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Low temperature phase transition predicted in the compound B13C2/B4C[1]

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The experimental phase diagram of boron-carbon exhibits the compound boron-carbide over a broad composition range that extends to low temperatures, in seeming contradiction to the third law of thermodynamics. First principles total energy calculations suggest the presence of two energy-minimizing structures in the boron-carbon phase diagram, B13C2 and B4C. Both distribute boron and carbon atoms on the same 15-atom rhombohedral unit cell (hR15), consisting of 12-atom icosahedra at cell vertices plus three-atom chains at cell centers. However, only B13C2 respects the rhombohedral symmetry, while B4C breaks the symmetry by replacing one of the icosahedral boron atoms with carbon. Because B4C is incompatible with the experimentally observed rhombohedral symmetry, it must lose thermodynamic stability at elevated temperatures. We report a study of the configurational ensemble obtained by substitution of boron or carbon on different sites using a semi-grand canonical ensemble. Varying chemical potential at low temperature, we find sharp transitions from beta-rhombohedral boron to B13C2 then to B4C and finally to graphitic carbon. Only the rhombohedral-symmetry phase B13C2 survives at high temperature while the symmetry-broken phase B4C loses stability around room temperature.

[1]In collaboration with Will Huhn