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A cold energy mixture theory for the equation of state in solid and porous metal mixtures

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Porous or solid multi-component mixtures are ubiquitous in nature and extensively used as industrial materials such as multifunctional energetic structural materials (MESMs), metallic and ceramic powder for shock consolidation, and porous armor materials. In order to analyze the dynamic behavior of a particular solid or porous metal mixture in any given situation, a model is developed to calculate the Hugoniot data for solid or porous mixtures using only static thermodynamic properties of the components. The model applies the cold energy mixture theory to calculate the isotherm of the components to avoid temperature effects on the mixtures. The isobaric contribution from the thermodynamic equation of state is used to describe the porous material Hugoniot. Dynamic shock responses of solid or porous powder mixtures compacted by shock waves have been analyzed based on the mixture theory and Hugoniot for porous materials. The model is tested on both single-component porous materials such as aluminum 2024, copper, and iron; and on multi-component mixtures such as W/Cu, Fe/Ni, and Al/Ni. The theoretical calculations agree well with the corresponding experimental and simulation results. The present model produces satisfactory correlation with the experimentally obtained Hugoniot data for solid porous materials over a wide pressure range. © 2011 American Institute of Physics. [doi:10.1063/1.3603018]

I. INTRODUCTION

As a result of material processing requirements, explosion synthesis of new materials, projectile impacts, nuclear explosions, and shock compression of materials have become popular subjects that have been studied by many researchers in recent years. Here high pressure equations of state (EOS) and the dynamic mechanical properties of materials have been investigated by using shock wave loadings. The Hugoniot of a material is a locus of final pressure-volume-energy states that can be attained by shock compression. Compared with solid materials, porous materials show different behaviors under shock wave loadings due to their energy absorption or shock isolation properties. As a pressure is applied to a porous material the consolidation behavior is characterized by several phases.¹ Initially the porosity is high and densification occurs by particle rearrangement, and the phase change is resisted by inter-particle friction and interlocking. As the porosity reduces, a point is reached when the particle interlock and rearrangement cease. Thereafter the material behaves as a porous solid with densification occurring by means of elastic and plastic deformations or fracture if the material is brittle, then ultimately by bulk compression.

Porous mixtures are ubiquitous in nature and extensively used as multifunctional energetic structural materials (MESMs), metallic and ceramic powders for shock consolidation, and porous armor materials. These materials include thermites, intermetallics, metal-polymer mixtures, metastable intermolecular composites (MICs), matrix materials, and hydrides.^{2,3} Chemical reactions may occur in powder systems due to shock loading, which can be separated in two categories, i.e., shock induced reaction and shock assisted reaction.⁴ In order to analyze the dynamic behavior of a particular porous solid mixture in any given situation, a constitutive equation describing the porous mixture is required.

In the case of porous material for a single element, a number of EOS are available in the literature based on work by McQueen and Marsh,⁵ Herrmann,⁶ and Salvadori et al.⁷ Here a "snow plow" model, which neglects the compaction process, was used for porous materials with an assumption of the porosity being removed at a very low stress. Dijken and De Hossen⁸ gave different methods for Hugoniot curves for normal and anomalous cases based on the assumption that a powder at zero pressure from V_{00} (the specific volume for a porous material) to V_0 (the specific volume for a solid material) does not alter the internal energy. Oh and Persson⁹ derived eight equations for porous materials using the linear relationship between the shock wave velocity and the particle velocity. Simons and Legner¹⁰ obtained the Hugoniot pressure in terms of the cold pressure, energy, and density for a porous material. Wu and Jing and colleagues^{11–13} and Boshoff-Mostert and Viljoen¹⁴ derived an alternative equation of state that has the same form as the Mie-Grüneisen EOS by using the specific enthalpy. For a solid multi-component mixture, an important acknowledged contribution is the so-called zero temperature mixture theory recommended by Meyers,¹⁵ and McQueen et al.,¹⁶ which eliminates the temperature effect of different components. Such a theory was used to calculate the 0 K isotherm for two constituents by using mass averages of the specific volume, the cold internal energy, and the Grüneisen coefficient. Yoshida¹⁷ developed

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a computer code based on the above theory for EOS of multi-component mixtures. By assuming that the components are in thermal equilibrium, Duvall and Taylor¹⁸ used a mixture method that relies on knowing the component's Gibbs free energy. Barry and Thad¹⁹ presented a Hugoniot theory for solid or powder mixtures by assuming a linear dependence of the isothermal bulk modulus with pressure. Reding and Hanagud^{20,21} proposed two new EOS algorithms which could be used to physically interpret both the homobaric and the uniform strain assumptions. Recently, Reding²² introduced a multiscale modeling approach to simulate the mechanical response in porous energetic mixtures under shock loading within a multiscale framework. The pore collapse model introduced parameters that could capture microstructural effects due to changes in mixture morphology, which were incorporated into the gas-gun simulations and experimental results for the Ni + Al mixture.

