Experimental study on the phase transition of graphite to hexagonal diamond

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Hexagonal diamond (lonsdaleite) is a metastable polymorph of carbon and occurs as microscopic crystals associated with cubic diamond in some meteorites such as the Canyon Diablo meteorite. Recent theoretical studies reported a possibility that hexagonal diamond has indentation strength and a bulk modulus comparable to or even greater than those of cubic diamond. However, such physical properties of hexagonal diamond have not experimentally investigated due to a difficulty in synthesizing a single-phase bulk sample. Here, we investigated the P-T conditions required to obtain single-phase hexagonal diamond from graphite.

We performed a series of high-pressure and -temperature experiments using a laser-heated diamond anvil cell (DAC) at pressures of 25 and 50 GPa and temperatures ranging from 1400-3300 K. Highly oriented graphite (starting material) was compressed in a DAC without using a pressure transmitting medium and rapidly heated to a target temperature for ∼1 min using fiber laser. The sample became transparent upon laser heating above 2300 K at 25 GPa and above 1400 K at 50 GPa, suggesting that the phase transition of graphite to diamond phase(s) occurred under those P-T conditions. Interestingly, the transparent area became apparently smaller or almost disappeared (especially in the case of the experiments at 50 GPa) after decompression to room pressure.

The recovered samples were first examined by Raman spectroscopy for phase identification and then by transmission electron microscopy (TEM) for microtextural observations and electron diffraction analysis. The Raman spectra collected from the transparent area in the samples showed a broad peak at 1350-1450 cm⁻¹, but no cubic diamond peak (at 1332 cm⁻¹). TEM observation revealed that the transparent area in each recovered sample consists of hexagonal diamond with a layered structure similar to that of the graphite starting sample. The electron diffraction pattern collected from the sample is complex and can be interpreted as a superposition of three types of reciprocal patterns in which [100], [002] and [-212] of hexagonal diamond are all arranged in a coaxial relation with graphite [002]. This suggests that the martensitic phase transition from graphite to hexagonal diamond proceeds as a result of 1/2a or 1/3(1/2)a layer shifts of graphene layers along graphite [100].

Keywords: Hexagonal diamond, Highly oriented graphite, Laser-heated diamond anvil cell