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A new equation of state for porous materials with ultra-low densities

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Abstract

A thermodynamic equation of state is derived which is appropriate for investigating the thermodynamic variations along isobaric paths to predict compression behaviours of porous materials. This equation-of-state model is tested on porous iron, copper, lead and tungsten with different initial densities. The calculated Hugoniot are in good agreement with the corresponding experimental data published previously. This shows that this model can satisfactorily predict the Hugoniot of porous materials with wide porosity and pressure ranges.

1. Introduction

The equation of state (EOS) for porous materials has already been well studied, especially in the low-porosity and low-pressure region, where the shock temperature is just thousands of kelvins and the contribution of thermoelectrons is negligible [1–6]. Among the theories, the one given by Wu Qiang and Jing Fuqian is particularly appropriate for it combines the P – α model with a modified Mie–Grüneisen EOS along isobaric paths, and is capable of making perfect predictions for the whole Hugoniot locus [5].

However, the situation is entirely different if high initial porosity and high pressure are introduced, for the heat generated in compression is so abundant that the contribution of thermoelectrons would rise enormously and lead to abnormal Hugoniot [7]. The EOS for porous materials under these conditions are more complicated than those mentioned above. The classical formalism of the pressure–volume relation is also invalid for it cannot describe the abnormal Hugoniot locus of shock-dilated materials.

Though some theories on the EOS for low-initial-density porous materials have been proposed, they are not all satisfactory [8–11]. In this paper, a thermodynamic EOS for thermoelectrons is derived which is appropriate for investigating the thermodynamic variations along isobaric paths. On the basis of this, we deduce a new Hugoniot EOS model including the thermoelectronic contribution, which is proposed to predict the compression behaviours of porous materials with ultra-low densities.

2. New Hugoniot EOS for porous materials

Consider a new EOS for thermoelectrons in crystals, which is a typical multiparticle system consisting of atomic nuclei and electrons, and the interactions among them. The equations of motion for this system can be written down easily. However, it is impossible to solve these complicated Schrödinger equations strictly. It has been proved that these equations can be divided into two parts: one for the electrons and the other for the nuclei, if use has been made of the Born–Oppenheimer adiabatic approximation. Here interactions between electrons and nuclei are taken as perturbations [12]. For metals, it is a good approximation to take thermoelectrons as a free Fermi gas that moves in a potential trap with an infinite depth surrounded by the surface of the crystal. In this way, the Hamiltonian of the thermoelectrons is independent of the lattice, and vice versa. In addition, the particle numbers of lattices and electrons should be conservative at shock final states. Thus, we can employ the relation [13]

$$P_e V = P V_e. \quad (1)$$

Here the subscript e labels variables contributed by thermoelectrons.

Following the suggestion by a Russian group that the electron Grüneisen parameter for most metals should be $\gamma_e \approx 1/2$ when the shock temperature $T \leq 30\,000\text{--}50\,000$ K [7], we have $V_e = \beta T^2/4P$; here β is the electronic specific heat and can be determined from $\beta = \beta_0(V/V_0)^{1/2}$ in general.

Now, we return to the lattice part of the EOS. It is convenient to ignore the phase described by the P – α model in Wu–Jing EOS model. Thus we can write down this part of the EOS directly [14]:

$$V_p - V_s = \frac{R_s}{P}(H_p - H_s). \quad (2)$$

Here subscript s labels the variables of the corresponding solid matrix and p labels those of porous materials. After some simple treatments, the final result reads

$$V_p = V_s + \frac{R_s}{2 - R_s}(V_{00} - V_0). \quad (3)$$

Here use has been made of the relationship of the enthalpy and internal energy and the definition of the Hugoniot function. V_{00} and V_0 are the initial specific volumes of the porous material and solid matrix, respectively. In fact, we have made some computations using equation (3) and compared the results with those based on the primary EOS; little deviation is observed.

