Potential super-hard phases and the stability of diamond-like $B_nC_m$ structures

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Metastable complexes of diamond structured B-C-N complexes are now established with the recent synthesis of the metastable material BC$_2$N[1]. The precursor to the BC$_2$N super-hard phase has a graphitic structure with the same stoichiometry. Claims that such a material is the second hardest material to date have inspired further studies of hard materials having a potential diamond-like structure and quite recently a B-C phase has been synthesized[2] and where an extreme hardness was also claimed.

The properties of some potential super-hard diamond like boron carbon phases are examined using ab-initio computational modelling. Both the bulk and shear modulus show a steady decrease with boron concentration. The electronic density of states suggest that each of the materials has a strong conducting character. Two specific phases, namely BC$_3$ and BC$_7$, are singled out and their possible graphitic precursor phases considered. Finally energies of the graphitic phases are related to the super-hard phases with the same stoichiometry.

References:
