Shock wave response of porous materials: from plasticity to elasticity

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Abstract

Shock wave reaction results in various characteristic regimes in porous materials. The geometrical and topological properties of these regimes are highly important in practical applications. Via morphological analysis of characteristic regimes with high temperature, we investigate the thermodynamics of shocked porous materials whose mechanical properties span a wide range from hyperplasticity to elasticity. It is found that, under fixed shock strength, the total fractional area $A$ of the high-temperature regimes with $T \geq T_{th}$ and its saturation value first increase and then decrease with increasing initial yield stress $\sigma_{Y0}$, where $T_{th}$ is a given threshold value of temperature $T$. In the shock-loading procedure, the fractional area $A(t)$ may show the same behavior if $T_{th}$ and $\sigma_{Y0}$ are chosen appropriately. Under the same $A(t)$ behavior, $T_{th}$ first increases and then decreases with $\sigma_{Y0}$. At the maximum point $\sigma_{Y0M}$, the shock wave contributes maximum plastic work. Around $\sigma_{Y0M}$, two materials with different mechanical properties may share the same $A(t)$ behavior even for the same $T_{th}$. The characteristic regimes in the material with larger $\sigma_{Y0}$ are more dispersed.

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(Some figures in this article are in colour only in the electronic version.)

1. Introduction

Porous materials are ubiquitous in nature and are extensively used as industrial materials. Examples include wood, bricks, metals, foams, ceramics, carbon and explosives. The use of porous materials in parts may lead to reduced weight, improved structural and mechanical properties, better heat transfer, greater motion and deformation control, etc [1, 2]. Among others, they have also been used in surgical implant design to fabricate devices to replace or augment soft and hard tissues [3, 4]. Although the study of shock wave reaction on porous materials has a long history, most of the previous studies were focused on global behavior, such as the Hugoniot [5–12] and the equation of state [13–15]. The dynamical procedures involve much richer physical behavior but in fact are much less extensively investigated.

The main challenges for studying the dynamical behavior in shocked porous materials are twofold: the first is the numerical tool and the second is the scheme to analyze the simulation data. From the simulation side, an appropriate simulation tool must overcome two constraints. The first is the scale limitation. Molecular dynamics can discover some atomistic mechanisms of shock-induced void collapse [16, 17], but the spatial and temporal scales it may cover are far from being comparable with experiments. To overcome the scale limitation, one solution is to develop some mesoscopic particle methods. The second constraint is the numerical stability. Traditional simulation methods, both Eulerian and Lagrangian ones, when treating the dynamics of structured and/or porous materials, encountered severe difficulties. The reason is that the material under investigation is generally highly distorted during the collapse of cavities. The Eulerian description is not convenient for tracking interfaces. The Lagrangian formulation has to rezone the meshes to restore proper shapes. The mapping of state fields of mass density, velocities and stresses from the distorted mesh to the newly generated one is not easy and introduces errors. In this study, we use a mixed method, the material-point method (MPM) [18, 19], to study the shock wave reaction on porous materials. As a step to approach the shock wave dynamics in...
porous materials, we have carefully studied the cavity collapse in shocked materials [19, 20].

As for the second challenge, data analysis and picking up information, a relatively straightforward way is to study the local averaged values and the corresponding fluctuations of state variables [21]. In [21], the evolution of local turbulence mixing and volume dissipation were also studied. Shock wave reaction results in various characteristic regimes in porous materials, for example, regimes with high temperature, regimes with high pressure, regimes with high particle speeds, etc. These characteristic regimes are generally highly important in practical applications. Regimes with high temperature are places where initiation may start in energetic materials. Regimes with high pressure are places where phase transition may occur. Regimes with high particle speed are places where jet phenomena may occur. To understand the behavior, where the Minkowski functionals to measure their morphological properties, a relatively straightforward way is to study the characteristic regimes defined by the Minkowski functionals to measure their morphological behavior, where is a physical variable under consideration, such as the temperature, density, some specific stress, particle velocity or its components, and is a given threshold value.

Previous studies showed that the porous metal aluminum (Al) [22] and porous HMX-like material [23] show significant differences under shock wave reaction. To clarify the effects of single material parameters and present indicative information for material design, it is of interest to have a thorough study of the shock behavior in relation to the mechanical properties ranging from hyper-plastic to pure elastic [24].

In the present paper, we focus on characteristic regimes with high temperature. We organize the paper as follows. Section 2 briefly introduces the material model and the numerical method. Section 3 outlines the morphological characterization for characteristic regimes manifested by Turing patterns. Simulation results are shown and analyzed in section 4. Section 5 gives the conclusion.

