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Shock wave equation of state of powder material

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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_p and initial powder specific volume V_{00} . The model is tested on Cu, Al2024, and Fe. Calculated U_s vs u_p curves agree well with experiments provided V_{00} 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 quasistatic powder compaction models¹⁻⁵ 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 = 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 by¹⁰

$$P = \frac{2P_C V - 2\Gamma(V)E_C}{2V + \Gamma(V)V - \Gamma(V)V_{00}}.$$
 (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 $V_{00} > V_0[1+2/\Gamma(V_0)]$, the increasing linear denominator crosses the specific volume axis at the right of V_0 at $V = \{\Gamma(V)/[2+\Gamma(V)]\}V_{00}$. Now P is calculated between V_0 and $V = \{\Gamma(V)/[2+\Gamma(V)]\}V_{00}$ 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 work¹¹ 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_p . 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 $E_0 = E_{00}$.

(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-

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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'_p ($u_p = u'_p$). The shock-wave velocity is U_s or U'_s . (b) The powder is represented by separate solid plates collapsing sequentially on the shock-wave front.

uted 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

$$VU_{s} = V_{0}(U_{s} - u_{p}), \tag{2}$$

where for powder material

$$V'U'_{s} = V_{00}(U'_{s} - u'_{p}).$$
⁽³⁾

Taking u_p equal to u'_p ,

$$U_s(V_0 - V)/V_0 = U'_s(V_{00} - V')/V_{00}.$$

C. Conservation of momentum

The change of momentum of material impacted by a flyer plate with surface A in a time lapse δt is given by $\delta p = mv$, where $m = AU_s \delta t/V_0$ 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 δt in order to obtain the (mean) pressure difference over the shock front. Taking $P_0 = 0$,

$$P = \delta P = \frac{\delta p}{A\delta t} = \frac{U_s u_p}{V_0},\tag{4}$$

where for powder material

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$$P' = \frac{U'_{s} u'_{p}}{V_{00}}.$$
 (5)

Taking u_p equal to u'_p leads to $PV_0/U_s = P'V_{00}/U'_s$.

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 δt is given by $dE = mv^2/2$, where $m = AU_s \delta t/V_0$ and $v = u_p$. The change of internal energy δE is defined as the change of internal energy per unit mass, i.e.,

$$\delta E = E - E_0 = \frac{1}{2}u_p^2,\tag{6}$$

and for powder material

$$E' - E_{00} = \frac{1}{2} u_p^{\prime 2}.$$
 (7)

By taking u_p equal to u'_p and since $E_{00}=E_0$ [assumption (a)], the increase in internal energy is exactly the same for solid and powder material, i.e., $E-E_0=E'-E_{00}$, 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^2 in which $\frac{1}{2}u_p^2$ per kg is converted in increasing the internal energy of the compressed material and $\frac{1}{2}u_p^2$ 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,

$$E' - E_{00} = \frac{1}{2}P'(V_{00} - V') = \frac{1}{2}P(V_0 - V).$$
(8)

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 .^{6,14} 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,

$$P = \frac{C^2(V_0 - V)}{[V_0 - S(V_0 - V)]^2}.$$
(9)

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.¹⁵

III. CALCULATIONS

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

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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 $(0 \rightarrow 2)$; only explosive compaction of solid material; $(0\rightarrow 1)$ explosive compaction $(0\rightarrow 2)$ and heating at constant volume $(2\rightarrow 1)$; $(0\rightarrow 4)$; only heating at zero pressure; $(0\rightarrow 3)$; heating at zero pressure $(0\rightarrow 4)$ and heating at constant volume $(4\rightarrow 3)$.

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_{00} to V_0 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_0 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_0 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 $(00 \rightarrow 1)$ (Fig. 2) is given by Eq. (8),

TABLE I. Calculated copper state point values on different equienergy curves (Fig. 2). $E-E_0$ is the internal energy increase, u_p is the corresponding flyer-plate velocity, P_A is the pressure on the solid Hugoniot, and T_B is the zero-pressure temperature (energy in MJ/kg, velocity in m s⁻¹, pressure in Pa, temperature in K).

	b	с	d	е	f
$\overline{E-E_0}$	0.25	0.50	0.75	1.00	1.25
<i>u</i> _n	707	1000	1225	1414	1518
ŕ,	31.4	48.4	63.0	76.3	88.9
T_B	829	1314	1761	2177	2567

$$E_1 - E_{00} = E_1 - E_0 = \frac{1}{2} P_1 (V_{00} - V_1) = \frac{1}{2} u_p^2.$$
(10)

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

$$E_2 - E_0 = \frac{1}{2} P_2 (V_0 - V_1), \tag{11}$$

and the internal energy along the isochore $(2 \rightarrow 1)$,

$$E_1 - E_2 = \frac{(P_1 - P_2)V_1}{\Gamma(V_1)}.$$
 (12)

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

$$P_2 = \frac{C^2(V_0 - V_1)}{[V_0 - S(V_0 - V_1)]^2}.$$
(13)

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 by¹⁵

$$\Gamma(V) = \frac{\alpha(T)VK_S(T)}{C_P(T)} = \frac{\alpha(T)VK_T(T)}{C_V(T)}.$$
 (14)

