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Mechanical properties of icosahedral boron carbide explained from first principles ROMAN RAUCOULES[1], NATHALIE VAST, EMMANUEL BETRANHANDY, JELENA SJAKSTE, LSI - Ecole Polytechnique — An exhaustive DFT study of the structural defects of icosahedral B_4C and of their behavior under high pressure has been performed. Among the possible atomic structures, the lowest value of the formation energy has been found for the *polar* model B_4C^P, which consists of one distorted icosahedron and of one CBC chain. This result, together with the inspection of the vibrational and NMR spectra, has proved that B_4C^P is the proper structural model for B_4C.[1,2] Consequently, B_4C^P has been used as a matrix to isolate the defects. The native defects have been identified and shown to be energetically stable at high pressure. Most vacancy locations in B_4C^P are found to be energetically unstable and only a boron vacancy in the CBC chain is stable. A cluster of this vacancy is shown to induce a dynamical instability of the icosahedra when the pressure is increased. The dynamical failure of shocked B_4C [3] is attributed to the increase in the concentration of these unstable vacancies under plastic deformation. 1. R. Lazzari, N.Vast, J.M. Besson, S. Baroni and A. Dal Corso, Phys. Rev. Lett. 83 (1999) 3230. 2. F. Mauri, N. Vast and C.J. Pickard, Phys. Rev. Lett. 87 (2001) 085506. 3. T. Vogler, W. Reinhart and L. Chhabildas, J. Appl. Phys. 95 (2004) 4173.

[1]Membership pending

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