A popular approach for multi-component mixtures is the zero temperature mixture theory developed by McQueen *et al.*¹⁶ A common drawback of it, however, is that it uses mass averages for the Grüneisen coefficient, which assumes the Grüneisen coefficient is linearly related to the specific volume. In fact, according to Vocadlo *et al.*'s results,²³ the Grüneisen coefficient has a non-linear relationship with the specific volume. A more accurate equation for the Grüneisen coefficient should be used for the zero temperature mixture rules.

The purpose of this paper is to present a cold energy mixture theory for equation of state in solid or porous metal mixtures subjected to shock compression. It is a combination of the cold energy mixture theory and an extension of Wu and Jing's^{11–13} work. In the model the cold internal energy mixture theory at zero temperature is used to calculate the isotherm of the components to avoid temperature effects on the mixtures. Here Wu and Jing's method is used for the Hugoniot of porous material. Dynamic shock response of solid or porous powder mixtures compacted by shock waves has been analyzed based on the mixture theory and the Hugoniot for porous materials. The model is tested on both single-component porous materials, such as aluminum 2024, copper, and iron; and on two or three component mixtures such as W/Cu, Fe/Ni, and Al/Ni.

II. BACKGROUND

A. Hugoniot relations for solid materials

With the assumption that the shock profile is steady in time, the Rankine-Hugoniot equations are derived from the mass, momentum, and energy conservation equations. In Lagrangian coordinates the jump conditions can be expressed as

$$\rho_0 U_s = \rho \left(U_s - U_p \right) \tag{1}$$

$$P - P_0 = \rho_0 U_s U_p \tag{2}$$

$$E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V)$$
(3)

where $\rho_0(1/V_0)$ is the initial density of the solid, $\rho_1(1/V)$ is the shocked density, U_p is the particle velocity, U_s is the shock wave velocity, P_0 is the initial pressure, P is the shock pressure, and E_0 and E are the initial and final specific internal energy of the material, respectively.

The shock pressure P(V,T) and internal energy E(V,T) can be written as:

$$P(V,T) = P_c(V) + P_T(V,T) + P_e(V,T)$$
(4)

$$E(V,T) = E_c(V) + E_T(V,T) + E_e(V,T)$$
(5)

where $P_c(V)$ and $E_c(V)$ are the cold (elastic) pressure and cold (elastic) internal energy, respectively. $P_e(V,T)$ and $E_e(V,T)$ are the pressure and internal energy contribution due to thermal excitation of the electrons, respectively. For most of the materials, the electronic contributions are negligible at temperatures below approximately 101000 K.²⁴

Internal energy E is the function of the heat capacity at a constant volume C_V and temperature T,

$$E = C_V T. (6)$$

One model that is used extensively is the Mie-Grüneisen EOS given by Eliezer *et al.*, 25

$$P_T(V,T) = \frac{\gamma(V)}{V} E_T(V,T).$$
(7)

From Eq. (4) there is

$$P - P_c = \frac{\gamma(V)}{V} (E - E_c) \tag{8}$$

where $\gamma(V)$ is the Grüneisen coefficient, which is assumed to be a function of the specific volume *V*.

