

Experimental study on the graphite-diamond phase transition -Influence of local stress state and crystallinity of graphite

Hiroaki Ohfuji[1]

[1] GRC, Ehime Univ.

Direct conversion of graphite to diamond under static high-pressure and temperature has recently been investigated in detail (e.g. Irifune et al., 2003) and two different pathways are suggested for the phase transition process on the basis of the micro-textural analysis. One is a diffusion process, which involves nucleation and subsequent crystal growth of cubic diamond via diffusion of carbon atoms, and the other is a martensitic process where the transition proceeds by the rearrangement of atoms with maintaining the original structural framework of graphite. These two pathways result in the formation of different types of microtextures; in the former granular texture composed of euhedral crystals with random orientation is formed, whereas in the latter lamella structure made up of layered crystals stacked in the 111 direction (Sumiya and Irifune, 2005). Sumiya and Irifune (2005) reported that such graphite-diamond transition pathways may be controlled by the local stress state of graphite compressed to high pressures. In this study, to experimentally investigate the influence of local stress state in graphite under pressures on the graphite-diamond transition mechanism, a series of high-pressure experiments were conducted and the micro-structure of the recovered products were examined in detail.

High pressure and temperature experiments were conducted in a laser-heated diamond anvil cell. Highly oriented pyrolytic graphite (HOPG) sheet was used as a starting material. It was laser-cut into small pieces and placed in a pre-indented Re gasket so that (1) the graphite c-axis direction is oriented parallel to the compression axis of DAC and (2) the c-axis is perpendicular to the compression axis. No pressure transmitting media was used. The sample is compressed to pressures of 50-60 GP at room temperature and heated to 2000~2500 K using fiber laser (1072 nm). Experiments using polycrystalline graphite (0.5-2 μm) and finely-grinded graphite (10-100 nm) were also conducted. The quenched products were analyzed by SEM and TEM.

TEM observation of the samples synthesized by the parallel compression experiments showed that the original layered structure (lamella structure) of graphite is thoroughly preserved, but phases identified are mainly hexagonal and cubic diamonds and no or only small amounts of graphite is found. Detailed electron diffraction analysis revealed that coaxial relationships among graphite 002, hexagonal diamond 100 and diamond 111, which are all perpendicular to the layered structure, and between hexagonal diamond 001 and cubic diamond 111. The result clearly indicates that the martensitic phase transition from graphite to hexagonal diamond to cubic diamond is involved in the formation process. On the other hand, samples synthesized by the perpendicular compression showed a mixture of two types of microtextures, lamella structure and fine matrix. The former consists of layered hexagonal diamond and smaller amounts of cubic diamond, which are considered to have formed via martensitic process, whereas the latter consists mainly of fragmented hexagonal diamond with almost random crystallographic orientations. However, the evidence of diffusion transition pathway such as the formation of euhedral cubic diamond grains was not observed. On the other hand, the recovered products from experiments using polycrystalline graphite show granular texture composed of euhedral diamond particles with 20-30 nm in size and no lamella structure and hexagonal diamond phase were found, suggesting that the transition occurred via diffusion process. The result of the present study suggests that graphite-diamond phase transition process is controlled mainly by the initial structure (such as crystallinity and crystallite size) of the graphite rather than the local stress state in the graphite under high pressure. More details will be presented in the talk.