

Abstract Submitted
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Melting and phase stability of high-density beryllium ANDREA TRAVE, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, FRANCOIS GYGI, GIULIA GALLI, University of California, Davis and Lawrence Livermore National Laboratory — First-principles Molecular Dynamics calculations have been performed to determine the liquid vs. solid phase boundary for beryllium up to 250 GPa. Shock Hugoniot curves have been calculated for both solid and liquid beryllium in this range of pressures and temperatures to determine the shock melting onset conditions and pressure range of liquid-solid coexistence. The results of these simulations also provide insights on the problem of relative stability of various crystalline forms of beryllium at high temperature. This work was performed under the auspices of the US Department of Energy by the University of California at the LLNL under contract no W- 7405-Eng-48.

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