The pressure obtained in the Hugoniot is much higher than atmospheric pressure. Therefore, the initial conditions for pressure in Eqs. (2) and (3), $P_0 = 0$, are equivalent to the initial conditions for shock wave experiments. According to Eq. (3), the Hugoniot pressure in terms of V, $P_c(V)$, and $E_c(V)$ is written as

$$P(V) = \frac{\frac{V}{\gamma(V)}P_c(V) - E_c(V)}{\frac{V}{\gamma(V)} - \frac{1}{2}(V_0 - V)}.$$
(9)

B. Equation of state for solid powder mixtures

As discussed before, a popular approach for multi-component mixtures is the zero temperature mixture theory developed by McQueen *et al.*¹⁶ From the 0 K isotherm for the mixture/alloy, obtain the shock Hugoniot for the alloy using the same equation,

$$(P_H - P_{0K}) = \frac{\gamma_0}{V_0} (E_H - E_{0K})$$
(10)

where volume, cold energy, and the ratio V/γ are obtained based on a mass fraction basis,

$$V = \sum m_i V_i \quad \frac{V}{\gamma} = \sum m_i \left(\frac{V}{\gamma}\right)_i \quad E_K = \sum m_i E_i.$$
(11)

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From the Hugoniot theory for two-component mixtures proposed by Barry,¹⁹ two preliminary assumptions are made, i.e., (1) the components are at an equal pressure, and (2) particle velocity and average methods are used to determine the properties:

$$V(P) = \sum_{i=1}^{N} m_i V_i(P)$$
 (12)

$$E_C(V) = \sum_{i=1}^{N} m_i E_{Ci}(V)$$
 (13)

$$\sum_{i=1}^{N} m_i = 1$$
 (14)

where m_i is the mass fraction of component materials. The cold (elastic) internal energy can be calculated by using the zero-mixture theory in Eq. (13).

From the Born-Meyer theory for cold (elastic) pressure and internal energy,²⁶ the $P_c(V)$ and $E_c(V)$ are expressed in the form of

$$E_C(\delta) = \frac{3Q}{\rho_{0\mathrm{K}}} \left\{ \frac{1}{q} \exp\left[q\left(1 - \delta^{-1/3}\right)\right] - \delta^{1/3} - \frac{1}{q} + 1 \right\}$$
(15)

$$P_{C}(\delta) = Q\delta^{2/3} \left\{ \exp\left[q\left(1 - \delta^{-1/3}\right)\right] - \delta^{2/3} \right\}$$
(16)

$$\delta = \frac{\rho}{\rho_{0\mathrm{K}}} = \frac{V_{0\mathrm{K}}}{V} \tag{17}$$

where Q, q, and $\rho_{0\rm K}(V_{0\rm K})$ are parameters for cold energy and the initial density of a material or mixture at 0 K, respectively. $\delta(V_{0\rm K}/V)$ is the compressibility.

Following the descriptions given by Hu and Jing,²⁷ the parameters Q, q can be written as:

$$\lambda = \frac{1}{12} \frac{q^2 + 6q - 18}{q - 2} \tag{18}$$

$$C_0^2 = \frac{Q(q-2)}{3\rho_{0\rm K}}$$
(19)

$$C_0 = C'_0 \left[1 + \left(2\lambda' - \frac{\gamma_0^2}{4} - 1 \right) \alpha_\nu T_0 \right]$$
(20)

$$\lambda = \lambda' \left[1 + \left(\frac{\lambda'}{2} - \frac{1}{8} \frac{\gamma_0^2}{\lambda'} - 1 \right) \alpha_v T_0 \right]$$
(21)

where C_0 is the zero pressure bulk sound speed, λ is related to the binding energy and repulsive potential of the solid material, α_v is the coefficient of cubic expansion, and C'_0 and λ' are the material constants at 0 K.

III. EQUATION OF STATE FOR A MULTI-COMPONENT MIXTURE WITH POROSITY

A. Wu and Jing's Method

The present method for porous materials in this paper is based on Hugoniot curves for porous materials proposed by Wu and Jing and colleagues^{11–13} and Boshoff-Mostert and Viljoen.¹⁴ Following Wu and Jing's theory, the relevant equation of state for a solid and the corresponding porous material can be written in the following forms:

$$V_H - V_C = \frac{R}{P} (H - H_C) \tag{22}$$

$$V'_{H} - V'_{C} = \frac{R}{P} \left(H' - H'_{C} \right)$$
 (23)

where V_H , V'_H , V_C , V'_C , H, H', H_C , and H'_C are the specific volume, the cold specific volume, the specific enthalpy, and the cold specific enthalpy for a solid and porous material, respectively.

