The 445th Geodynamics Seminar

Synthesis of a new cubic carbon nitride with a diamond-like structure

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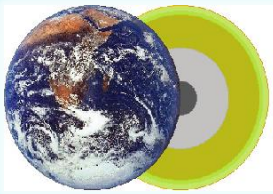

EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

Abstract

Carbon nitride is long believed to be harder material than diamond due to the short bond length of C-N. Generally, carbon nitride has the "C_3N_4" stoichiometry based on the atom substitution of the known A_3B_4 structure. Although there are many experimental studies by various methods in terms of the synthesis of "C_3N_4" compounds, these results are doubtful because of the small amount and heterogeneity of the products. Recently, a hydrogen bearing carbon nitride possessed the chemical formula of C_2N_2X (X= NH, CH_2) has been successfully synthesized under high-pressure and -temperature conditions using a hydrogen-containing starting material. This result indicates that carbon nitride stabilizes a C-N-H ternary compound in the presence of hydrogen.

Here in this work, a new cubic carbon nitride with a diamond-like structure is successfully synthesized using tetracyanoethylene (TCNE) as a hydrogen-free starting material. Phase relation of TCNE was investigated in 1980s-1990s, which revealed that TCNE has three polymorphs: cubic structure at LT, monoclinic structure at HT and amorphous phase at HP(-HT) conditions. Up to now, no further phase transition has been reported. In the present study, the phase transition to the new phase can observe at more than 53 GPa and 5000 K with a "flash heating". The unit cell is determined to be fcc structure with lattice parameter of a= 3.5124(2) Å, and the isothermal bulk modulus K_0 and its pressure derivative K'_0 are estimated to be 398(38) and 3.7(15), respectively, under nonhydrostatic condition. This value is comparable to the bulk modulus of cubic boron nitride (360-380 GPa). TEM examination shows that two crystalline phases can be observed: the new phase with ca. 1 μm in grain size and diamond with ca. 20 nm in grain size. Existence of diamond indicates the (partial) decomposition of the new phase under high pressure and high temperature conditions. In recent study of Stavrou *et al.*, an orthorhombic *Pnnm* CN has been synthesized at above 50 GPa and 7000 K with a reaction between graphite and nitrogen. Taking their and the present study into account, crystallization of 3D-networked carbon nitride requires very high driving force for overcoming a high kinetic barrier.

詳細は当センターホームページ: http://www.grc.ehime-u.ac.jp/をご覧ください
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