Shock wave equation of state of powder material

D. K. Dijken and J. Th. M. Do Hoeson
Department of Applied Physics, Material Science Center, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

(Received 24 March 1993; accepted for publication 6 October 1993)

A model is proposed to predict the following quantities for powder materials compacted by shock waves: the pressure, the specific volume, the internal energy behind the shock wave, and the shock-wave velocity $U_s$. They are calculated as a function of flyerplate velocity $u_f$ and initial powder specific volume $V_0$. The model is tested on Cu, Al2024, and Fe. Calculated $U_s$ vs $u_f$ curves agree well with experiments provided $V_0$ is smaller than about two times the solid specific volume. The model can be used to predict shock-wave state points of powder or solid material with a lower or higher initial temperature than room temperature.

I. INTRODUCTION

Since the 1960s various approaches have been followed in describing the shock-wave equation of state (EOS) of powder materials. Roughly speaking modeling was done in two different ways: i.e., semiempirically, using quasi-static powder compaction models$^{1-5}$ and purely theoretically.$^{6-11}$ Except for Ref. 11 these models adopt the Mie–Grüneisen EOS, which relates the change in internal energy to the change in pressure at constant specific volume: $dE = \frac{V}{dP}$, $\Gamma(V)$. In many materials the Mie–Grüneisen constant $\Gamma(V_0)$ ranges between 1.6 and 2.6.

These models, however, have some drawbacks because the internal energy and the pressure are divided into separate contributions of cold isothermal compressive and thermal components: $E = E_C + E_T$ and $P = P_C + P_T$, respectively. It follows that the pressure behind the shock wave is given by

$$P = \frac{2P_C V - 2\Gamma(V)E_C}{2V + \Gamma(V)\Gamma(V) \Gamma(V) V_0 \cdot} \quad (1)$$

$P_C$ is always represented by the second-order isothermal Birch–Murnaghan EOS. This relationship is not very accurate and rather questionable.$^{12,13}$ Further, for the cold isotherm $E_C$ is supposed to be $E_C = \int P_C \, dV$. This is certainly not the case as it only holds for the adiabat and a large error is introduced. In addition the derivative of the isothermal bulk modulus $K_0$ with respect to pressure is needed as an input parameter for the Birch–Murnaghan relation. This value is difficult to determine experimentally.

Finally, it is clear that when $V_0 > V_0 = \frac{1}{2} + 2.5 (V_0)$, the increasing linear denominator crosses the specific volume axis at the right of $V_0$ at $V = \left\{ \frac{\Gamma(V_0)}{2 + \Gamma(V)} \right\} V_0$. Now $P$ is calculated between $V_0$ and $V = \left\{ \frac{\Gamma(V)}{2 + \Gamma(V)} \right\} V_0$ using the negative part of $P_C$. Since the Birch–Murnaghan EOS is only estimating $P_C$ in the case of compression, Eq. (1) fails.

In this article another theoretical approach is reported that takes Oh and Persson's work$^{11}$ as a starting point while using the Mie–Grüneisen EOS instead.

II. BASIC CONCEPTS

A. Shock-wave conservation EOS for solid and powder material

Suppose a rigid planar flyer plate of infinite mass propagates at a constant velocity $u_f$. When it impacts onto solid or powder materials these will be compressed and a shock wave with velocity $U_s$ will propagate through the material. The situation is schematically displayed in Fig. 1. The pressure, specific volume, internal energy, and temperature ahead and behind the shock front are represented by $P_0$, $V_0$, $E_0$, and $T_0$, and $P$, $V$, $E$, and $T$ respectively for solid material and $P_{00}$, $V_{00}$, $E_{00}$, and $T_{00}$ and $P'$, $V'$, $E'$, and $T'$ respectively, for powder material.

Figure 1(b) shows what happens to a powder material during shock-wave compaction. The powder is represented by separate infinite thin material plates. When the first plate collapses on the shock front, it behaves exactly like a solid material. Since there is some space left between the first and the second material plate, the first plate, after being compacted, starts to expand. Its compressive energy is transformed into internal kinetic energy. Then, more plates collide leaving the first plate oscillating between the flyer plate and the second plate. This goes on until all its internal kinetic energy is transformed to random thermal energy. Eventually the first flyer plate is "locked" in its final specific volume. For material with a higher $V_{00}$ behind the shock wave, more compressive energy is transformed to thermal energy. At first instance this transformation step does not take place in solid material. During pressure release the (remaining) compressive energy part is transformed and/or transferred to the surrounding material.

In order to derive EOS for shock compacting solid and powder material, the following four assumptions have to be made.