Following the definition of the specific enthalpy, for solid materials there are the following equations:

$$H_C = PV_C + E_C \tag{24}$$

$$H = E_0 + \frac{1}{2}P(V_0 + V)$$
(25)

and, for the porous materials

$$H_{C}^{'} = PV_{C}^{'} + E_{C}^{'}$$
 (26)

$$H' = E_{00} + \frac{1}{2}P(V_{00} + V')$$
(27)

where E_0 and E_{00} are the initial specific internal energy of solid and porous materials, respectively. V_0 and V_{00} are the initial specific volume of solid and porous materials.

According to Wu and Jing's^{11–13} assumption, the parameter *R* has the same value for both solid and porous materials under isobaric conditions. Combining Eqs. (22)–(27) results in a relationship between the porous Hugoniot and the solid Hugoniot under isobaric conditions,

$$\frac{V_H - V_C}{E_0 + \frac{1}{2}P(V_0 + V_H) - PV_C - E_C} = \frac{V'_H - V'_C}{E_{00} + \frac{1}{2}P(V_{00} + V'_H) - PV'_C - E'_C}.$$
 (28)

Equation (28) is the combined Hugoniot EOS of porous and solid materials, and can be used to solve for V'_{H} . Note the cold specific volume V'_{C} and the cold internal energy E'_{C} for porous material should be determined before calculations.

B. Cold specific volume of solid and porous materials

The Born-Mayer potential is used to describe the 0 K isotherm of a solid as:

$$P = Q\left(\frac{V_{0K}}{V_C}\right)^{2/3} \left(\exp\left\{q\left[1 - \left(\frac{V_{0K}}{V_C}\right)^{-1/3}\right]\right\} - \left(\frac{V_{0K}}{V_C}\right)^{2/3}\right)$$
(29)

where Q and q are two material constants and V_{0K} is the initial specific volume of the material at 0 K. Eq. (29) shows

Material	$\rho_0 (\text{g/cm}^3)$	$C_{0}^{'}$ (km/s)	λ'	γ _o	$\alpha_v (10^{-5}/\mathrm{K})$	Y (GPa)
Copper ^a	8.924	3.973	1.498	1.97	5.01	0.448
Aluminum-2024 ^a	2.784	5.370	1.290	2.18	6.93	0.276
Iron ^a	7.856	3.780	1.652	1.81	3.51	0.456
Nickel ^a	8.875	4.590	1.440	2.00	3.81	0.380
Tungsten ^a	19.200	4.040	1.230	1.78	1.38	1.729
Hematite ^b	5.274	4.450	1.323	1.99	1.50	/
Epoxy ^b	1.198	2.480	1.395	0.58	3.5	/

TABLE I. The material parameters related to the calculations.

^aRef. 31.

^bRef. 22.

the relationship that links V_C to P for a solid material. When the value of pressure is known, the cold volume can be calculated by using interpolation methods in Eq. (29).

As shown by Wu and Jing,¹¹ a parameter of porosity for a porous material at 0 K, α_C , is defined as

$$\alpha_C = \frac{V'_C}{V_C} \tag{30}$$

The porosity α_C can be described by Carroll and Holt's²⁸ model, i.e.,

$$\alpha_C \approx \begin{cases} \alpha_0 & 0 < P < P_{\text{crit}} \\ \frac{1}{1 - \exp(-3P/2Y)} P_{\text{crit}} < P < \infty \end{cases}$$
(31)

where α_0 is the initial porosity at ambient conditions and $\alpha_0 = V_{00}/V_0$; *Y* and *P*_{crit} are the strength of the matrix material and the elastic critical pressure of a porous material at ambient conditions, respectively. The value of *P*_{crit} can be given in the form of¹¹

$$P_{\rm crit} = \frac{2}{3} Y \ln \frac{\alpha_0}{\alpha_0 - 1}.$$
 (32)

C. Variation of the Grüneisen coefficient y with volume

The Grüneisen coefficient is an important quantity in physics, as it often appears in equations that describe the

thermo-elastic behavior of a material under high pressures and temperatures. The parameter γ is simply dependent on volume *V*, and can be expressed as $\gamma(V) = \left(\frac{K_T}{C_V}\right) \left(\frac{\partial V}{\partial T}\right)_P$. It has been experimentally demonstrated for most metallic materials that the Grüneisen coefficient γ can be described by the Dugdale-MacDonald relationship⁵ as

$$\gamma(\delta) = -\frac{V_C}{2} \frac{d^2 \left(P V_C^{2/3}\right) / dV_C^2}{d \left(P V_C^{2/3}\right) / dV_C} - \frac{1}{3}.$$
 (33)

