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Equation of State Model for Delocalization of 4f Electrons in Ce

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The elemental metal Ce has an isostructural phase transition under pressure, from the low density γ phase to the high density α phase, with a line of first order transitions terminating at a critical point. This leads to anomalies under dynamic compression such as large dissipative heating and non-monotonic variation of the bulk modulus with pressure. The transition is generally understood to be associated with delocalization of the 4f electron states. The thermodynamics of the low density γ phase are accurately described by a combination of phonons, itinerant electrons, and a local 4f electron on each atom. The 14-fold degeneracy of the 4f state is broken by a ~ 260 meV spin orbit splitting and a ~ 17 meV crystal field splitting. I will describe our EOS model, which allows for a continuously varying degree of localization as a function of compression. I will show comparisons with static and dynamic data. Finally, I will comment on the prospects for an analogous phase transition in the liquid.