(a) It is assumed that compaction of a powder at zero pressure quasistatically from $V_{00}$ to the solid specific volume $V_0$ does not cost any energy, so that $E_{00} = E_{00}$.

(b) Behind the shock wave there are no voids present, i.e., the material is completely compacted.

(c) The increase in internal energy is equally distrib-
FIG. 1. (a) A rigid flyer plate impacts onto a solid or powder material. Area I is the flyerplate, area II is the compacted powder or solid material, area III is the uncompacted powder or solid material at rest. The flyerplate velocity is $u_P$ or $u_i$ ($u_p = u_i$). The shock-wave velocity is $U_s$ or $V_i$. (b) The powder is represented by separate solid plates collapsing sequentially on the shock-wave front.

uated inside the compacted material. It implies that the pressure and the temperature fields are uniform.

(d) There are no volume or energy changes due to deformations or phase transformations.

B. Conservation of mass

The condition that the mass flux in and out the shock front must be equal is expressed by

$$VU_s = V_0(U_s - u_p),$$

where for powder material

$$V'U'_s = V_0(U'_s - u'_p).$$

Taking $u_p$ equal to $u'_p$,

$$U_s(V_0 - V)/V_0 = U'_s(V_0 - V')/V_0.$$  

C. Conservation of momentum

The change of momentum of material impacted by a flyer plate with surface $A$ in a time lapse $\delta t$ is given by $\delta p = mv$, where $m = AU \delta t/V_0$ and $v = u_p$. Pressure is the change of momentum per unit area per unit time, so the momentum has to be divided by the impact area $A$ and the impact time $\delta t$ in order to obtain the (mean) pressure difference over the shock front. Taking $P_0 = 0$,

$$P = \frac{\delta p}{A \delta t} = \frac{U_s u_p}{V_0},$$

where for powder material

$$P = \frac{U'_s u'_p}{V_0}. $$

Taking $u_p$ equal to $u'_p$ leads to $PV_0/U_s = P'V_0/U'_s$.

D. Conservation of energy

Suppose the compacted material is at rest and the uncompacted material collides with a velocity $u_p$ onto the shock front. Then the change of compressive and thermal energy of material impacting onto an area $A$ in a time lapse $\delta t$ is given by $dE = m v^2/2$, where $m = AU \delta t/V_0$ and $v = u_p$. The change of internal energy $\delta E$ is defined as the change of internal energy per unit mass, i.e.,

$$\delta E = E - E_0 = \frac{1}{2}u_p^2,$$

and for powder material

$$E' - E_0 = \frac{1}{2}u'_p^2.$$  

By taking $u_p$ equal to $u'_p$ and since $E_0 = E_0$ [assumption (a)], the increase in internal energy is exactly the same for solid and powder material, i.e., $E - E_0 = E' - E_0$, and only depends on $u_p$.

Recall that the work done by the flyer plate per kg of compressed material initially at rest is $u'_p$ in which $u'_p$ per kg is converted in increasing the internal energy of the compressed material and $u'_p$ per kg is converted in increasing the kinetic energy. By combining Eqs. (2) and (4) and Eqs. (3) and (5) the powder $P', V'$ state points can be related to the solid $P, V$ state points,

$$E' - E_0 = \frac{1}{2}P'(V_0 - V') = \frac{1}{2}P(V_0 - V).$$  

E. Solid system

The three solid conservation relations Eqs. (2), (4), and (6) contain four known variables, $E_0, P_0, V_0$, and $u_p$, and four unknown variables, $E, P, V$, and $U_s$. One more relation between any two variables is necessary.

For solid and powder materials $U_s$ can be measured at different values of $u_p$. From these data it is known that the relationship between $U_s$ and $u_p$ for solid material is always nearly linear, i.e., $U_s = C + Su_p$, where $C$ is approximately the zero pressure sound velocity and $S$ is a constant. Combining Eqs. (2) and (4) with the linear relationship of $U_s$ with $u_p$ leads to an expression for the pressure behind the shock wave,

$$P = \frac{C(V_0 - V)}{[V_0 - S(V_0 - V)]^2}.$$  

Equation (9) describes the solid Hugoniot which is the locus of the final shock state, but not the thermodynamic path followed by the material. The Hugoniot is an adiabat, neither an isotherm or an isentrope. The actual thermodynamic path followed is a straight line from the initial to the final state, called the Rayleigh line.

