A Sample of Some New Equations of State

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Recently, we have been exploring several different categories of materials: metals, glasses, liquids, and ceramics. By using electronic structure calculations and the best experimental data available to guide our standard Equation of State (EOS) models, we have created new baseline EOS and made improvements on existing EOS. Some of the materials include baseline EOS such as gallium and boron, for which no SESAME table existed, and improved EOS such as boron carbide, lithium fluoride, and vanadium.

Gallium melts slightly above room temperature and has three known solid phases. A new EOS was created by using theoretical calculations and published parameters, which reproduce two of the three solid phases and the liquid phase of the EOS. Figure 1 illustrates how well the new EOS predicts the shock response of the liquid. It is also in agreement with preliminary quantum molecular dynamics (QMD) simulations of Stephane Mazevet, formerly of T-4.

The boron and boron carbide EOS were created in parallel. Both materials exhibit high strength along with other similar characteristics. These EOS were created uniquely to compensate for the strength effect in the shock data. Figures 2 and 3 illustrate the shock response of the new EOS compared with the data.

The new vanadium EOS is similar to the older SESAME EOS at moderate compression, but the Hugoniot for the new EOS agrees much better with the shock data at higher compression than its predecessors (Fig. 4). This new EOS also takes into account melting, for which it correctly reproduces the available melt data.

The final example, lithium fluoride, is used as a window for VISAR measurements in shock experiments. The new EOS was created using a similar process as the gallium EOS. This new EOS Hugoniot matches new shock data from Sandia National Laboratories, which ranges from two to ten Mbars in pressure. Figure 5 compares this new EOS with the older shock data, QMD calculations, and a previous SESAME table.

In summary, with every new theoretical development and new data from EOS experiments we continually improve SESAME EOS database.

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[1] S. Crockett and L. Burakovsky, "Gallium Equation of State (SESAME 2370)," Los Alamos National Laboratory report, LA-UR-06-8390 (2006).
[2] S. Crockett, "Creating New Equations of State for High Strength Materials (Boron and Boron Carbide," Los Alamos National Laboratory report, LA-UR-06-8402 (2006).
[3] S. Crockett and S. Rudin, "Vanadium Equation of State (SESAME 2552): A Comparison of Old and New SESAME Tables," Los Alamos National Laboratory report, LA-UR-06-8389 (2006).
[4] S. Crockett and S. Rudin, "Lithium Fluoride Equation of State (SESAME 7271)," Los Alamos National Laboratory report, LA-UR-06-8401 (2006).

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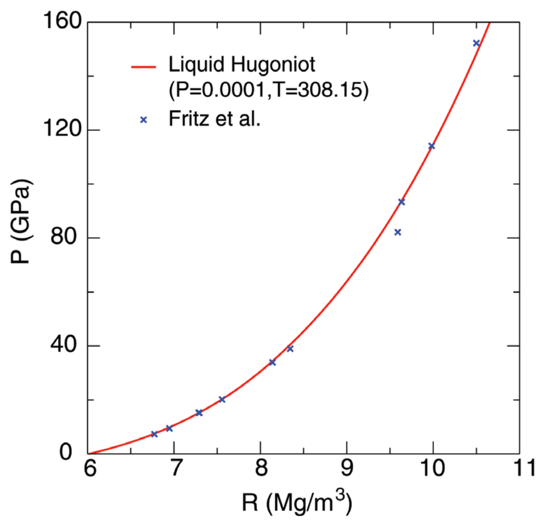


