Carbon and boron nitride materials: basic science and broader impact

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(i) On Earth circa 2025 significantly more natural graphite (G) than diamond (D) is mined/processed, and significantly more synthetic G than D is made. In metric tons: ~1,500,000 to ~24 (G to D, natural) and ~3,500,000 to ~3,100 (G to D, synthetic).
D&G are almost isoenergetic at 273K and 1 atm and the same is true for hexagonal boron nitride (hBN) and cubic boron nitride (cBN).
A pure carbon sample containing only D&G at chemical equilibrium would have 22 mol% D at STP and 34.5 mol% D at 2000K (per HSC Chemistry). ΔH_f of D at STP is about the same as ΔH_{vap} of liquid neon at its boiling point of 27K, and about 1/10 the enthalpy of an H-bond in liquid water. (We recall that graphite is the standard state at STP.)
My perspective: Kinetic control and not thermodynamic control dictates why it has been simpler to synthesize G than D at 1 atm pressure. And: (I suggest) that it is also kinetic control and not thermodynamic control that favors synthesis of D vs G in high temperature-high pressure (HTHP) synthesis in metal flux (pressure in the range 5 – 10 GPa; typically but not always, a seed crystal is used). Almost invariably the explanation for each case (e.g., in textbooks, the published literature, etc.) has been based on thermodynamics and I suggest this is “simply wrong.”
I discuss possibilities to synthesize D (please see [1]) in new ways. The parameter space for the elemental compositions of metal fluxes that might dissolve the needed amount of C (or for cBN the needed amount(s) of B and/or N) at ~1 atm pressure is very large per combinatorics and the relevant elements in the Periodic Table. Fortunately (for opportunities for basic science as well as technology) there is a great deal that is “not studied at all” about dissolution of carbon, phase equilibria, and other interesting issues, in many possible choices of metal fluxes.
I will, furthermore, discuss new ideas about establishing/controlling the spatiotemporal distribution of solute elements in metal flux, from “time = 0” onwards (as the metal flux/solute(s) system evolves, so to speak). With retrosynthesis (terms such as inverse design and/or inverse optimization are also apt) and kinetic control in mind, I foresee a new—and very promising— horizon for synthesis of diamond and cubic boron nitride.
(ii) The macroscale tensile loading mechanics of monolayer single crystal graphene (SCG) is presented. We have measured the Young’s modulus, strain at failure, and tensile strength, as a function of crystallographic orientation. SCG is grown on either single crystal Cu(111) or on Ni(111) foils, and ‘dog bone’ samples with gauge length of 10 mm and width 2 mm have been found to have remarkably high tensile strength values, which we suggest bodes well for applications, particularly for ‘lightweighting’ in space and aerospace, among others. An earlier version of this study (in progress) has been archived, please see [2]. Supported by the Institute for Basic Science (IBS-R019D1).

References

[1] Yan Gong, Da Luo, Myeonggi Choe, Won Kyung Seong, Pavel Bakharev, Meihui Wang, Seulyi Lee, Tae Joo Shin Zonghoon Lee, Rodney Ruoff. Growth of diamond in liquid metal at 1 atmosphere pressure. Nature. 2023, 629, 348-354.
[2] https://arxiv.org/abs/2411.01440v1