The High-Pressure Structure of Silicate Melts and the Impact on Magma Ocean Evolution

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Abstract

The early evolution of terrestrial planets is strongly influenced by the high P-T properties of silicates liquids. Planets like Earth are expected to experience multiple giant impacts during accretion which bury tremendous heat sufficient to melt a significant fraction of the rocky mantle and produce deep magma oceans. From this initial molten state, the mantle cools and solidifies, but its evolutionary path is highly uncertain. This coupled thermodynamic and fluid dynamic process is highly sensitive to the thermophysical properties of both liquid and solid along the melting curve. The curvature and slope of the melting curve, as compared to the adiabatic profiles of the magma ocean, directly determine the depth of initial crystallization. Two competing endmember hypotheses argue that the mantle would crystallize from the bottom-up (e.g. Andrault et al., 2011) or the center-outwards (e.g. Stixrude et al. 2009), and resolving this puzzle requires a careful assessment of the properties of high pressure melts. We thus develop a new high-pressure equation of state (EOS) for liquids and combine it with a simple model for the structural degrees of freedom of silicate melts. Our new liquid-specific EOS, RTPress, gives a high-pressure extension of Rosenfeld Tarazona model. We apply this model to molecular dynamics (MD) simulations of MgSiO3 melt (Spera et al. 2011), and validate it against the experimental shock wave Hugoniot of enstatite glass (Mosenfelder et al. 2009). The magma ocean crystallization depth is obtained by comparing the adiabats given by our model with the mantle melting curve. There is not a current consensus about the shape of the deep mantle melting curve, with dramatic differences in the degree of curvature across experiments and simulations. To help resolve this issue, we adopt an independent thermodynamic approach of modifying the pure MgSiO3 melting curve to account for realistic mantle chemistry. The structure of these melts play a central role in determining their entropy, which directly influences the slope of the melting curve. By analyzing previous MD studies, we model the configurational entropy effect on the shape of the mantle liquidus. The non-negligible curvature of the resulting liquidus is shown to favor center-outwards, rather than bottom-up, crystallization.

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