Fluid driven *sp*^{3}-to-*sp*^{2} transformation in carbon at 1300K and 1GPa: experimental studies

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Although in materials science *sp3-sp2* transformations in carbon are well-studied by both laboratory experiments and *molecular dynamic* simulations, challenges still exist in understanding the mechanisms of diamond-to-graphite transformation in geological environments. Because the structures of diamond (*sp3-tetrahedral bonding*) and graphite (*sp2-trigonal bonding*) are very dissimilar, the reaction of diamond-to-graphite is slaggish because of existing kinetic barrier. Assuming that a fluid can be one of the more plausible factors to trigger *sp3-sp2* transformation, we conducted anhydrous and hydrous experiments in a piston-cylinder apparatus at T=1300K and P=1GPa, *t*=5hrs to transform synthetic diamond to graphite. Run products were studied with STEM, FIB, and Raman spectroscopy combined with SEM "in-situ". Powder of $Mg(OH)_2$ was added as the H_2O supply. Anhydrous experiments showed that there is no direct transformation of diamond-to-graphite at 1300K, 1GPa and t=5hrs. Hydrous experiments conducted at the same PT,t conditions, showed the formation of amorphous carbon, "globular carbon" particles, and tiny flakes of graphite which were nicleated at the {100} and {111} diamond surfaces. We conclude that sp3-to-sp2 transformation was triggered by a fluid and accomplished through the following processes:

(1) Diamond reacts with a supercritical H_2O (fluid) producing an intermediate 200-500 nm size "globular carbon" C_{2n}-H_n formed on the {111} planes of diamond. This is a metastable phase of carbyne. (2) Flakes of disordered graphite were crystallized during the decomposition of the metastable phase of carbyne due to re-organisation of its linear *sp*-bonds into more stable *sp*^{2} bonds (graphite).

The hydrous experiments illustrated the possibilities for synthesis of carbyne (hydrocarbone), a metastable phase, during diamond transformation to graphite. It suggested that intermediate metastable phase (hydrocarbon) is required for transformation from sp^3 C-bonds of diamond into sp^2 C-bonds of graphite, which fits well to Ostwald's Rule operating, as we see, also in many other high-pressure geological environments.