Prediction of Phase Diagrams for Hard Materials

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Hard materials and refractory materials are generally quite stable, which means not flexible as the other side of the stability. Diamond is a good example. These materials have high melting points, and the phase diagrams exhibit relatively simple structures; there is poor variety in the compound. For example, for B-C system, it is believed that only B_4C is a stable compound over the whole range of $B_{1-x}C_x$. However, recent progress of high-pressure experiments along with theoretical prediction by density-functional-theoretic (DFT) methods has disclosed rich of new structures, which attract attentions of material researchers. For example, a diamond-structure compound BC_5 has been recently discovered. Even for elemental boron crystals, a lot of stable and metastable structures are known. However, it is only recently that the phase diagram has been established. In the process of creating the phase diagram for boron, a new structure of g-phase has been discovered. See a recent review [1]. Now, we have to admit that hard materials are rich of material researches. This is because a lot of metastable phases are hidden behind the widely accepted phase diagrams. How to discover these hidden phases is one of the central issues for material research. In this paper, I like to describe our experience on the phase diagram of boron by theoretical approach. Hopefully, this gives a good guideline for efficient material researches. A combination of microscopic method of DFT and macroscopic approach of thermodynamics is an extremely powerful tool.

[1] K. Shirai, J. Superhard Materials, **32**, 205 (2010); **32**, 336 (2010).