Substituting the Born-Mayer potential from Eq. (16) into Eq. (33), γ can be expressed as

$$\gamma(\delta) = \frac{1}{6} \frac{q^2 \delta^{-\frac{1}{3}} \cdot \exp\left[q\left(1 - \delta^{-\frac{1}{3}}\right)\right] - 6\delta}{q \cdot \exp\left[q\left(1 - \delta^{-\frac{1}{3}}\right)\right] - 2\delta}.$$
 (34)

IV. APPLICATIONS TO SOLID AND POROUS TWO-COMPONENT MIXTURES

In the present research, we first determine the Hugoniot for a solid mixture by using the mixture theory of the cold internal energy E_C in Eq. (13). We also find the cold pressure of the solid mixture, which is computed by $P_C = dE_C/dV_C$.



FIG. 1. Comparison of the present method and the zero-temperature isotherm (Ref. 16): (a) γ/V vs compressibility δ ; (b) pressure vs the relative volume relationship.

TABLE II.	Results	of Hugoniot	calculations	for s	single-compo	nent	materials.	т	is	the	inverse	of	porosity
$m = V_{00}/V_0;$	C_0^* and L	S [*] are linear i	terative value	es fro	m experiment	ts (R	ef. <mark>30</mark>).						

Material	$\rho_0 ({\rm g/cm^3})$	C_0^* (km/s)	m/s) S^* C_0 (Calc.) (km/s)		S (Calc.)
Copper					
m = 1.00	8.924	3.910	1.509	4.034	1.517
m = 1.13	7.900	2.551	1.769	2.478	1.826
m = 1.22	7.314	2.077	1.778	1.975	1.844
m = 1.42	6.326	1.411	1.789	1.328	1.818
m = 1.57	5.742	1.050	1.830	1.106	1.449
m = 1.98	4.508	0.941	1.514	1.021	1.412
Aluminum 20	24				
m = 1.00	2.784	5.370	1.295	4.995	1.413
m = 1.09	2.559	3.843	1.602	3.866	1.568
m = 1.25	2.224	2.503	1.781	2.496	1.701
m = 1.42	1.955	1.717	1.782	1.728	1.711
m = 1.68	1.661	1.161	1.750	1.194	1.665
Iron					
m = 1.00	7.856	3.834	1.627	3.570	1.834
m = 1.13	6.972	2.571	1.775	2.509	1.902
m = 1.31	5.982	1.871	1.737	1.715	1.885
m = 1.65	4.743	0.644	1.911	0.624	1.880
m = 2.33	3.368	0.146	1.730	0.136	1.724

Then E_C-V and P_C-V curves are determined for multi-component mixtures. The material constants Q and qare calculated using the non-linear iterative method known as the Levenberg-Marquardt algorithm²⁹ for obtaining the best fit of the E_C-V and P_C-V curves. Then the Hugoniot for the porous material is determined using Wu and Jing's theory based on the Hugoniot for the solid material. Eq. (28) does not require the parameter R and other additional information, e.g., the Hugoniot Elastic Limit (HEL) required by the method of Wu and Jing.

In order to estimate validity of the proposed methods for solid and porous metal mixtures, another equation for the Hugoniot curve that is based on the linear relationship for the shock wave velocity U_s and the particle velocity U_p is used to compare the calculated Hugoniot with the experimental results. From experimental data it is known that the relationship between U_s and U_p can be approximated very well by¹⁷

$$U_s = C_0 + SU_p. \tag{35}$$

The expression for the pressure behind the shock wave is given by^{17}

$$P(V) = \frac{C^2(V_0 - V)}{\left[V_0 - S(V_0 - V)\right]^2}$$
(36)



FIG. 2. The calculated and experimental (Ref. 30) Hugoniots for porous copper with different initial densities: (a) pressure vs relative volume relationship; (b) shock velocity vs particle velocity relationship.



FIG. 3. The calculated and experimental (Ref. 30) Hugoniots for porous aluminum-2024 with different initial densities: (a) pressure vs relative volume relationship; (b) shock velocity vs particle velocity relationship.

where V_0 is the initial specific volume for both solid and porous materials.

