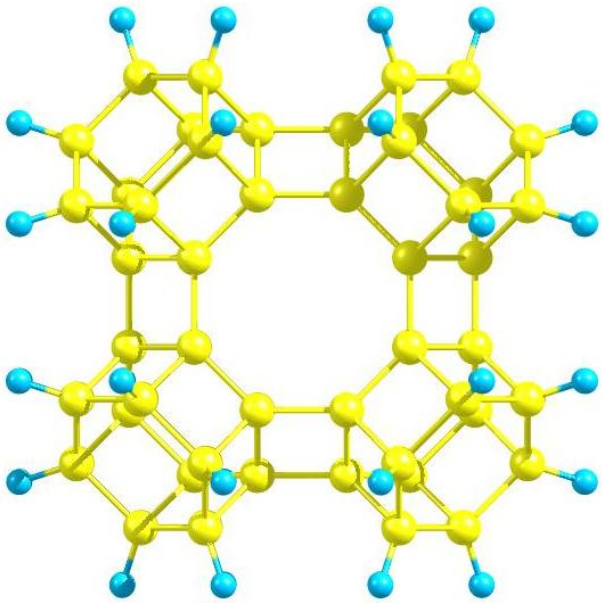

Fig.1 Nanocluster of KFI zeolite as the unit cell, where the atoms of hydrogen imitating periodical boundary conditions are shown with the circles of less sizes

Hardness is calculated by the formula of $120*\rho^{2/3}/d^{5/2}$, where ρ is the density, and d is the average bond length, and equals to about 70 GPa, that is few less than that of diamond (93 GPa).

Thus, the structure of cube graphite remains discussional and requires further systematic researches.

1. R. B. Aust, H. G. Drickamer, Science, 140, 817 (1963).
2. V.V. Pokropivny, A.V. Pokropivny, Physics of the Solid State 46, 392 (2004).