Consequently, the new EOS including the thermoelectronic contribution is obtained by summing these two parts:

$$V = V_s + \frac{R_s}{2 - R_s}(V_{00} - V_0) + \frac{\beta_0 T^2}{4P} \left(\frac{V_s}{V_{0K}} \right)^{1/2}. \quad (4)$$

Here V_s is the specific volume of the corresponding solid materials at the same pressure and can be determined from the solid Hugoniot relation [7]

$$P = \rho_0 C_0^2 (1 - V_s/V_0)/(1 - \lambda(1 - V_s/V_0))^2.$$

In addition, the Wu–Jing parameter of the lattice part R_s can be calculated approximately on the shock Hugoniot of solid materials.

In order to determine the temperature appearing in equation (4), one has to reconstruct the method developed by Walsh from the differentials of enthalpy and other thermodynamic relations:

$$dH - V dP = \left(\frac{\partial H}{\partial T} \right)_P dT + \left(\frac{\partial H}{\partial P} \right)_T dP - V dP = C_P dT - T \left(\frac{\partial V}{\partial H} \right)_P \left(\frac{\partial H}{\partial T} \right)_P dP. \quad (5)$$

Table 1. Parameters for solid materials used in the calculations. (l is the anharmonicity parameter.)

	ρ_0^a (g cm ⁻³)	$\rho_0 \kappa^a$ (g cm ⁻³)	λ^a	Q^a (GPa)	q^a	C_0^a (km s ⁻¹)	l^a	β_0^a (erg g ⁻¹ K ⁻²)	C_{P0}^b (cal g ⁻¹)
Fe	7.85	7.96	1.92 ^b	39.96	11.28	3.574	8	193.9	0.091
Cu	8.93	9.05	1.51	59.72	9.89	33.91	9	174.4	0.0845
Pb	11.34	11.56	1.47	14.88	11.27	2.03	30	104.5	0.0304
W	19.2	19.31	1.23	129.59	8.58	4.04	8	83.85	0.0321

^a Xu and Zhang (see [12]).

^b Handa (see [18]).

Considering an alternative expression for the Wu–Jing EOS [5]

$$\left(\frac{dH}{dV}\right)_P = \frac{P}{R}, \quad (6)$$

and substituting it into equation (5), a relationship of the enthalpy and shock temperature is yielded:

$$dH - V dP = C_P dT - C_P T \frac{R}{P} dP. \quad (7)$$

On the other hand, from the Hugoniot relation and $H = E + PV$, an alternative expression for $dH - V dP$ is

$$dH - V dP = \frac{1}{2} \left(V_0 - V + P \frac{dV}{dP} \right) dP.$$

So, combining these relations, we obtain the equation for the shock temperature for porous materials with ultra-low densities:

$$\frac{dT}{dP} - \frac{R_s/(3R_s + 1)}{P} T = \frac{1}{2C_P} \left(V_{00} - V + P \frac{dV}{dP} \right). \quad (8)$$

Here $C_P = C_{P0}[1 + (1 + Z)^{-2}]/2 + 3\beta T/2$, Z is the degree of deviation from solid [15], and we have taken the electron Wu–Jing parameter $1/3$ and the specific heat of the electrons into account. The slope of the shock Hugoniot can be derived directly from equation (4). By just numerically solving this ordinary differential equation of order one for the shock temperature, one may acquire the shock temperature at certain pressures for certain materials.

3. Calculations and discussion

Our Hugoniot EOS model (equations (4) and (8)) is tested on porous iron, copper, lead, and tungsten with different initial densities. The agreement of the calculated temperatures with the data given by Gryaznov which were calculated using a non-ideal plasma EOS model [11, 16] validates the applicability of equation (8) in the high-temperature zone (see figure 1(a)). In fact, we have also calculated the shock temperatures of solid aluminium and iron below 10 000 K, which are all in full accord with the calculations given by Al'tshuler and McQueen, to test the application of this EOS model at low temperature. However, in view of space limitations, we have not included our findings. The calculated Hugoniots for these materials are in good agreement with the corresponding experimental data published previously [9, 11, 16, 17] (see figure 1(b)–(f)). This shows that this Hugoniot EOS model can satisfactorily predict the Hugoniots of porous materials with wide porosity and pressure ranges. However, in this EOS model we did not take the influence of phase transition into account. It seems from figure 1 that this influence should be small. We suppose this may be partly attributed to the vitrification