III. CALCULATIONS

When a flyer plate impacts onto a sample, either solid or powder material, the internal energy increase equals the
Copper

Specific volume \( \text{m}^3/\text{kg} \)

FIG. 2. (a) Copper Hugoniot and equienergy curves (b) \( E - E_0 = 0.25 \) MJ; (c) \( 0.50 \) MJ; (d) \( 0.75 \) MJ; (e) \( 1.00 \) MJ; (f) \( 1.25 \) MJ. The internal kinetic energy is zero. At fixed flyer-plate velocity, behind the shock wave, the internal energy of both the compacted solid and the powder material are the same. Therefore, the final \( P, V \) point must lie somewhere on the equienergy curve (0-2); only explosive compaction of solid material; (0-1) explosive compaction (0-2) and heating at constant volume (2-1); (0-4); only heating at zero pressure; (0-3); heating at zero pressure (0-4) and heating at constant volume (4-3).

kinetic energy increase \( E - E_0 = E' - E_0 = u_p^2/2 \). In the \( P-V \) plane of Fig. 2 equienergy lines are depicted. It is assumed that compacting a powder material from \( V_0 \) to \( V \) does not cost any energy. It means that starting from \( V_0 \), final states on the equienergy curve (d) at the left-hand side of \( V \) are calculated by shock compacting solid material from \( V_0 \) to \( V_2 \) along the Rayleigh line and then heating the material at constant volume to \( P_1 \). Starting from \( V_0 \), energy states on the equienergy curve at the right-hand side of \( V \) are calculated by heating solid material at zero pressure from \( V_0 \) to \( V_4 \) resulting in a thermal expansion and then heating the material at constant volume to \( P_3 \). Dense powders are compacted to states close to point A. Highly porous powders are compacted to states close to B, Fig. 2. In Table I for different equienergy curves (Fig. 2), values are listed for \( E - E_0 \), \( u_p \), \( P_A \), and \( T_B \) (Fig. 2).

A. \( U_s \) vs \( u_p \) calculation for powder materials: \( V_1 < V_0 \)

The total amount of internal energy, deposited by the flyer plate to the powder (00-1) (Fig. 2) is given by Eq. (8).

\[
E_1 - E_0 = E_1 - E_0 = \frac{1}{2} P_1 (V_0 - V_1) = \frac{1}{2} u_p^2.
\]

This amount of internal energy can be stored in the system by adding the shock-wave energy along the Rayleigh line (0-2).

\[
E_2 - E_0 = \frac{1}{2} P_2 (V_0 - V_1),
\]

and the internal energy along the isochore (2-1),

\[
E_1 - E_2 = \frac{(P_1 - P_2) V_1}{\Gamma(V_1)}.
\]

By choosing \( V_1 \), the pressure \( P_2 \) is given by Eq. (9),

\[
P_2 = \frac{C_0^2(V_0 - V_1)}{[V_0 - S(V_0 - V_1)]^2 2[\Gamma(V_1)(V_0 - V_1) - 2V_1]}.
\]

For some materials such as Al, Cu, In, Fe, Pb, and NaCl, at room temperature, zero pressure, \( \Gamma(V_0) \) is determined experimentally by Ref. 16.

At other temperatures the Grüneisen constant is calculated by

\[
\Gamma(V_1) = \Gamma(V_0) \left( \frac{V_1}{V_0} \right)^{\frac{q-\gamma}{\gamma}}.
\]

where \( q \) is a constant. For the above-mentioned materials \( q \) is determined experimentally as well. When no values for \( q \) are available \( q \) is assumed to be equal to unity.

Finally, the pressure in the fully shock-compacted powder material is calculated from Eqs. (10), (11), (12), and (13),

\[
P_1 = \frac{C_0^2(V_0 - V_1)}{[V_0 - S(V_0 - V_1)]^2 2[\Gamma(V_1)(V_0 - V_1) - 2V_1]}.
\]

B. \( U_s \) vs \( u_p \) calculation for powder materials: \( V_1 > V_0 \)

The total amount of internal energy, deposited by the flyer plate in the powder (00-3) (Fig. 2) is given by Eq. (8),

\[
E_3 - E_0 = E_3 - E_0 = \frac{1}{2} P_3 (V_0 - V_3) = \frac{1}{2} u_p^2.
\]

This amount of internal energy can quasistatically be stored in the system by heating solid material at zero pressure from \( V_0 \) to \( V_4 \) (0-4) and then heating at constant volume \( V_4 \) from \( P_4 \) to \( P_3 \) (4-3).
So, at first the material is thermally expanded to a volume $V_0$ ($0 \to 4$), after which $T_4$ and $E_4 - E_0$ are calculated from the temperature-dependent thermal-expansion coefficient $\alpha(T)$ and the specific heat at constant pressure $C_p(T)$.

