The 386th Geodynamics Seminar

Synthesis of carbon nitride under high pressure and high temperature, and the problems toward synthesizing super-hard phases of carbon nitride

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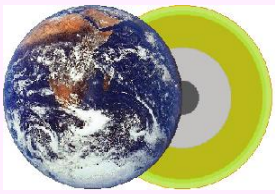

EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

Abstract

There have been considerable interests on carbon nitride (C_3N_4) since the theoretical calculation predicted that β-C_3N_4 is potentially harder than diamond (Liu and Cohen, 1989). In five polymorphs proposed by Teter and Hemley (1996), cubic-C_3N_4 has the highest bulk modulus, K_0 = 496 GPa, and is the most stable at high pressure. This phase can be synthesized at 12 GPa using graphitic-C_3N_4, which is stable at ambient pressure, as a starting material. Although many attempts were performed to synthesize a super-hard phase of C_3N_4, none of them has shown clear evidence of a crystalline phase of C_3N_4. On the other hand, Horvath-Bordon *et al*. (2007) reported that hydrogen-bearing carbon nitride $C_2N_2(NH)$, which has an orthorhombic structure, has been synthesized at 27 GPa and 1973 K using dicyandiamide as a starting material. Sougawa et al. (2010 - 2013) also showed that graphitic-$C_3N_4H_xO_y$ transformed to the orthorhombic phase with the chemical composition of $C_2N_2(CH_2)$, however, the lattice parameter has the large difference between experimental and theoretical data. In my study, graphitic-$C_3N_4H_x$ transformed to the hydrogen-bearing orthorhombic phase ($C_2N_2[(NH)_{6/7}, (CH_2)_{1/7}]$) which was stable up to 125 GPa and 3000 K (Kojima and Ohfuji, 2013). And also the annealed graphitic-$C_3N_{4.4}H_{1.8}$ changed to the orthorhombic phase at 30 GPa and 1800 K. As a result, ternary C-N-H system favors the orthorhombic framework included hydrogen under high-pressure and high-temperature, thus super-hard phases of C_3N_4 cannot synthesize unless hydrogen-bearing carbon nitride is used for a starting material.

Recently, several experiments using hydrogen-free carbon nitride have been conducted, but super-hard phases of C_3N_4 have not synthesized yet. In this presentation, I will talk about the phase relation and stability of carbon nitride under high pressure and high temperature, and the problems for the synthesis of super-hard phases of C_3N_4.

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