The 415th Geodynamics Seminar

Phase relation on tetracyanoethylene under high pressure and temperature: For hydrogen-free carbon nitride

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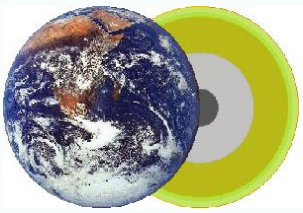

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Abstract

Carbon nitride (C_3N_4) is a potentially harder material than diamond on the basis of theoretical calculation. On the other hand, none of experimental reports have achieved a synthesis of C_3N_4 so far. In our previous study, it is revealed that carbon nitride take hydrogen in its structure to form an orthorhombic C_2N_2X (X=NH, CH_2). Thus, hydrogen-free carbon nitride is needed for synthesis of super-hard phases of C_3N_4. Tetracyanoethylene (TCNE, C_6N_4) is a candidate as a hydrogen-free starting material for C_3N_4. High pressure studies on TCNE have been conducted elsewhere, and it is known that there is a cubic phase at low temperature and a monoclinic phase at room temperature. However, high pressure and high temperature (HPHT) studies have been few.

In this study, we conducted HPHT experiments using TCNE as a starting material in laser-heated DAC. Firstly, TCNE compressed to ~30 GPa with SiO_2 thermal insulator was heated up to ~2000 K. The opaque sample was changed to transparent, suggesting that phase-change has been occurred. Two unindexed peaks in XRD profile appeared (d=~1.90 Å and 1.51 Å at 1 atm), and there is currently no suitable solution in terms of the lattice parameter for these. To estimate the bulk modulus K_0 of the unknown phase, $(d/d_0)^3$ can be approximated as V/V_0. The estimated K_0 is 386 ± 20 GPa, this value is higher than cubic BN (362 GPa). On the other hand, TCNE without thermal insulator at 30 GPa, 2000 K also changed to transparent, but XRD profiles show a broad peak (d= ~2.04 Å) and three weak peaks. These results suggest that new hard phase has been obtained, although TCNE seems to react with SiO_2.

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