A. Comparison of methods with the zero-temperature isotherm

Comparing with the well known zero-temperature mixture theory developed by McQueen,^{17,18} the present method for EOS of multi-component solids can complement it by using an accurate equation for the Grüneisen coefficient. Some comparisons between the present method and the zerotemperature Isotherm were presented by calculating the γ/V and Hugoniot curves for tungsten, sintered with 24 wt. % infiltrated copper. The data that were needed for each method are given in Table I. Figure 1 shows variation of the ratio of the Grüneisen coefficient to the specific volume against the compressibility and the Hugoniot curves of different methods. As can be seen from Fig. 1, the Grüneisen coefficient shows a non-linear relationship with the specific volume in the present method. The Hugoniot of the zero-temperature isotherm and the present method are indistinguishable, and agree closely with the experimental data at thelow pressures. However, at pressures higher than 300 GPa the present method gives higher prediction values than those given by McQueen's method for the same relative volume.

B. Applications to a single-component material

Hugoniot curves for a solid single-component material were calculated using the methods outlined in the previous section, i.e., Eqs. (15) and (16) for the cold pressure and cold internal energy, Eq. (34) for the Grüneisen coefficient γ , and Eq. (9) for the *P*-*V* relationship. The data required for comparisons between the experimental and the calculated results for solid and porous materials are available for copper, aluminum-2024, and iron. The material parameters related to



FIG. 4. The calculated and experimental (Ref. 30) Hugoniots for porous iron with different initial densities: (a) pressure vs relative volume relationship; (b) shock velocity vs particle velocity relationship.

TABLE III. The calculated values of solid mixtures.

Material	$\rho_{0\mathrm{K}} (\mathrm{g/cm^3})$	$C_{0\mathrm{K}}$ (km/s)	$\lambda_{0\mathrm{K}}$	Q (GPa)	q
W/Cu (76/24)	15.171	4.009	1.307	121.478	8.022
W/Cu (68/32)	14.165	4.214	1.330	108.522	8.280
W/Cu (55/45)	12.787	3.998	1.365	91.853	8.676
W/Cu (25/75)	10.442	4.123	1.431	60.551	9.312
Fe/Ni (90/10)	8.025	3.915	1.621	38.227	11.656
Fe/Ni (82.1/17.9)	8.094	3.982	1.601	40.869	11.423
Fe/Ni (73.8/26.2)	8.168	4.051	1.581	43.778	11.188

the calculations for seven elements are tabulated in Table I, which were taken from Xu and Zhang³¹ and Reding.²² The comparison between the calculated and experimental³⁰ results is listed in Table II and Figs. 2-4. As can be seen in Table II, the calculated values of both the zero pressure sound velocity C_0 and constant S match the experimental data reasonably well. Also it is shown from these figures that the calculated results agree well with the corresponding experimental results over a wide pressure range. The comparison between the calculated and experimental results indicates that the theory can be used to quantitatively determine the Hugoniot of single-component material. It is important to point out that the present model requires only limited thermodynamic static parameters of solid materials. The Hugoniots calculated for different porosities are in close agreement with the experimental data. This, together with the results discussed for solid materials, shows that the shock response of a porosity material can be accurately described using the present methods. This implies that the extension of the model to porous mixtures may be sufficiently accurate when a Hugoniot of a multi-component mixture is determined. In the following section, the Hugoniots of two-component mixtures are discussed.

C. Applications to solid two-component mixtures

The key point of this paper is to present the Hugoniot theory for two-component mixtures. Experimental results of sintered tungsten infiltrated with copper, and of iron with nickel from the literature³⁰ are used for estimating the validity of the proposed methods for two-component mixtures. The calculated static values for solid mixtures are shown in Table III, where the material constants Q and q are determined by using the averaged properties of the cold internal energy E_C and the non-linear iterative method. The calculated and experimental results for solid mixtures with differ-

ent mass fractions of the components are shown in Table IV and Figs. 5 and 6. The experimental and calculated zero pressure sound velocity C_0 and the material constant S are tabulated in Table IV as well. The pressure P versus relative volume (V_H/V_{00}) plots for W/Cu and Fe/Ni mixtures are shown in Figs. 5 and 6, respectively. There is a little difference between the average density ρ_{00} and the theoretical density from the mixture theory, which means the mixtures may have some porosity properties. A good fit to experimental data from the calculated Hugoniot is observed (Table IV) by assuming averaged properties of the cold internal energy of mixture components. It is interesting that the calculated Hugoniots are nonlinear at lower particle velocity especially for W/Cu mixtures (Fig. 5(b)), although the limited experimental points are also nonlinear. This phenomenon is due to the smaller thermal energy at the low particle velocity. As can be seen from Fig. 5, the pressure versus relative volume curves are different from one another, due to the different mechanical properties of W and Cu (Table I). When the static mechanical parameters have little difference between the components, the calculated Hugoniots have almost no differences with one another, which can be seen in Fig. 6 for the mixtures of Fe and Ni.

