Pure Phases of C_3N_4 Synthesized at High Pressure and High Temperature

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Since A. Y. Liu and M. L. Cohen predicted that beta phase of C_3N_4 may be comparable to diamond in hardness [1], and then D.M.Teter and R.J.Hemley predicted that cubic phase of C_3N_4 will be harder than beta phase C_3N_4 and a particular challenger to diamond [2], thousands of laboratories around the world launched into preparation of beta and cubic phase of C_3N_4 by use of various experimental metholds [3]. Unfortunately, they failed to get pure phases of C_3N_4 with stoichiometric ratio. We have obtained pure phases of graphite phase, beta phase of C_3N_4 synthesized from carbon-natrogen organic compounds as stating material with different catalysts under high pressure and high temperature. We also got beta phase and cubic phase of C_3N_4 starting from its graphite phase by use of laser heating method at high pressure and high temperature in DAC. Phase transitions from graphite phase C_3N_4 to beta phase C_3N_4, and from beta to cubic C_3N_4 under high pressure and room temperature have been investigated by XRD and electrical resistance measurement up to 104 GPa. A phase transition of C_3N_4 looks like an electronic phase transition from direct band gap to indirect band gap by ab initio calculation of energy band at 40 GPa.The physical properties of C_3N_4 will be reported in present paper.

References:

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