2. The material model and MPM

The porous material is fabricated by a solid body with a number of randomly distributed voids embedded. The solid body follows an associative von Mises plasticity model with linear kinematic and isotropic hardening [21]. The pressure is calculated by using the Mie–Grüneissen equation of state, which can be written as 

\[ P = P_H = [\gamma(V)/V][E - E_H(V)], \]

where and are pressure, specific volume and energy on the Rankine–Hugoniot curve, respectively. The relation between and can be estimated by experiments and can be written as

\[
P_H = \begin{cases} 
\rho_0 c_0^2 \left( \frac{1 - V_H}{V_0} \right)^2, & V_H \leq V_0, \\
\frac{\rho_0 c_0^2}{(\lambda - 1)^2} \left( \frac{\lambda}{\lambda - 1} \times \frac{V_H}{V_0} - 1 \right), & V_H > V_0,
\end{cases}
\]  

(1)

where and are the initial density and specific volume of the solid material, is the sound speed and is the characteristic coefficient in the Hugoniot velocity relation. Both the shock compression and the plastic work are due to temperature increase of temperature. The increase of temperature from shock compression can be calculated as

\[
dT_H = \frac{c_v^2 \cdot \lambda (V_0 - V_H)^2}{c_l (\lambda - 1) V_0 - \lambda V_H} - \frac{\gamma(V)}{V_H} T_H.
\]  

(2)

where is the specific heat. Equation (2) can be derived from the thermal equation and the Mie–Grüneissen equation of state [21]. The increase of temperature from plastic work can be calculated as 

\[ dT_p = \frac{dW_p}{c_v}. \]

We model shocked materials with continuously varying mechanical properties. The reference material is the metal aluminum. The corresponding parameters are as given below: density in the solid portion is kg m\(^{-3}\), Young’s modulus is MPa, Poisson’s ratio is 0.33, initial yield is MPa, tangential modulus is MPa, sound speed is km s\(^{-1}\), characteristic coefficient in the Hugoniot velocity relation is 1.34, specific heat is J (kg K\(^{-1}\)), heat conduction coefficient is W (m K\(^{-1}\)), and the Grüneissen coefficient is 1.96. The initial temperature of the material is 300 K. In simulations, a wide range of the yield will be used.

The MPM is a relatively new particle method in computational solid mechanics. This method uses a regular structured grid as a computational scratchpad for computing spatial gradients of field variables. The grid is convected with the particles during deformations that occur over a time step, eliminating the diffusion problems associated with advection on a Eulerian grid. The grid is restored to its original location at the end of a time step. In addition to avoiding the Eulerian diffusion problem, this approach also circumvents problems with mesh entanglement that can plague fully Lagrangian-based techniques when large deformations are encountered. The MPM has also been successful in solving problems involving impact, etc. It has an advantage over traditional finite-element methods in that the use of the regular grid eliminates the need for costly searches for contact surfaces. For details of the scheme, refer to our previous publications [18, 19].

3. Outline of the morphological description

A variety of techniques can be used to describe the complex spatial distribution and time evolution of physical quantities in a shocked porous material. In this study, we concentrate on the set of statistics known as Minkowski functionals [25–27]. The Minkowski functionals have been successfully used to characterize patterns in reaction–diffusion systems [28], spinodal decomposition [29, 30], fluctuations of the cosmic microwave background [31] and block copolymer systems [32, 33] and to reconstruct complex materials [34].

Assume that is a physical quantity of interest to us; then the regions with are the characteristic regimes, where is a threshold value of . To simplify the analysis of the complex physical field, we first condense the physical field as two kinds of characteristic regimes: the white and the black. The white correspond to regimes with and the black correspond to regimes with . For such Turing patterns, a general
Theorem of integral geometry states that all the properties of a d-dimensional convex set that satisfy motion invariance and additivity (called morphological properties) are contained in \( d + 1 \) numerical values [35]. For a condensed temperature field, the white corresponds to the high-temperature regimes and the black corresponds to the low-temperature regimes. The high-temperature regimes are also generally referred to as ‘hot spots’.

For a two-dimensional temperature map, the three Minkowski functionals correspond geometrically to the total fractional area \( A \) of the high-temperature regimes, the boundary length \( L \) between the high- and low-temperature regimes per unit area and the Euler characteristic \( \chi \) per unit area (equivalent to the topological genus). When we increase the temperature threshold \( T_{th} \) from the lowest temperature to the highest one, the high-temperature area \( A \) will decrease from 1 to 0; the boundary length \( L \) first increases from 0, then arrives at a maximum value and finally decreases to 0 again. There are several ways to define the Euler characteristic \( \chi \). The simplest one is \( \chi = (Nw - Nb)/N \), where \( Nw \) (\( Nb \)) is the number of connected white (black) regimes and \( N \) is the total number of pixels. In contrast to the area \( A \) and boundary length \( L \), the Euler characteristic \( \chi \) describes the connectivity of the characteristic regimes in the material. It describes the patterns in a purely topological way, i.e. without referring to any kind of metric. It is negative (positive) if many disconnected black (white) regimes dominate the image. A vanishing Euler characteristic indicates a highly connected structure with an equal amount of black and white regimes. The ratio \( \kappa = \chi / L \) describes the mean curvature of the boundary line separating black and white regimes. For more discussions and calculation schemes of the Minkowski functionals, refer to [26, 28, 36].

