The relation between the shock-induced free-surface velocity and the postshock specific volume of solids[a)]

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The release of solids from a state of shock compression at a free surface is examined. For isentropic release, the postshock specific volume V'_0 is shown to be constrained by $V'_0 \geq (U_{fs} - U_p)^2/P_1 + V_1$, where (P_1, V_1) is the pressure-volume Hugoniot state of shock compression and U_{fs} and U_p are the free-surface and shock particle velocities, respectively. When a sudden phase change occurs during the release process, this lower bound is increased, subject to simplifying assumptions about the phase transition.

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I. INTRODUCTION

The use of strong shock waves induced in solids provides a valuable tool for the study of high-pressure equations of state. Such measurements find applications in broad areas of solid-state physics, geophysics, and related fields.

The present work concerns the adiabatic release of materials from a Hugoniot state of shock compression and, specifically, the information that is obtained by measuring the final rarefaction-wave particle velocity. In practice, when a single shock wave with particle velocity U_p interacts with a free surface at normal incidence, it is reflected as a simple rarefaction wave which increases the particle velocity by an amount U_r. The quantity which is often determined experimentally is the velocity of the free surface,

$$U_{fs} = U_p + U_r. \tag{1}$$

Since both U_p and U_{fs} are typically measured experimentally, U_r is known.

It is well known that for such an isentropic release wave, U_r is given by the Riemann integral[1]

$$U_r = \int_0^{P_1} \left(-\frac{dV}{dP}\right)^{1/2}_{\text{adi}} dP, \tag{2}$$

where the subscript adi denotes the specific path in the pressure-volume P-V plane known as the release adiabat. Equation (2) is valid as long as the density is a single-valued function of the pressure, such as in the case of an isentropic or isenthalpic process. A fluid rheology is considered here for simplicity.

Recent developments in high-pressure physics have seen the registration of time-resolved release adiabats, using in-material stress gauges as well as laser velocimeter records.[2] However, the majority of high-pressure shock-wave data, such as those which are relevant to geophysical problems, do not include such detailed release information. The results presented here have been and continue to be of practical use in interpreting the results of such shock-wave experiments. It is the authors' intention to derive here the results relevant to simple free-surface velocity measurements without reference to complementary techniques of direct release adiabat measurements using in-material gauges.

Figure 1 shows the Hugoniot state (P_1, V_1) and possible release adiabats which take the material from this shocked state to zero pressure and post shock specific volume V'_0. By making an approximation to the form of this adiabat, a limit can be placed on the final specific volume V'_0, given the measured value of U_r. There are two cases which are of specific practical interest in approximating the adiabat.

In the first of these cases, no shock-induced phase change occurs in the material at high pressure. Examples of this behavior are found in a large class of metals such as Ag, W, Al, Cu, and others. For such materials, Walsh and Christian[3] show that U_r and hence V'_0 are well constrained, and in the region of a single phase, the problem is well treated. The usually tabulated values of specific volume and enthalpy H as functions of temperature can, furthermore, be used to obtain $H(V)$, the enthalpy as a function of volume, and

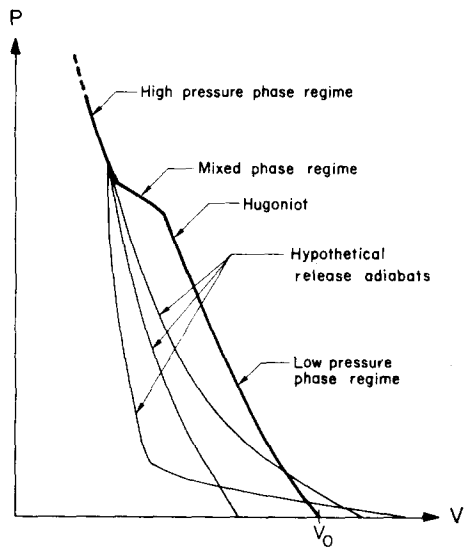

FIG. 1. Possible release paths from a Hugoniot state for a material which undergoes a shock-induced phase change. V_0 denotes the specific volume of unshocked material at the foot of the Hugoniot.

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provide a constraint on the Gruneisen parameter $\gamma = V(\partial P/\partial E)_v$ along the release adiabat.[1] Here, E denotes the specific internal energy.

The second case concerns a shock-induced phase change in the material. In virtually all known examples of transition to a high-pressure phase, partial or complete reversion to the original or other low-pressure (and high-temperature) phase is observed to occur upon unloading. Examples of complete reversion are found in iron[4] and alkali halides.[5] Partial reversion occurs in many silicate minerals.[6]

II. STRAIGHT-LINE ESTIMATE

The calculus of variations[7] can be employed to find the trial adiabat which gives a maximum value for the integral in Eq. (2). In the absence of any further constraints, the Euler-Lagrange equation applied to the integrand of Eq. (2) gives

$$\frac{d}{dP}\left[-\frac{1}{2}\left(-\frac{dV}{dP}\right)^{-1/2}\right]=0. \tag{3}$$

