Abstract Submitted
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An improved multiphase equation of state for beryllium GREGORY ROBERT, ARNAUD SOLLIER, PHILIPPE LEGRAND, CEA/DIF — In our previous articles on beryllium (1)(2), a new theoretical phase diagram with three phases (hcp+bcc+liquid) of beryllium has been proposed : - Melting curve is obtained from quantum molecular dynamics (QMD) calculations along isochors. - Using phonon densities of states and a quasi-harmonic model, solid-solid transition is modeled. Our attempt to construct a three phases equation of state (EOS) failed due to our representation of the liquid phase based on Wallace's approach with the bcc phase, instable at low pressure, as reference. Here, we propose to deal with the instability of bcc phase at low pressure and the discontinuity of physical properties at melting. We also present an improved three phases (hcp+cc+liquid) EOS using simple analytic model constrained by the QMD calculations for the liquid. (1) G. Robert and A. Sollier, J. Phys IV 134, 257 - 2006. (2) G. Robert, A. Sollier and Ph. Legrand, to be published in APS-SCCM, June 2007.

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