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Multiphase EOS development at LLNL – improving EOS fidelity by collective knowledge of experiment and theory: the cases of Beryllium & Gallium[1] CHRISTINE WU, CARRIE PRISBREY, JOEL VARLEY, Lawrence Livermore Natl Lab — Equation of state (EOS) describes how materials respond to changes in energy, pressure, density, and temperature. The availability and quality of EOS are vital for achieving realistic hydrodynamic simulations. Over the past few years, we have successfully developed an object-oriented multiple EOS generation code (MEOS) at LLNL, which substantially reduces turn-around time in multiphase EOS generation, and provides a wide collection of EOS models. With this new tool, we began an accelerated effort at LLNL to develop global EOSs in the multiphase representation. First, we started with the metals of Beryllium (Be) and Gallium (Ga). Be is a potential ablator material for NIF experiments, and Ga has an unusual liquid phase that is denser than the Ga-I solid phase leading to a melt line of negative slope near ambient conditions. Recent dynamic experiments at Z also show interesting features of phase transitions in Ga. In this work, we present our construction of the baseline multiphase models for Be and Ga utilizing the collective knowledge of experiment and first principle's DFT calculations. In addition, we will discuss our preliminary effort to assess EOS uncertainties, in particular our study of DFT uncertainties due to the choice of exchange-correlation functions.

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