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Analytic multiphase equation of state for MgO O. HEUZE, Commissariat a l.Energie Atomique, D.C. SWIFT, Lawrence Livermore National Laboratory, N.D. DRUMMOND, University of Lancaster, R.G. KRAUS, Harvard University, G.J. ACKLAND, University of Edinburgh — MgO is an important prototype and end-member constituent for the mantle of rocky planets. Planetary structures and the response to impacts depend on the equation of state (EOS), notably including any phase transitions. MgO adopts the B1 crystal structure under ambient conditions, and has been predicted to change to B2 under compression. There are large variations in theoretical predictions of this transition and of the conditions for shock melting; experimental observations are inconsistent or unclear. We have previously constructed equilibrium B1-B2 EOS for MgO, in tabular form, using ab initio electronic structure calculations based on density functional theory and the quasiharmonic approximation for lattice vibrations. Here, we use our new formalism for thermodynamically-complete Mie-Grueneisen EOS to construct an analytic, multiphase EOS for MgO. We also constructed an approximate liquid EOS as a perturbation of the B1. We investigated the effect of phase change kinetics, including an asymptotic case in which the Maxwell construction is omitted. The principal shock Hugoniot calculated using kinetics appears to agree closely with pressure-temperature states measured for a decaying shock, corresponding to the B1-B2 region of the EOS.

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