D. Applications to porous multi-component mixtures

As discussed above, most of the MESMs have porous properties, and a direct way for determining the Hugoniots is to understand the necessary porous nature of the MESMs under shock loading. Unfortunately, few Hugoniots of well-characterized mixtures have been determined experimentally. However, limited data are available in the literature^{21,32} that give comparisons of porosity in slightly distended mixtures of an epoxy-bonded thermite system $(Al + Fe_2O_3)$ and aluminum/nickel. The input material parameters are listed in Table I. Due to the limited parameters for epoxy, a non-linear iterative method is used to determine the zero pressure sound velocity C_0 and constant S based on the experimental data from Ref. 30 for epoxy. The input parameters for Fe₂O₃ are obtained from the simulation work of Reding and Hanagud.^{20,21} The material constants are calculated first, which are shown in Table V. The comparisons between the calculated and the experimental results are listed in Table VI and Figs. 7 and 8. The zero pressure sound velocity C_0 and constant S are obtained from the discrete particle simulation results of Al/Ni mixtures presented by Eakins and Thadhani.³²

TABLE IV. Results of Hugoniot calculations for solid mixtures. C_0^* and S^* are linear iterative values from experiments (Ref. 30).

Material	$\rho_0 ({\rm g/cm^3})$	$\rho_{00} ({ m g/cm}^3)$	C_0^{*} (km/s)	S^*	C_0 (Calc.) (km/s)	S (Calc.)
W/Cu (76/24)	15.171	14.852	3.473	1.485	3.540	1.451
W/Cu (68/32)	14.165	13.812	3.693	1.438	3.545	1.466
W/Cu (55/45)	12.787	12.315	3.276	1.590	3.219	1.567
W/Cu (25/75)	10.442	9.691	2.789	1.780	2.853	1.742
Fe/Ni (90/10)	7.940	7.886	4.071	1.507	3.823	1.543
Fe/Ni (82.1/17.9)	8.008	7.962	4.179	1.511	3.885	1.583
Fe/Ni (73.8/26.2)	8.080	7.974	4.088	1.494	3.835	1.611



FIG. 5. The calculated and experimental (Ref. 30) Hugoniots for W/Cu mixtures: (a) pressure vs relative volume relationship; (b) shock velocity vs particle velocity relationship.

As can be seen from Table VI and Fig. 7, there are relatively large discrepancies between the calculated and the experimental values (C_0 and S) for Al/Ni mixtures initially. This may be due to the error of the simulation results; as an extreme example, the simulated zero pressure sound velocity is consistently higher than the average value of Al and Ni for porosity of 0.8. This indicates that further theoretical and experimental work is needed to determine a reasonably accurate value. The $P - U_p$ and $U_s - U_p$ relationships calculated from the model and from the experimental results are plotted in Fig. 8. The shock velocity calculations agree well with the experimental data in the low-velocity regime with $U_p < 1200$ m/s and the differences between them become somewhat large in the high-velocity regime with $U_p > 1200$ m/s. This is probably due to the isothermal volumetric compression caused artificial pressure-volume effects, which has been analyzed by Reding.²⁰

V. DISCUSSION

The proposed thermodynamics EOS for porous and solid multi-component mixtures discussed in this paper are essentially based on two assumptions: (1) The components are under equal pressures and particle velocities behind the shock discontinuity, which is often called homobaric. (2) A rigid elasto-plastic model is used during the compression process of volume change V_{00} to V_0 given by Carroll and Holt.²⁸

The first assumption is based on the fact that no contradictory experimental evidence has been found in the previous experimental results. Most of the experimental evidence shows that the pressure equilibration will occur during the shock rising time within tens of nanoseconds and the components have an equal particle velocity behind the shock discontinuity. The second assumption is based on the volume change from V'_C to V_C being within a very small range during



FIG. 6. The calculated and experimental (Ref. 30) Hugoniots for Fe/Ni mixtures: (a) pressure vs relative volume relationship; (b) shock velocity vs particle velocity relationship.

