Detailed structure and stability of hexagonal diamond (lonsdaleite)

Akira Yoshiasa[1], Osamu Ohtaka[2], Tomoo Katsura[3]

[1] Earth and Space Sci., Osaka Univ., [2] Earth and Space Science, Osaka Univ, [3] ISEI, Okayama Univ.

Hexagonal diamond powders were synthesized using a large volume cell high pressure appalatus and the essential detailes of the structures were examined by Rietveld refinements in order to investigate the thermodynamic stability and the transition mechanism. Mass fraction of hexagonal diamond and cubic diamond was 50:50 for the products annealed between 800 and 1400 C. Higher temperature than 1600 C seem to favor the formation of cubic diamond or to commence the conversion from hexagonal diamond to cubic diamond. Structure refinements revealed that decrease and increase in the basal and the apical distances of C C bonds in hexagonal diamond are introduced by lowering the symmetry from cubic to hexagonal (Yoshiasa et al. (2003) Jpn. J. Appl. Phys.). Based on analogous features observed in the synthetic hexagonal diamond and lonsdaleite, the formation mechanism of lonsdaleite is proposed.