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Properties of MgO to 1.2 TPa from high-precision experiments on Sandia's Z machine and first-principles simulations using QMC and DFT

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MgO is a major constituent of Earth's mantle, the rocky cores of gas giants and is a likely component of the interiors of many exoplanets. The high pressure - high temperature behavior of MgO directly affects equation of state models for planetary structure and formation. In this work, we examine MgO under extreme conditions using experimental and theoretical methods to determine the phase diagram and transport properties. Using plate impact experiments on Sandia's Z facility a low entropy solid-solid phase transition from B1 to B2 is clearly determined. The melting transition, on the other hand, is subtle, involving little to no signal in us-up space. Theoretical work utilizing density functional theory (DFT) provides a complementary picture of the phase diagram. The solid-solid phase transition is identified through a series of quasi-harmonic phonon calculations and thermodynamic integration, while the melt boundary is found using phase coexistence calculations. The calculation of reflectivity along the Hugoniot and the influence of the ionic structure on the transport properties requires particular care because of the underestimation of the band gap and attendant overestimation of transport properties due to the use of semi-local density functional theory. We will explore the impact of this theoretical challenge and its potential solutions in this talk. Finally, understanding the behavior of MgO as the pressure releases from the Hugoniot state is a key ingredient to modeling giant impact events. We explore this regime both through additional DFT calculations and by observing the release state of the MgO into lower impedance materials. The integrated use of DFT simulations and high-accuracy shock experiments together provide a comprehensive understanding of MgO under extreme conditions. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.