TRANSITION FROM GRAPHITE TO HEXAGONAL DIAMOND

by

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A new crystalline form of carbon-hexagonal diamond has been synthesized in the laboratory under conditions of static pressure exceeding about 130 kb and temperatures greater than 1000°C. The crystal structure is related to that of ordinary cubic diamond in the same way that the wurtzite structure is related to that of zincblende. The hexagonal unit cell has dimensions close to the values expected for regular tetrahedra with bond distance of 1.54Å, namely a = 2.52Å and c = 4.12Å. The density and hardness are essentially the same as for cubic diamond.

It is necessary for the synthesis of hexagonal diamond not only that the graphite be crystalline but that the c-axes of the crystallites be parallel to each other and to the direction of compression. Thus, pyrolitic graphites which satisfy these conditions as well as single crystal specimens yield hexagonal diamond. Graphites with random orientations of the c-axes do not. The formation of the new phase is accompanied by large increases in resistivity. The rise in resistivity is observed also at temperatures below 1000°C but then no hexagonal diamond is retrieved. It is not known whether at the lower temperatures hexagonal diamond is formed and reverts back to graphite upon release of pressure or whether the carbon is in a still different state.

X-ray diffraction studies of material prepared from single crystals of graphite reveal an interesting and unexpected epitaxial relationship between the graphite and the resulting hexagonal diamond. Although the hexagonal base cells are rather closely matched for both phases (a = 2.46Å for graphite and 2.52Å for hexagonal diamond) it is not a parallelism of (001) planes that occurs but instead the following orientation relationships:

(100) 11 (001) graphite

[001] 11 [210] graphite

or [010] 11 [010] graphite.

Thus, a buckling of the graphite planes appears to be involved in the formation of hexagonal diamond.

To date, the new phase has been made only in the form of very small crystallites (less than 0.1μ) and generally together with substantial amounts of cubic diamond, although some preparations appear to be predominantly hexagonal diamond. Typical specimens would seem to contain a considerable number of imperfections. The x-ray diffraction patterns do not, therefore, allow usually any great precision in the determination of lattice parameters or in a complete characterization of the specimen as to mature of imperfections, possibilities of polytypes, stacking disorders and the like. Nonetheless, continued investigation with a large variety of examples indicates now that the lattice parameter of hexagonal diamond may deviate from the "ideal" values associated with the presence of regular tetrahedra. Rather than the ideal values of a = 2.52Å and c = 4.12Å, more typical values are a = 2.50Å and c = 4.15Å (± 0.005Å), with c/a = 1.66 compared to 1.63 for the former.

Hexagonal diamond has been prepared in another laboratory (1) by intense shock compression and strong thermal quenching. Also, it has been discovered recently to be present to an appreciable extent in the Canyon Diablo meteorites (2).

1. Netherlands Patent Release No. 6506395, Nov. 22, 1965, E.I. du Pont de Nembars and Company.

2. R. E. Hanneman, H. M. Strong and F. P. Bundy, Science 155, 989 (1967).