This implies that dV/dP is constant along the extremal path. Thus, the value of U_r given by Eq. (2) is an extremum for the linear adiabat

$$V(P)=V_0'-(V_0'-V_1)P/P_1. \tag{4}$$

The value of the integral in this case is

$$U_r^{\max}=\int_0^{P_1}\left(\frac{V_0'-V_1}{P_1}\right)^{1/2}dP=[(V_0'-V_1)P_1]^{1/2}. \tag{5}$$

This value is indeed a maximum, provided nonphysical discontinuities in $V(P)$ are excluded. In particular, other choices of the trial adiabat such as that of a parabola or higher-degree polynomial yield values smaller than the result of Eq. (5). Furthermore, it is easily shown that for the choice Eq. (4),

$$\lim_{\epsilon\to 0}\{U_r[V(P)+\epsilon h(P)]-U_r[V(P)]\}\leq 0, \tag{6}$$

where $h(P)$ is a smooth function which vanishes at the endpoints of integration, $P=0$ and $P=P_1$. This means that Eq. (4) is at least a "weak local maximum" of the functional of Eq. (2).

Now, given experimentally measured values of P_1, V_1, U_p, and U_{fs}, it follows from Eqs. (1) and (5) that

$$V_0'\geq V_1+\frac{(U_{fs}-U_p)^2}{P_1}. \tag{7}$$

If the state $(P_1,\ V_1)$ is achieved via a single shock transition from $(0, V_0)$, then by the Rankine-Hugoniot conservation equations, the above result may be rewritten

$$V_0'\geq V_0\left(1-2\frac{U_{fs}}{U_s}+\frac{U_{fs}^2}{U_pU_s}\right), \tag{8}$$

where U_s is the shock-wave velocity. This result has been used previously in the literature, as in Ahrens and Rosenberg,[6] but is now derived here. The possibility of further constraining the maximum value of U_r by requiring the trial adiabat to conserve internal energy in a manner similar to that developed by Walsh and Christian for metals has been investigated. It has been found, however, that for simple materials like metals, little additional constraint is obtained. For materials of greater interest, such as silicates and other materials undergoing phase changes, *a priori* knowledge of the nature and internal energy of the released state is so uncertain as to prevent any useful conclusions from being drawn.

III. PHASE TRANSITION DURING RELEASE

As stated earlier, many materials which are transformed into a high-pressure phase upon shock loading undergo further usually retrograde phase changes during release. Knowledge of such transitions, such as can be inferred from shock recovery experiments, can provide an improved estimate of V_0'.

Suppose that the release adiabat for a material can be approximated by assuming that at a certain pressure P_2 a phase change occurs with an associated change in specific volume ΔV. Consider the straight-line estimate for the process described with onset of phase change occurring at $(P_2,\ V_2)$, as shown in Fig. 2. For this idealized model of the phase transition, the condition of isentropicity still holds individually for the two branches of the adiabat.

The horizontal section which joins these branches may or may not satisfy the isentropicity condition. Furthermore, this horizontal line in P-V space has the appearance of an isothermal phase change, rather than an adiabatic one. However, approximating the phase change in this way allows the contribution to U_r which is due to the phase change to be neglected, since the pressure drop ΔP in going from the high-to low-pressure phase vanishes in this limit. Therefore, U_r will be assumed to be given by the Riemann integral (2) applied successively to the two single-phase branches only.

Now, if P_2 and V_2 can actually be estimated from buffer or in-material gauge measurements along the adiabat, then the straight-line estimate gives directly

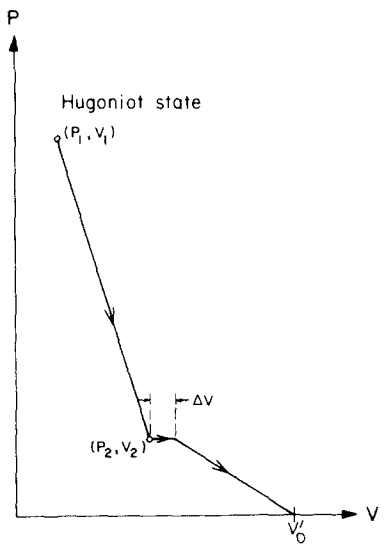

FIG. 2. Linear approximation to a release adiabat which incorporates a retrograde phase change. ΔV denotes the change in specific volume upon phase transition. V_0' is the final post-shock specific volume.

$$U_r^{\max} = [(V_2 - V_1)(P_1 - P_2)]^{1/2} + [(V_0' - V_2 - \Delta V)P_2]^{1/2}. \tag{9}$$

However, the results of the present work are of most use when detailed information regarding the actual adiabat are not known. In such cases, the best that can be done is to maximize Eq. (9) with respect to V_2. The result will turn out to be independent of P_2.

Equation (9) is differentiated with respect to the unknown parameter V_2, and this derivative is equated to zero, in order to obtain a grand maximum of $U_r^{\max}$. Solving for V_2 in this case, the maximum occurs when

$$V_2 = [(P_1 - P_2)/P_1](V_0' - V_1 - \Delta V) + V_1. \tag{10}$$

Inspection shows that this maximum happens to correspond to the case that the linear segments of the adiabat on each side of the phase change have equal slopes. This result is an artifact of the straight-line estimate and bears no real physical significance.

