AN HIGH-PRECISTION SEMI-ANALYTICAL ON-HUGONIOT EOS FOR GEOLOGIC MATERIALS.

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Introduction: 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 [1] and M-ANEOS [2], 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 C_v from Dulong-Petit limit due to molecular dissociation and ionization [e.g., 3,4]. 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 hydrocode 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.

Furthermore, when a new range of shock pressures is explored, thermodynamic measurements are usually very limited. Also, the vast majority of shock compressed EOS data are taken only along Hugoniot curves. However, many thermodynamic data including both on-Hugoniot and off-Hugoniot conditions are needed to revise sophisticated EOS's accurately. Such revisions often take time and have to wait for data accumulation. Nevertheless, when new experimental data are obtained, one would wish to examine the significance of such new data promptly. Thus, a simple EOS that works only on Hugoniot curves but can describe the experimental data accurately would be very useful for shock compression experimental data analysis.

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.

Analytical Formulation: Most condensed matter under shock compression is known to follow the linear velocity relation between particle velocity U_p and shock velocity U_s:

$$U_s = C_o + s\, U_p, \qquad (1)$$

where C_o, 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 [5]. Despite the wide applicability of this relation, most EOS's do not take advantage of this relation. One of the few exceptions is the analytical EOS by Tillotson [6]. It is simple and accurate (for compression) and has been used widely. However, it is not thermodynamically self-consistent and cannot calculate entropy gain due to shock heating.

Besides the U_p-U_s relation (1), we use only general thermodynamic relations, the differential form of Rankine-Hugoniot relations, and Grüneisen EOS.

From these relations, we obtain ordinary differential equations for temperature T and entropy S:

$$\frac{dT}{dU_p} = C_o \Gamma_o T \frac{\left(U_s - U_p\right)^{q-1}}{U_s^{q+1}} + \frac{sU_p^2}{C_v U_s} \qquad (2)$$

$$\frac{dS}{dU_p} = \frac{sU_p^2}{TU_s} \qquad (3)$$

Density and pressure can be obtained with frequently used analytical solutions for Hugoniot curves:

$$p = \rho_o U_s U_p, \quad \rho = \rho_o \frac{U_s}{U_s - U_p}. \qquad (7)$$

Then, all the basic thermodynamic variables can be calculated for Hugoniot without having knowledge of an off-Hugoniot EOS. This EOS needs only six model parameters ρ_o, C_o, s, C_v, Γ_o, and q.

Experimetal Validation: We compared the results of our calculations and literature values in order to examine the validity of the new on-Hugoniot EOS,.

Fig. 1 compares our EOS and ice shock experiment data with single-stage powder gun [7]. Because all the parameter values are well established, there is no room for adjustment for fitting. However, the comparison indicates that our semi-analytical EOS can reproduce shock temperature and entropy very well.

Our semi-analytical EOS are alo compared with shock data of both diopside and quartz obtained by 2-stage light-gas gun [9,10] (Fig. 2). The shock temperatures measured around 150 GPa are well reproduced by our EOS with Dulong-Petit assumption.

These good reproductions of well-established shock temperature data and entropy estimates support the validity of our new EOS for Hugoniot conditions.

Planetary-Velocity Impacts: For extremely high-pressure shocks, C_v is not approximated by a constant value well; it may become well above Dulong-Petit limit [e.g., 3,4]. 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) in Fig. 2B, different EOS's yield significantly different results at higher shock pressures (several hundred GPa) [4]. 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 C_v is a very important property to characterize condensed matter, the capability to derive C_v from temperature data is very useful. A couple of examples of comparisons between our recent experimental data and our EOS predictions are shown in Fig. 2. The quartz data at 150 GPa requires C_v significantly larger than $3R$, but the shock temperatures of diopside at ~300 GPa is consistent with the Dulong-Petit value. Such difference in C_v among different silicates is of great importance in planetary science.

Planetary Applications: Perhaps, the most important thermodynamic variable that an on-Hugoniot EOS is expected to provide is entropy. Once shock-induced entropy gain is known, its final thermodynamic state after adiabatic decompression can be accurately calculated. There are a number of applications of such entropy calculations in Earth and planetary science. For example, the degrees of melting and vaporization, post-decompression temperature of impact-induced vapor can be calculated relatively easily once entropy gain is given. Furthermore, this EOS is useful for matching thermodynamic conditions between laser-induced and impact-induced vapor plumes [12].

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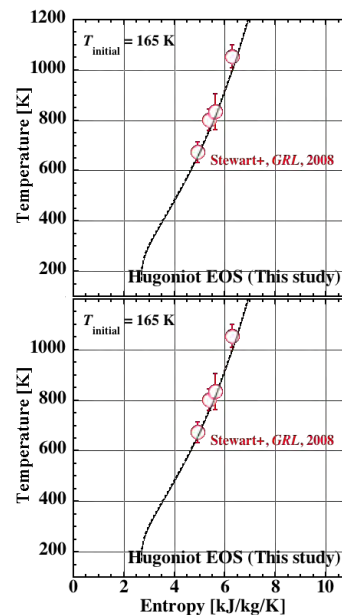
Figure 1. Comparison between shock experimental data [7] and our proposed EOS calculations. The results of Both temperature and entropy are reproduced well by our semi-analytical EOS.
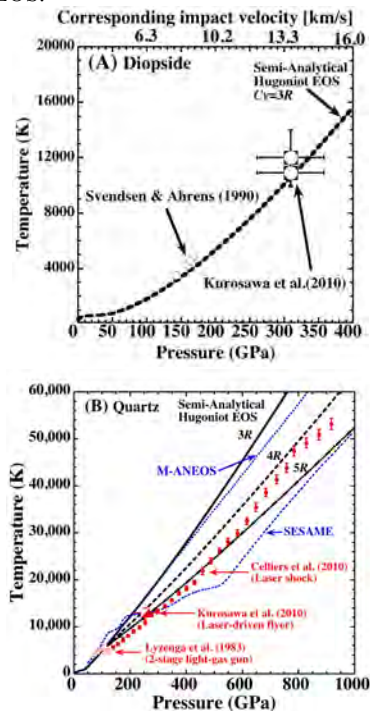
Figure 2. Comparison between EOS calculations and shock experimental data for diopside [8,11] and quartz [9,10,11]. Temperature and entropy for both diopside and quartz at shock pressures below 200 GPa are reproduced well by our semi-analytical EOS and Dulong-Petit C_v, but temperature measurements at much higher shock pressure for quartz with intense laser [11] requires higher C_v than Dulong-Petite ($3R$). For comparison, M-ANEOS and SESAME calculations by [4] for the same conditions are also shown.