

# Geodynamics Seminar

## 第359回ジオダイナミクスセミナー

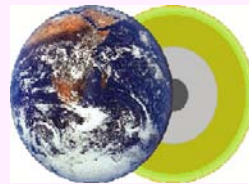
### Structure and stability of carbon nitride under high pressure and high temperature

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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  $\beta$ - $C_3N_4$  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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