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TABLE V. The calculated values of solid mixtures.

Material	$\rho_{0k} (g/cm^3)$	$C_{0\mathrm{K}}$ (km/s)	$\lambda_{0\mathrm{K}}$	Q (GPa)	q
Al/Ni (70/30)	3.576	5.182	1.312	47.485	8.067
Al/Fe ₂ O ₃ /epoxy (12.63/37.37/50)	1.894	3.804	1.345	15.375	7.312

TABLE VI. Results of the Hugoniot calculations for porous solid power mixtures. C_0^* and S^* are linear iterative values from experiments (Refs. 32 and 33).

Material	$\rho_0 ({\rm g/cm^3})$	$ ho_{00} ({ m g/cm}^3)$	C_0^* (km/s)	S^{*}	C_0 (Calc.)(km/s)	S (Calc.)
Al/Ni(70/30)	3.506	3.506	/	/	4.761	1.451
		2.805	5.667	2.185	3.223	1.485
		2.104	2.242	1.863	2.033	1.418
	1.874	1.823	1.363	1.698	1.161	1.476
		1.578	0.796	1.593	0.767	1.461
Al/Fe ₂ O ₃ //PETF (12.63/37.37/50)		1.850	3.180	1.160	3.371	1.401



FIG. 7. The calculated Hugoniots for porous Al/Ni with different initial densities: (a) pressure vs relative volume relationship; (b) shock velocity vs particle velocity relationship.



FIG. 8. The calculated Hugoniots for $Al/Fe_2O_3/epoxy$ mixture: (a) shock velocity vs particle velocity relationship; (b) pressure vs particle velocity relationship.

the shock compression. Compared with the existing models, the advantages of the currently proposed method are as follows: (1) The proposed method uses only the averaged quantities of the volume and energy mass fraction, so that mass averaging of the bulk modulus is avoided. (2) The method does not require either additional information about HEL or the integration constant, as do the methods of Wu and Jing¹¹ or Boshoff-Mostert and Viljoen.¹⁴ The input material constants can be relatively easily determined from solid materials. (3) In contrast to the popular approach developed by McQueen and Marsh,⁵ a thermodynamics expression for the Grüneisen coefficient $\gamma(V)$ is used to determine the Hugoniot curves of two-component mixtures, which gives a physical description of the dependence of the Grüneisen coefficient on the specific volume.

Although a good agreement has been obtained between the calculated and the corresponding experimental results, the following remarks need to be pointed out.

- (1) A drawback of the calculated results is a little deviation from those of the experiments in the low pressure region. It is probably due to the simplification of the elasto-plastic model proposed by Carroll and Holt.²⁸ A modified expression for α_C of a porous material is to be developed in the next step in order to obtain more accurate predictions in the low pressure region.
- (2) The proposed model shows a good correspondence with the experimental results and a good capability, especially for porous single component and solid multi-component mixtures. However, for porous multi-component mixtures, only limited experimental data is available for verification of the proposed model. More experimental work needs to be carried out to validate the calculated results.

VI. CONCLUSIONS

A theory based on the cold internal energy mixture method has been presented to determine the Hugoniots of solid and multi-component powder mixtures using only static input parameters. The Hugoniot of the zero-temperature isotherm and the present method are indistinguishable, and agree closely with the experimental data at low pressures. However, at pressures higher than 300 GPa the present method gives higher prediction values than those given by McQueen et al.'s method for the same relative volume. For a single constituent, the Mie-Grüneisen model with cold pressure and internal energy and the Wu-Jing model were used to determine the Hugoniot curves of porous materials. For multi-component mixtures, the cold mixture theory and the Wu-Jing model were used to obtain the Hugoniot curves. The model uses empirical data to test the validity of this theoretical Hugoniot EOS for porous single components such as 2024 aluminum, copper, and iron; for solid multi-component mixtures such as W/Cu and Fe/Ni; and for porous multicomponent mixtures such as Al/Ni and Al/Fe₂O₃/epoxy. It has been shown that the theoretical calculations agree well with the corresponding experimental results, and the model presented is capable of satisfactorily predicting the Hugoniots of solid porous mixtures over a wide pressure range.

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