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Boron carbides from first principles[1] EMMANUEL BETRANHANDY, JELENA SJAKSTE, NATHALIE VAST, Laboratoire des solides irradiés Ecole polytechnique-CEA-CNRS — In this work, we focus on the understanding gained from the investigation of the physical properties of boron-carbides with theoretical methods based on density functional theory (DFT). Comparison of computed and experimental vibrational or NMR spectra has shown that the atomic structure of B_4C consists in C-B-C chains linking mostly $B_{11}C$ icosahedra, and a few percent of $B_{10}C_2$ icosahedra. In particular, C-C-C chains are excluded and can not be responsible for B_4C amorphization under shockwaves. In this work we find that at lower carbon concentration all models are metastable with respect to B_4C plus α-boron. This could explain actual difficulties in the synthesis of clean samples. Furthermore we discuss effects of temperature and/or pressure on stabilities and properties. Finally, the idea of combining high hardness and superconductivity in the same material by doping boron-rich solids has emerged. We show results on the strength of the electron-phonon coupling constant obtained with DFT-based methods in $B_{13}C_2$.

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