Constants for the isothermal and the adiabatic bulk modulus $K_T(T)$ and $K_S(T)$, respectively, and the specific heat at constant volume $C_V(T)$ are scarcely available in the literature. $C_P(T)$ is the specific heat at constant pressure. $\alpha(T)$ is the temperature-dependent thermal-expansion coefficient. Consequently, it was proposed¹⁷

$$\Gamma(V_1) = \Gamma(V_0) \left(\frac{V_1}{V_0}\right)^q, \tag{15}$$

where q is a constant. For the above-mentioned materials q is determined experimentally as well.¹⁶ When no values for q are available q is assumed to be equal to unity.¹⁷

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

$$P_{1} = \frac{C^{2}(V_{0} - V_{1})}{[V_{0} - S(V_{0} - V_{1})]^{2}} \frac{[\Gamma(V_{1})(V_{0} - V_{1}) - 2V_{1}]}{2[\Gamma(V_{1})(V_{00} - V_{1}) - 2V_{1}]}.$$
(16)

At given V_{00} and V_1 , P_1 can be calculated using Eq. (16). u_p and $E_1 - E_{00}$ are calculated using Eq. (10) after which U_s can be calculated either with Eq. (3) or Eq. (5).

B. U_s vs u_p calculation for powder materials: $V_3 > V_0$

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

$$E_3 - E_{00} = E_3 - E_0 = \frac{1}{2} P_3 (V_{00} - V_3) = \frac{1}{2} u_p^2.$$
(17)

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 \rightarrow 4) and then heating at constant volume V_4 from P_4 to P_3 (4 \rightarrow 3).

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So, at first the material is thermally expanded to a volume V_4 (0 \rightarrow 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

$$\int_{V_0}^{V_4} \frac{1}{V} dV = \int_{T_0}^{T_4} 3\alpha(T) dT.$$
 (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 $\alpha(T) = \alpha(T_0) + \beta(T)(T - T_0)$. Substituting $\alpha(T)$ in Eq. (18) relates V_4 to T_4 ,

$$\ln \frac{V_4}{V_0} = 3\alpha(T_0)(T_4 - T_0) + \frac{3}{2}\beta(T)(T_4 - T_0)^2.$$
(19)

The energy needed to expand to V_4 is given by

$$E_4 - E_0 = \int_{T_0}^{T_4} C_P(T) dT.$$
 (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 $C_P(T) = C_P(T_0) + \gamma(T)(T - T_0)$. Substituting $C_P(T)$ in Eq. (20) leads to

$$E_4 - E_0 = C_P(T_0) (T_4 - T_0) + \frac{1}{2} \gamma(T) (T_4 - T_0)^2, \quad (21)$$

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 $(4 \rightarrow 3)$

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

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

$$P_{3} = \frac{2\Gamma(V_{3})}{[\Gamma(V_{3})(V_{00} - V_{3}) - 2V_{3}]} \int_{T_{0}}^{T_{4}} C_{P}(T) dT. \quad (23)$$

Since V_{00} 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_s is calculated with Eq. (3) or Eq. (5).

The model can calculate U_s 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 detona-



FIG. 3. U_s vs u_p relationship for Cu (solid line: calculated; dashed line: experiment).

tion 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_s 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 $V_{00} < \pm 1.8V_0$ powder $U_s - u_p$ calculations fit well with experiment. The amount of energy E_G needed to compact a homogeneous powder quasistatically to full density mainly depends on the particle shape and is fixed. For powder material, the larger the u_p , the larger the ratio $E - E_{00}/E_G$ and in that case the better the model. So, the violation of assumption (a) in Sec. II depends on the flyer-plate veloc-



FIG. 4. U_s vs u_p relationship for Al2024 (solid line: calculated; dashed line: experiment).

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

ity. From the U_s vs u_p figures it can be concluded that even for relatively low values of u_p the model is still appropriate.

For $V_{00} > \pm 1.8V_0$ the difference between experimental and calculated U_s values for Cu increases with u_p when $u_p > \pm 2000$ m/s. The most probable reason is the following.

Because of the low density every particle oscillates many times before it finally comes to rest. With every collision a part of the internal energy is leaking away in the form of elastic shock waves through the already compacted material. At other places in the compacted powder this energy may be consumed in the form of heat or fracture. In the calculation procedure no energy is leaking away, resulting in higher U_s values. Depending on the material qualities and the demands of the compactor, the principal parameters have to be adjusted to optimum values. In order to get crack-free well-sintered material, the adjustment should be a high-flyer-plate velocity and highly porous material, i.e., the adiabatic compressive energy is transformed to thermal energy already during the compaction process. Further, the grain size should not be too small, i.e., the thermal energy is mainly deposited in the surface²² so the surface grains become hotter which favors the sintering process. In addition the initial temperature should be above room temperature resulting in a higher temperature behind the shock wave, leading to a better sinter behavior of the material. Next, the batches should be large and thick by which the material may remain for a longer time at high pressure and at high temperature. Finally, a strong and heavy canning material should be applied since the canning material will absorb the adiabatic compressive energy.

V. CONCLUSIONS

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., $u_p > \pm 3000$ m/s, calculated U_s vs u_p lines may even cross.

For Cu, Al2024, and Fe, $V_{00} < \pm 1.8V_0$ the model predicts very well the U_s vs u_p relationship. At larger specific volume and $u_p > \pm 2000$ 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.

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