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The phase diagram and transport properties of MgO from theory and experiment¹

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Planetary structure and the formation of terrestrial planets have received tremendous interest due to the discovery of so called super-earth exoplanets. 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 of these 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 its phase diagram and transport properties. Using plate impact experiments on Sandia's Z facility the 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. One issue of particular import is the calculation of reflectivity along the Hugoniot and the influence of the ionic structure on the transport properties. Particular care is necessary 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. The integrated use of DFT simulations and high-accuracy shock experiments together provide a comprehensive understanding of MgO under extreme conditions.

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