Now the grand maximum given by condition (10) gives

$$U_r^{\max} = [P_1(V_0' - V_1 - \Delta V)]^{1/2} \tag{11}$$

and

$$V_0' \geq [(U_{fs} - U_p)^2/P_1] + V_1 + \Delta V. \tag{12}$$

Thus, the limit given by the straight-line estimate is increased by an amount ΔV for the case of a sudden phase change, subject to the validity of the assumptions regarding the phase change and its contribution to U_r.

As a simple example of the application of this method, we consider the shock compression of α-quartz in the regime of conversion to the high-pressure phase stishovite. Ahrens and Rosenberg[6] present data for this system, including free-surface and buffer-release measurements. Measurements of particle velocity along the release adiabat are transformed to points in the P-V plane by the Riemann integral, producing a release adiabat of the form shown in Fig. 3. The pronounced bend in this adiabat is suggestive of a sudden transition to a phase of lower density around ~5 GPa.

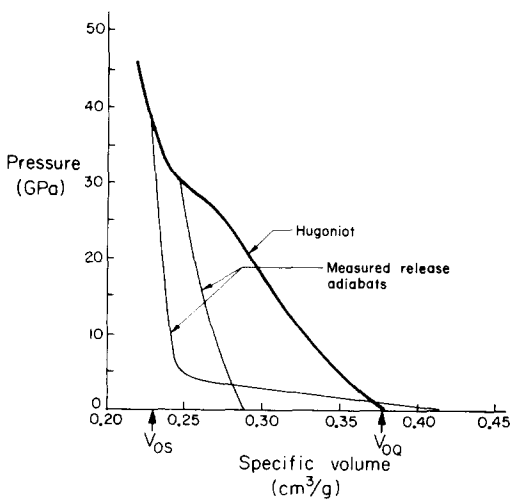

FIG. 3. Experimentally measured P-V release adiabats for polycrystalline quartz. Adiabats are shown for cases with and without retrograde phase change. V_{0Q} is the initial specific volume of quartz, while V_{0S} is specific volume of the uncompressed stishovite phase. Data from Ahrens and Rosenberg.

TABLE I. Quartz/stishovite release data (Ref. 5).

Hugoniot state	$P_1 = 38.2$ GPa $V_1 = 2.25 \times 10^{-4}$ m^3/kg $U_p = 2.380 \times 10^3$ m/sec $U_{fs} = 4.245 \times 10^3$ m/sec

Table I summarizes the data reported for release from a Hugoniot state with $P_1 = 38.2$ GPa. Using the simple straight-line estimate of Eq. (7), we obtain $V_0' \gtrsim 0.32$ cm^3/g. This is consistent with but substantially lower than the value $V_0' = 0.47 \pm 0.04$ cm^3/g obtained directly by transforming the release adiabat data.

Ahrens and Rosenberg suggest that approximately 75% of the compressed material consists of the stishovite phase, so that if this reverts suddenly to normal quartz upon release, a value of $\Delta V \cong 0.15$ cm^3/g can be used in the two-phase estimate of Eq. (12). This results in $V_0' \geq 0.47$ cm^3/g in agreement with the actual release adiabat measurements. It should be noted that the P-V adiabats reported by Ahrens and Rosenberg, and referred to here as giving "actual" values of V_0', are computed under the assumption of isentropic release. In such situations, this assumption has not been independently tested.

IV. CONCLUSIONS

As noted earlier, the results of the straight-line estimate applied to release adiabats have been of use in constraining the released density of materials in experiments where simple streak camera records of final free-surface velocity are made. The results are directly extended to the case of partial release and are being used to interpret experiments with the transmission of shock waves from geophysical materials into buffer materials at pressure levels approaching 100 GPa. Recent work by Jeanloz and Ahrens[8] on pyroxenes and olivines using the buffer method has used the straight-line estimate to constrain P-V release paths and the properties of high-pressure assemblages. Similarly, the adiabatic release of lunar material[9] and ilmenite[10] from pressures exceeding 100 GPa has been studied through buffer and free-surface particle velocity measurements. Constraints on density are important in the consideration of inferred or predicted high-pressure phases.

The results of the simple straight-line estimate hold as long as the isentropic condition of the Riemann integral holds. Neglecting the possibility of heat conduction as a significant form of energy transfer, this means that the estimate applies to reversible release processes. However, irreversible release should under most circumstances reduce the kinetic energy available in the form of rarefaction particle velocity and, therefore, retain Eq. (5) as an upper limit to U_r.

In summary, the approximation of linear P-V release adiabat yields a lower limit for postshock specific volume through Eq. (7), given a measured value of

U_{fs}. Furthermore, if phase changes can be assumed to occur during release over times short compared with the time required for unloading, the straight-line estimate may in some circumstances be generalized to include such cases through Eq. (12). Such information can in practice indicate where a more detailed study of the release adiabat of a given material would be fruitful.

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