Geodynamics Seminar

第307回ジオダイナミクスセミナー

The behavior of carbon nitride under high-pressure and high-temperature

Yohei Kojima

(Ph.D. Student, Ehime University)

主催:愛媛大学地球深部ダイナミクス研究センター

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Abstract

Since the prediction of β -C₃N₄, many researchers have found a strong interest in C₃N₄, which has high bulk modulus equal to or exceeding that of diamond. In five polymorphs reported by Teter and Hemley (1996), cubic-C₃N₄ has the highest bulk modulus and could potentially be synthesized from graphitic-C₃N₄ (g-C₃N₄) at 12 GPa in laboratory. Owing to these predictions, many of attempts were performed to synthesize a super-hard phase of C₃N₄ but none of them have yet shown distinct evidence for a form of crystalline C₃N₄. Ming et al. (2006) reported that although g-C₃N₄ was taken place a phase transition to an unknown high-pressure phase, this phase was transformed to a P-type cubic phase (a= 3.878(1) Å) at ambient pressure. This cubic phase was structurally different from the super-hard cubic phase (I-43I, a=5.3972 Å). Zinin et al. (2008) did an additional report for the cubic phase in multi-anvil apparatus; however, Fang et al. (2010) reported a decomposition of g-C₃N₄ despite the synthesis condition of such cubic phase.

In this seminar, I will talk about results of two series of experiments using in-situ XRD measurements and SEM-EDS and/or TEM analysis: (1) a new high-pressure phase ($Cmc2_1$, a= 7.625(2) Å, b= 4.490(1) Å, c= 4.042(1) Å) of C_3N_4 by no pressure transmitting experiments; (2) examining a reproducibility of Ming's report (using a g- C_3N_4 /NaCl mixture for pressure transmitting medium). The former set of experiments revealed that the orthorhombic phase had very close to an ideal C_3N_4 composition but was probably mixed in with hydrogen or hydroxyl because of using a low-crystalline starting material. In the latter, the P-type cubic phase mainly consisted of carbon and sodium, indicating that this cubic phase was not C_3N_4 .