Geodynamics Seminar

第359回ジオダイナミクスセミナー

Structure and stability of carbon nitride under high pressure and high temperature

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主催：愛媛大学地球深部ダイナミクス研究センター
日時：6/7（金）午後 4時30分～
場所：総合研究棟 4F 会議室

Abstract

Since the theoretical calculation predicted that β-C_3N_4 potentially has superior hardness and elastic property to those of diamond, there are considerable interests on carbon nitride (C_3N_4). In five polymorphs predicted by Teter and Hemley (1996), cubic-C_3N_4 is predicted to have the highest bulk modulus (K_0= 496 GPa) and transform from graphitic-C_3N_4 (g-C_3N_4) above 12 GPa. Based on these theoretical calculations, many researchers attempted to synthesize such a super-hard phase of C_3N_4, but none of them claimed clear evidence for successful synthesis . Sougawa et al. (2010) reported that g-C_3N_4 transformed to an orthorhombic phase (a=7.635, b=4.487, c= 4.040 Å) at 40 GPa and 1800 K, but, the structure of the obtained phase is similar to that of hydrogen-bearing carbon nitride, $C_2N_{2(}NH)$. Our LHDAC study showed that g-C_3N_4 also transformed to a similar orthorhombic phase (a=7.6251(19), b=4.4904(8), c= 4.0424 (8) Å), although the C/N ratio of the recovered sample was measured to be 3:4, which is apparently different from that of the carbon nitride imide phase. The chemical composition might be expressed as $C_2N_2(NH)_{2/3}$ or $C_2N_2[(NH)_{6/7}, (CH_2)_{1/7}]$. These results suggest that in the studied wide pressure and temperature range, hydrogen-bearing carbon nitride favors the orthorhombic structure with a fundamental composition of C_2N_2X where NH, CH_2, and even potentially vacancies can be flexibly accommodated in the X site.

The result of the present study suggests that the theoretically predicted superhard C_3N_4 phases can likely not be synthesized in laboratory unless preparing hydrogen-free starting materials. So, we recently conducted an annealing experiments on the starting carbon nitride under N_2 and Ar condition and found that the anneal is indeed effective to remove hydrogen, although it also causes the amorphization of the graphitic framework of the starting carbon nitride. I will talk detailed results in this seminar.

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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