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Modeling Thermodynamics of High-Pressure Liquids with Application to MgSiO3 for Understanding Magma Ocean Evolution AARON WOLF, Earth and Environmental Sciences, University of Michigan, DAN BOWER, ETH, Zurich — Accurately modeling high pressure thermodynamic properties for liquids is challenging due to the intimate link between liquid structure and thermodynamics. In the geological sciences, this issue arises for the early formation stages of rocky planets. Cooling and crystallization of magma oceans are dominated by the thermodynamics of high-pressure silicate melts. Even first-order properties like adiabats and melting curves are poorly understood, with strong disagreements between studies [e.g. Stixrude 2005, 2009; Mosenfelder 2009; Fiquet 2010; Andrault 2011]. We develop a new equation of state for compressed liquids and apply it to MgSiO3 melt. The High-Pressure Rosenfeld-Tarazona (RTpress) model extends the original Rosenfeld-Tarazona EOS by coupling it to physical compression models. We fit a new MgSiO3 melt EOS based on molecular dynamics simulations [Spera 2011], and show that it compares well with first-principles simulations and shock data. The relative slopes of the melting curve and liquid adiabat determine the crystallization depth of the magma ocean. Our model produces highly concave melting curves, consistent with recent experimental analog studies of MgSiO3 glass compression [Petitgirard 2015], and support the more complex center-outwards style of crystallization.

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