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High-density Modifications in Hydrogen-Rich Compound Diborane SERGE DESGRENIERS, Physics, U. of Ottawa, Canada, AKIO YOSHINAKA, Physics, U. of Ottawa, Canada, YANSUN YAO, Physics and Engineering Physics, U. of Saskatchewan, Canada, DENNIS KLUG, National Research Council of Canada — The study of dense hydrogen-rich compounds is regarded as a way to investigate pathways to metallic hydrogen. Compression of hydrides may lead to a metallic state at lower pressures than that required for hydrogen. Condensed diborane represents an interesting hydride as its high dipole polarizability yields to a prediction of a metallic state below 100 GPa. And, at lower density, theoretical results indicate the possible formation of complex molecular crystal structures, as a function of compression, comprising not only dimers of BH_3 (diborane) but also higher-order molecular assemblies, $(\text{BH}_3)_n$ with $n > 2$, and even polymeric chains. In this contribution, experimental results characterizing condensed phases of diborane, as obtained at high pressure at room temperature, are compared to predicted crystalline structures. Raman spectroscopy and x-ray diffraction with synchrotron radiation were carried out on single crystal as well as polycrystalline samples in diamond anvil cells for pressures up to 85 GPa. Results obtained at low pressures (< 4 GPa), across the liquid-solid phase boundary, indicate the existence of a phase with a crystalline structure different from that of the known b-phase ($P2_1/n$). Solid-to-solid transitions are observed at 6 and 14 GPa. The crystalline structures of the high-pressure phases, obtained by X-ray diffraction, are compared to molecular assemblies obtained theoretically. Finally, the possible metallization at high pressure is explored.

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