Structure of new form of super-hard carbon identified

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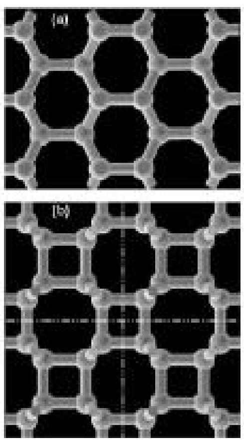

Views along [100]/[001], and [010] directions of 2x2x2 supercell of bct-Carbon,the dotted-dashed in (b) indicate the perpendicular graphene-like structure of bct-Carbon. Image credit: Xiang-Feng Zhou, http://arxiv.org/PS_cache/arxiv/pdf/1003/1003.1569v4.pdf

(PhysOrg.com) -- An experiment in 2003 formed what was believed to be a new form of carbon, but the findings were controversial. Now two teams of scientists have used different means to identify a three-dimensional network structure called "bct-carbon," which they say could have been the structure formed in 2003.

Pure carbon exists in a variety of structures, including graphite and diamond. The new structure, body-centered tetragonal carbon or bct-carbon, is unexpectedly simple and consists of sheets of squares of four carbon atoms each, joined by "short" bonds perpendicular to the sheets. This form of carbon is created when graphite is exposed to high pressure at normal temperatures.

It has been known for nearly 50 years that graphite subjected to cold compression (high pressure at ambient temperatures) undergoes a transformation that is reversible, and in 2003 researchers at Stanford University compressed graphite in a diamond anvil press, while simultaneously obtaining the x-ray diffraction pattern to help them study the bonds within the structure. They found that when the pressure exceeded 17 gigapascals (GPa) (170,000 atmospheres) the carbon atoms in the normally soft graphite formed a material hard enough to crack diamond, but its structure remained unclear.

Now a team of scientists led by Hui-Tian Wang of Nankai University at Tianjin, China, have shown through computer simulations that the super-hard carbon may be at least partly composed of bct-carbon, since this takes the least energy to form. Bct-carbon has a structure part-way between diamond's cubes of carbon atoms and graphite's linked sheets of carbon atoms in a hexagonal lattice. Bct-carbon consists of sheets of four-atom carbon rings linked together by strong bonds.

The team studied 15 possible structures and found the transparent bct-carbon not only required lower energies to form but that its shear strength is 17 percent greater than diamond's. If the results are confirmed, this means it may be possible to produce a material stronger than diamond at normal temperatures.

Another group of scientists, including Renata Wentzcovitch of the University of Minnesota and Takashi Miyake from the National Institute of Advanced Industrial Science and Technology in Japan, came to similar conclusions earlier this year, but by a different method. This group analyzed the proposed bct-carbon structure using quantum mechanical simulations. They found bct-carbon was more stable than graphite at 18.6 GPa, and that when mixed with M-carbon it would produce an x-ray diffraction pattern closely matched to that found in 2003. (M-carbon is a structure consisting of layers of carbon in rings of five and seven members.)

The paper from Hui-Tian Wang's team was published in the journal *Physical Review B*, while the US/Japan research was reported in *Physical Review Letters* in March this year.

More information:
-- Ab initio study of the formation of transparent carbon under pressure, *Phys. Rev. B* 82, 134126 (2010) DOI:10.1103/PhysRevB.82.134126

-- Body-Centered Tetragonal C_4: A Viable sp^3 Carbon Allotrope, Phys. Rev. Lett. 104, 125504 (2010) DOI:10.1103/PhysRevLett.104.125504