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Progress on Determining the alpha-beta Phase Boundary of Elemental Boron[1] TADASHI OGITSU, ERIC SCHWEGLER, LLNL — Recently, it was reported that the phase boundary between alpha-boron and beta-boron has been directly determined using high-pressure and temperature experiments down to P∼4GPa and T∼1400K [Scientific Reports 1, **96** (2011)]. Based on linear extrapolation of their results to lower pressure and temperature, these authors proposed that at P=0GPa alpha-boron is the stable form below about T∼933(20)K, in conflict with the recent theoretical works based on DFT total energy calculations [JACS **129**, 2458 (2007); PRB **77**, 064113 (2008); JACS **131**, 1903 (2009)], where it was concluded that beta-boron is the most stable at all temperature below melting temperature and down to zero Kelvin. At the talk, we show that the theoretical alpha-beta boundary obtained with a few approximations agrees well with the aforementioned experimental results within the error bars except for the lowest P, T point, and in this case, the ground state is still beta-boron [submitted]. We will also discuss on the recent experimental efforts in measuring the specific heat of boron allotropes that lead to a tentative conclusion supporting the aforementioned DFT results.

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