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An highly accurate semi-analytical EOS along Hugoniot curves

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Recent rapid development of shock compression technology has revealed many exciting properties of geologic materials under highly shock-compressed states. A number of very sophisticated thermodynamics-based equations of state (EOS), such as SESAME and M-ANEOS, have been developed. These numerical EOS codes, however, use many model parameters to reproduce experimental data. Thus, it is difficult to find the optimum model parameters uniquely, requiring extensive experiments covering a wide range of thermodynamic conditions.

Such complex EOS's have widely been considered necessary because physics behind the EOS of highly shock-compressed geologic materials is very complicated. In fact, recent experimental result using high-power laser have revealed further intricate properties of silicates under high compression conditions, such as large departure of isochoric specific heat Cv from Dulong-Petit limit due to molecular dissociation and ionization . In order to incorporate such complex properties into a thermodynamics-based EOS properly, physics behind these materials needs to model well.

Such thorough understanding of material properties is essential for building a versatile EOS for hydro-code calculations. However, many planetary applications requires only thermodynamic properties along Hugoniot compression curve. For example, estimation of the fractions impact melt/vapor and the final molecular composition of impact vapor plume requires only the entropy gain due to initial impact shock. In this study, we propose a semi-analytical formula of on-Hugoniot EOS derived from the differential form of Rankine-Hugoniot equation and compare it with conventional EOS's and experimental data.

Most condensed matter under shock compression is known to follow the linear velocity relation between particle velocity Up and shock velocity Us:

Us = Co + s Up, (1)

where Co, and s are bulk sound velocity and a constant, respectively. This relation is known to hold for a variety of materials over a wide range of impact velocity. Despite the wide applicability of this relation, most EOS's do not take advantage of this relation. Besides the Up-Us relation (1), we use only general thermodynamic relations, the differential form of Rankine-Hugoniot relations, and Gruneisen EOS. From these relations, we obtain ordinary differential equations for temperature T and entropy S.

For extremely high-pressure shocks, Cv is not approximated by a constant value well; it may become well above Dulong-Petit limit. The effect of specific heats can be calculated easily with our new EOS. Although there is good agreement among different EOS's at relatively low shock pressures (~150 GPa), different EOS's yield significantly different results at higher shock pressures (several hundred GPa). This scatter results from the fact that there are not many experimental data available in the higher shock pressure range. Under such conditions, our EOS is useful because it does not require many data points to make accurate predictions along a Hugoniot curve. It can also be used as an anchor for the more sophisticated EOS for Hugoniot conditions.

Furthermore, because Cv is a very important property to characterize condensed matter, the capability to derive Cv from temperature data is very useful. A couple of examples of comparisons between our recent experimental data and our EOS predictions are obtained. The quartz data at 150 GPa requires Cv significantly larger than 3R, but the shock temperatures of diopside at ~300 GPa is consistent with the Dulong-Petit value. Such difference in Cv among different silicates is of great importance in planetary science.

Keywords: shock compression, High pressure EOS, hypervelocity impact