Geodynamics Seminar

第333回ジオダイナミクスセミナー

Exploring stable structure for carbon nitride under high pressure and high temperature from experimental perspectives

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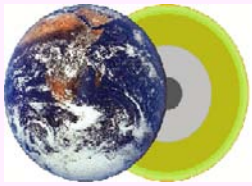
主催：愛媛大学地球深部ダイナミクス研究センター
日時：7/6（金）午後 4時30分～
場所：総合研究棟 4F 会議室



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Abstract

Carbon nitride (C_3N_4) has recently been studied extensively such as by shock and static high pressure and CVD experiments because of the increasing interest on its physical property as potential superhard materials. However, the phase stability and relation in the C-N system has yet been understood. We recently found that graphitic-C_3N_4 transforms to body-centered orthorhombic structure above 30 GPa and 1600 K based on in-situ XRD observations using a laser-heated DAC. The obtained cell parameters of the high pressure phase are a=7.625(2), b=4.490(1) and c=4.042 (1) Å at ambient condition. Interestingly, these cell parameters as well as the observed diffraction pattern are very similar to those of carbon-nitride-related materials such as $C_2N_2(NH)$ (Bordon et al., 2007) and $C_2N_2(CH_2)$ (Sougawa et al., 2010; 2012). However, our careful chemical quantification analysis revealed that the orthorhombic phase synthesized in our experiments has C/N ratio of 3:4, consistent with the ratio of the starting graphitic phase. Taking the results of the previous studies also into account, the orthorhombic structure could provide a flexible structural framework with substitutional C-X-C bonding (X= NH, CH_2, etc.). There is a possibility that our starting and synthesized materials also contain some amount of hydrogen (probably in the form of NH bonds), although it cannot be detected and quantified by the microprobe analysis we used.

In order to explore the stable structure for the pure C-N system, we are currently attempting to remove hydrogen (or hydroxyl) from the starting material. The method we choose for this is annealing of graphitic-C_3N_4 at 400 to 600 ° C in inert gas (Ar or N_2). The results obtained so far showed that with increasing annealing temperature, the crystallinity of graphitic-C_3N_4 becomes rather lower, while the amount of hydrogen decreases based on XRD and FT-IR analyses. The C/N ratio of the annealed products becomes closer to the stoichiometry of C_3N_4 with increasing temperature, indicating that the hydrogen has indeed been removed in the form of NH_3 from the structure of the graphitic C_3N_4. More details will be present in the 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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