The volume and the temperature are related according to

$$\int_{V_0}^{V_4} \frac{1}{V} dV = \int_{T_0}^{T_4} 3\alpha(T) dT. \tag{18}$$

For many solids, over a wide temperature range, i.e., $T_0 < T_4 < \pm 1300$ K, $\alpha(T)$ can be estimated accurately by

$$\alpha(T) = \alpha(T_0) + \beta(T)(T - T_0). \tag{19}$$

The energy needed to expand to $V_4$ is given by

$$E_4 - E_0 = \int_{T_0}^{T_4} C_p(T) dT. \tag{20}$$

For many solids, over a wide temperature range, i.e., $T_0 < T_4 < \pm 1300$ K, $C_p(T)$ can be estimated accurately by

$$C_p(T) = C_p(T_0) + \gamma(T)(T - T_0). \tag{21}$$

where $T_4$ can be calculated using Eq. (21). Note that $\alpha(T)$ and $C_p(T)$ are calculated from experimental values for $V_4(T)$ and $E_4(T) - E_0$, respectively. Whenever available it is better to use direct experimental values for $V_4$ as a function of $E_4 - E_0$.

The internal energy increase along the isochore from $P_4$ to $P_3$ is given by

$$E_3 - E_4 = \frac{(P_3 - P_4) V_3}{\Gamma(V_3)}, \tag{22}$$

where $\Gamma(V_3)$ is given by Eq. (15). Finally, the pressure in the fully shock-compacted powder material is given by

$$P_3 = \frac{2\Gamma(V_3)}{[\Gamma(V_3)(V_{oo} - V_3) - 2V_3]} \int_{T_0}^{T_4} C_p(T) dT. \tag{23}$$

Since $V_{oo}$ and $V_3$ are chosen, $T_4$ is calculated with Eq. (19), $P_3$ is calculated with Eq. (23), $u_p$ and $E_3 - E_0$ are calculated with Eq. (17), after which $U_f$ is calculated with Eq. (3) or Eq. (5).

The model can calculate $U_f$ vs $u_p$ values for powder and solid material as well at higher initial temperature than $T_0$. Further, in principle it is possible to calculate the solid Hugoniot, i.e., the constant $S$. Temperature calculations are presented in Ref. 8.22

IV. VALIDATION OF THE MODEL

In the compaction by shock waves of powder material there are six principal parameters having a main effect on the final compacted material. These are the particle or flyer plate velocity, which is mainly determined by the detonation velocity of the used explosive, next, the initial specific volume of the powder to be compacted, the particle grain size, the initial temperature, and the duration of the shock pressure, which is mainly determined by the size of the experiment. Finally, the compacted powder material, still at pressure, contains adiabatic compressive energy and thermal energy. The adiabatic part has to be transmitted to the surrounding material (flyer plate, canning material), otherwise extensive cracking will occur.

$U_f$ vs $u_p$ relations are calculated for Cu, Al2024, and Fe powder materials and compared with experimental data14 (Figs. 3–5). Other material data are from Refs. 14, 16, 19, 20, and 21. It can be concluded that for $V_{oo} < 1.8V_0$ powder $U_f - u_p$ calculations fit well with experiment. The amount of energy $E_g$ needed to compact a homogeneous powder quasi-statically to full density mainly depends on the particle shape and is fixed. For powder material, the larger the $u_p$, the larger the ratio $E - E_0/E_g$ and in that case the better the model. So, the violation of assumption (a) in Sec. II depends on the flyer-plate veloc-
A new EOS has been derived for shock-compacting powder material to full dense solid material. The model predicts the shock-wave velocity, the pressure, specific volume, and internal energy behind the shock wave, as a function of flyer-plate velocity, initial powder specific volume, and initial temperature. The model is based on the fact that the internal energy increase behind the shock wave is the same for both the solid and the powder compacted material.

The model indicates that, although at a given \( u_p \) for less dense powder more compressive energy is transformed to thermal energy the temperature behind the shock wave is roughly the same; at relatively high-flyer-plate velocities, e.g., \( u_p > \pm 3000 \text{ m/s} \), calculated \( U_s \) vs \( u_p \) lines may even cross.

For Cu, Al2024, and Fe, \( V_{oo} < \pm 1.8V_n \) the model predicts very well the \( U_s \) vs \( u_p \) relationship. At larger specific volume and \( u_p > \pm 2000 \text{ m/s} \) the calculated \( U_s \) values become too large. With the model it is easy to calculate \( U_s \) vs \( u_p \) relations of powders at temperatures other than room temperature.

**ACKNOWLEDGMENT**

The authors would like to thank Dr. A. C. van der Steen of Prins Maurits Laboratorium TNO (Rijswijk, The Netherlands) for his interest in this work and discussion.

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**FIG. 5.** \( U_s \) vs \( u_p \) relationship for Fe (solid line: calculated; dashed line: experiment).