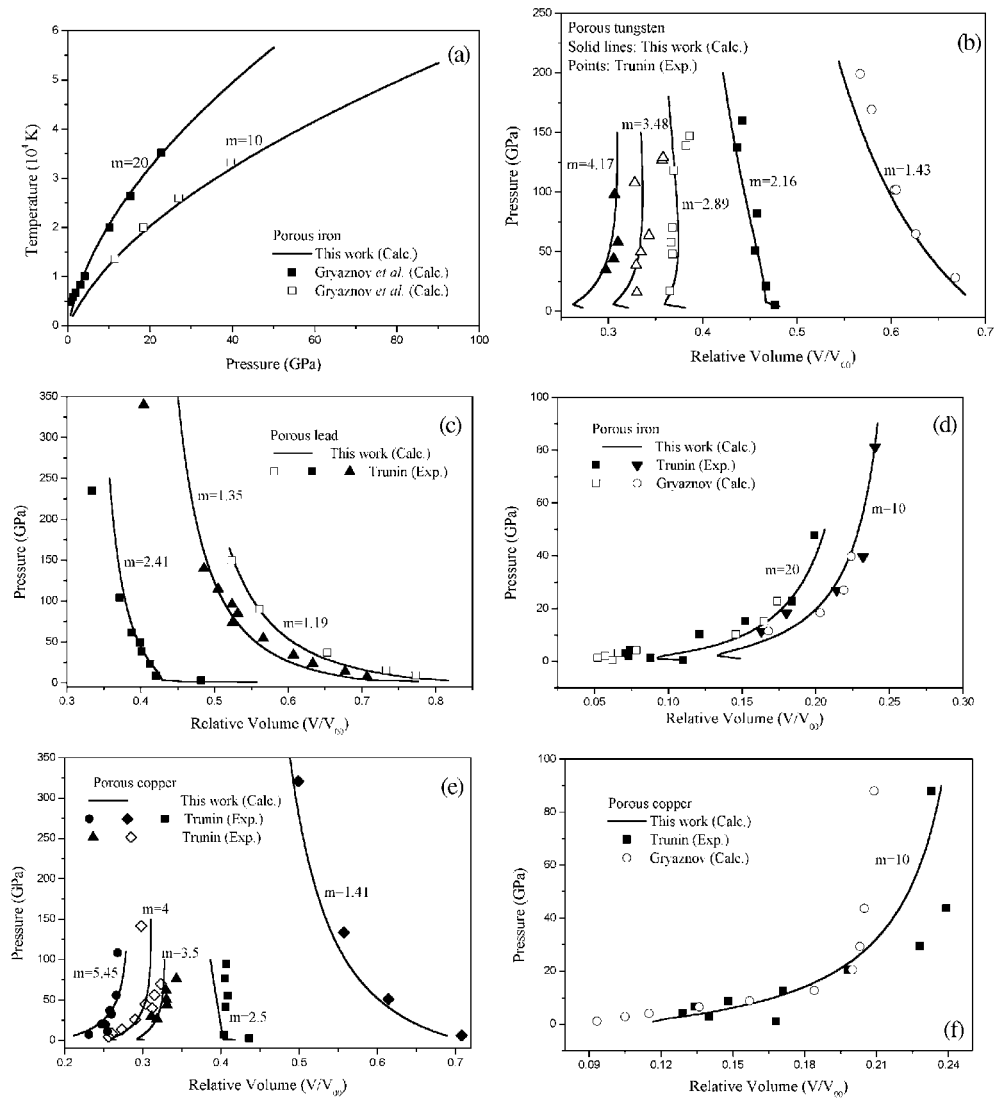


Figure 1. Calculated shock temperatures and Hugoniot for some standard porous materials with different initial densities compared with the corresponding experimental and theoretical data ($m = V_{00}/V_0$): (a) the temperature versus pressure relationship of porous iron [16]; (b)–(f) pressure versus relative volume relationships of porous tungsten, lead, iron, and copper, respectively (see [9, 17] and [16]).

of the phase transition of shocked porous materials and the fact that the region that we studied is far from the critical point.

In addition, all parameters for materials used in the calculations are listed in table 1, and no adjustable parameters were employed.

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