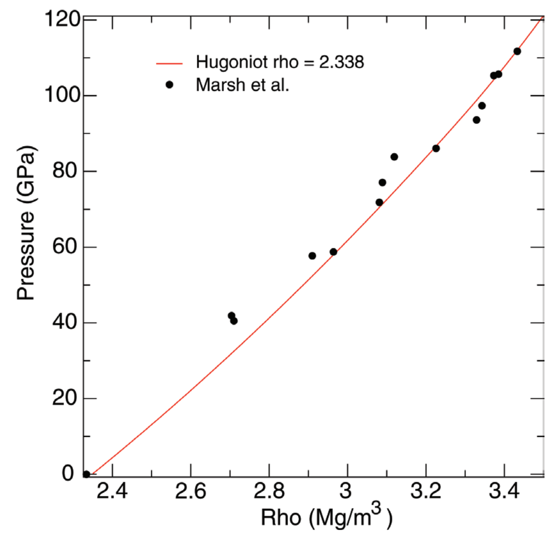
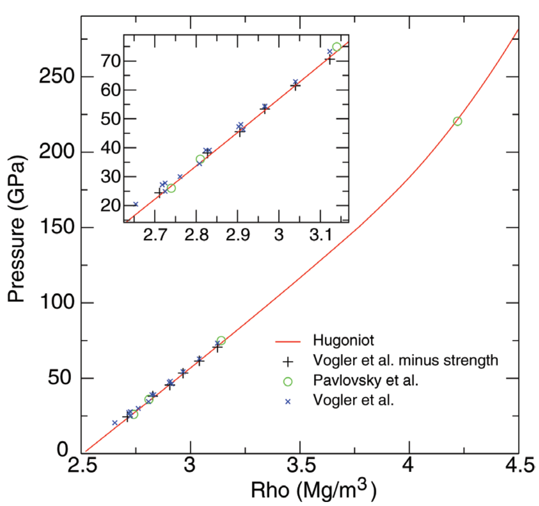


Fig. 1. Left
A gallium pressure Hugoniot compared with shock experiment [1].

Fig. 2. Right
A boron pressure Hugoniot compared with shock experiment [2].



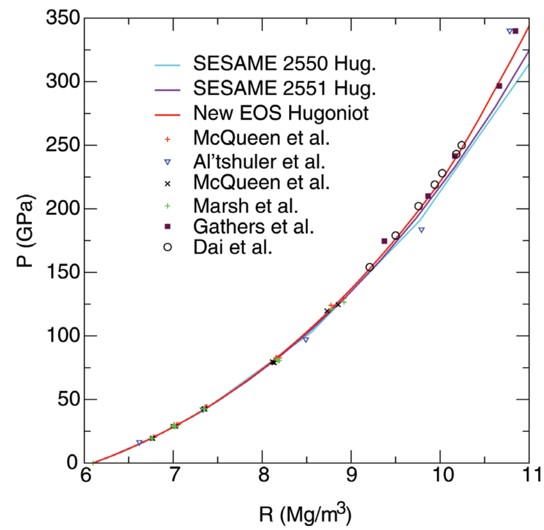


Fig. 3. Left
A boron carbide Hugoniot compared with shock experiments [2].

Fig. 4. Right
A vanadium Hugoniot compared with older EOS and shock xperiments [3].

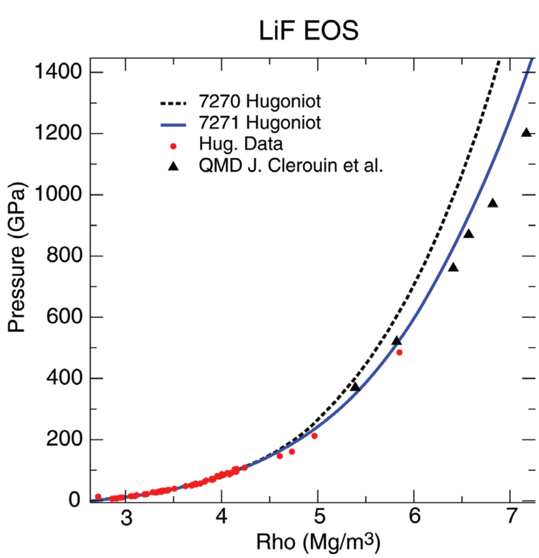


Fig. 5.
A lithium fluoride Hugoniot compared with QMD simulations, an older EOS, and older shock experiments [4].