Tabular Multiphase Equation of State for Plutonium

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The dynamical behavior of a material can be significantly impacted by the effects of transformations from one phase to another. Not only do such transitions introduce latent heats and volume changes that can be sizable, but aspects of material behavior such as strength can be phase-dependent as well. The equation of state (EOS) of a material should indicate the equilibrium phase in any situation, so the production of multiphase EOS which provide phase boundaries and phase-specific thermodynamic information is of some interest.

The importance of including these effects is shown in Fig. 1, which includes various thermodynamic curves for tin as functions of pressure and temperature. The light blue dots indicate the phase boundaries as determined by SESAME 2161, a multiphase EOS for tin constructed recently [1]. The three solid lines are the principal Hugoniot (black) and two release isentropes (blue and red) determined by the same EOS; the three dashed lines are the same three curves as determined by SESAME 2160, an older tin EOS that does not treat the solid-solid transition. The blue isentropes terminate in the solid at zero pressure, while the red isentropes terminate in the liquid at that same pressure. Notice that the two principal Hugoniots are rather similar; in effect, the old EOS averages over the shifts in the Hugoniot that the new EOS attributes to the crossings of the phase boundaries. The isentropes, on the other hand, are quite different, and as a result the two EOS give rather different predictions for the phase the system will relax into after a single shock. The old EOS predicts that the system will relax to pure solid after shocks below approximately 20 GPa and to pure liquid for shocks above about 27 GPa; after intermediate shocks the system will relax into a mixed solid-liquid state. The new EOS also places the lower limit at about 20 GPa, but the upper limit is much higher, at about 36 GPa. It is the inclusion of effects such as latent heat that significantly changes the isentropes, as the figure clearly shows, and thus the predictions for shock release.

We are currently using the multiphase techniques previously applied to tin to create a new EOS for plutonium. We have obtained model parameters for different phases of plutonium from experimental data and first principles calculations, and we have compared the results with additional experiments, leading to new predictions concerning the high-pressure phase diagram. Anomalous properties of the liquid have proved difficult to model consistently, and improving the liquid EOS will be a high priority for subsequent work. Details may be found in [2].

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[1] Greeff, C.W., et al., "SESAME 2161: An explicit multiphase equation of state for tin," Los Alamos National Laboratory report LA-UR-05-9414 (December 2005).
[2] Chisolm, E.D., et al., "Tabular Multiphase Equation of State for Plutonium (U)," Los Alamos National Laboratory report LA-CP-06-1365 (December 2006), to be published in *Proceedings of the Nuclear Explosives Code Developers Conference* (Los Alamos, New Mexico, October 23–27, 2006).

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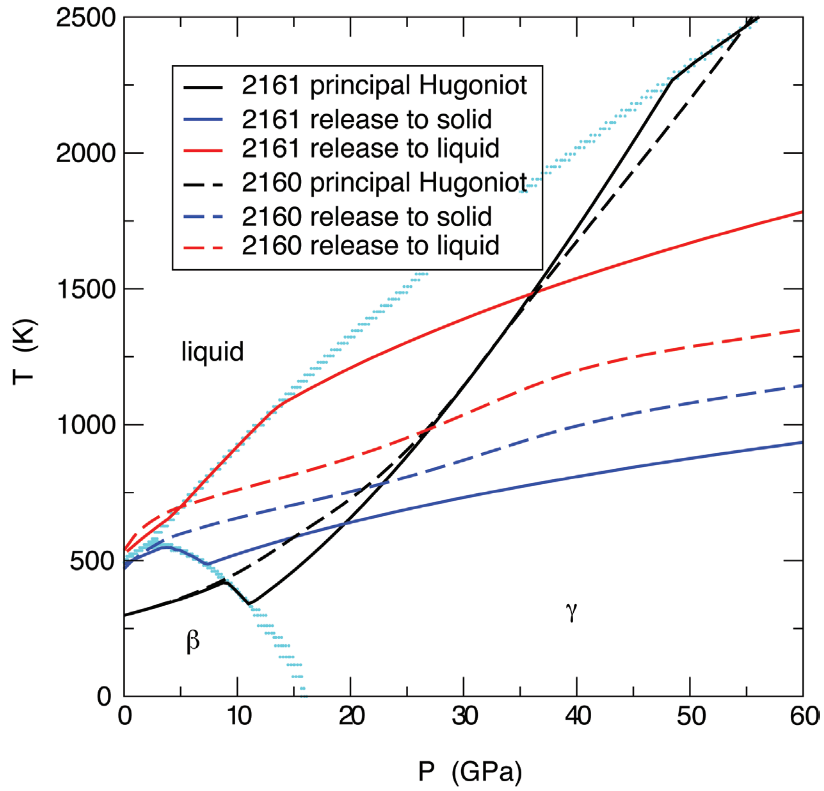

Fig. 1.
Predictions for shock release to pure solid and pure liquid for SESAME 2161 compared to SESAME 2160. Please see the text for detailed explanation.