Among the three Minkowski functionals, the high-temperature area \( A \) is the only one that monotonically increases in the shock-loading procedure and/or when the threshold value becomes smaller. For a given \( T_{th} \), its increase rate, \( D \), presents meaningful information. When the temperature threshold \( T_{th} \) becomes higher, \( D \) decreases. The variations of \( A \), \( L \) and \( \chi \) with \( T_{th} \) and time \( t \) form a scenario for the shock response of porous materials [22].

### 4. Simulation results and physical interpretation

If we denote the mean density of the porous body as \( \rho \), then the porosity of the material is \( \Delta = 1 - \rho / \rho_0 \). The shock to the target body is loaded by colliding with a rigid wall that is static at the bottom position \( y = 0 \). The initial velocity of the porous body \( \rho_{init} \). The collision starts at time \( t = 0 \). The height and width of the porous body are \( h \) and \( w \), respectively. Periodic boundary conditions are used in the horizontal directions, which means that the real system is composed of many simulated ones aligned periodically in the horizontal direction.

#### 4.1. The case with \( \rho_{init} = 1000 \text{ m s}^{-1} \)

Figure 1 presents a series of snapshots in the shock loading procedure, where the porosity \( \Delta = 0.5 \). Initial velocity \( \rho_{init} = 1000 \text{ m s}^{-1} \) and time \( t = 1000 \text{ ns} \). From left to right and from top to bottom, the two rows of snapshots are for the cases with \( \sigma_{y} = 12, 30, 8000, 10000, 12000, 15000 \) and 20 000 MPa, respectively. The points in the figure correspond to the material particles. The colors from blue to red correspond to increase of temperature. From figure 1, one can find the upper free surface moving down and the global compressive-waves series moving up. For each case, the initial shock wave is decomposed as a complex series of compressive and rarefactive waves. In the shock loading procedure, the compressive effects dominate. Within the shocked region, both the plastic work and shock compression make the temperature increase. In the present case, the plastic work dominates. The high-temperature regimes in materials with higher initial yields are more dispersed. The increase rate of the high-temperature area \( A(t) \) is different when the initial yield changes.

To quantify and get a more complete understanding of the shock wave response behavior, we show a set of morphological measures versus time in figure 2(a), where values of initial yields are shown in the legend. The temperature threshold here is \( T_{th} = 400 \text{ K} \). With the propagation of compressive-wave series in the porous material, the high-temperature area \( A \) first increases with time in a parabolic way, then approaches a saturation value slowly, maintains the saturation value for a period and finally decreases. The final decrease indicates that rarefactive waves are reflected back from the upper free surface and with decreasing mean pressure, a certain amount of material particles changed their temperature from \( T > T_{th} \) to \( T < T_{th} \). During the saturation period, more compressive waves arrived at the upper free surface; consequently, more rarefactive waves are reflected back into the porous body. The former tends to increase the temperature, while the latter tends to decrease it. The two effects are nearly balanced. Therefore, the high-temperature area \( A \) is nearly constant.

As for effects of the initial yield \( \sigma_{y} \), we can find two interesting phenomena: both the initial increasing rate and the saturation value of \( A \) first increase and then decrease when the material changes from being superplastic to pure elastic.

For cases checked in our numerical experiments, the increase rate \( D \) becomes larger when the initial yield \( \sigma_{y} \) increases from 0 to about 10 GPa. If \( \sigma_{y} \) further increases, \( D \) will decrease. The saturation value \( A_{S} \) of the high-temperature area becomes larger when \( \sigma_{y} \) increases from being very small to about 1 GPa. When \( \sigma_{y} \) becomes larger, the saturation value \( A_{S} \) decreases. For the time interval shown in figure 2(a), when \( \sigma_{y} > 10 \text{ GPa} \), the saturation value \( A_{S} \) decreases and the period for \( A \approx A_{S} \) becomes shorter with an increase of \( \sigma_{y} \). When \( \sigma_{y} = 12 \text{ GPa} \), \( A \approx 0.96 \) during the period 1430 ns < \( t < 2924 \text{ ns} \); when \( \sigma_{y} = 15 \text{ GPa} \), \( A \) increases slowly from 0.8 to 0.86 during the period 1245 ns < \( t < 2825 \text{ ns} \); when \( \sigma_{y} = 20 \text{ GPa} \), \( A_{S} \approx 0.52 \) and has a local minimum value 0.49 at about \( t = 1863 \text{ ns} \). When \( \sigma_{y} = 30 \text{ GPa} \), the area \( A \) remains very small.

Now we check the information given by the boundary length and Euler characteristic in figure 2(a). For all the cases shown in the figure, the boundary length \( L \) first increases and then decreases with time. The former increase corresponds to the propagation of compressive waves and the appearance
of more hot spots. The decrease of $L(t)$ is not monotonic. The initial decrease corresponds to the coalescence of some hot spots; the latter decrease corresponds to the coming in of the global rarefactive waves from the upper free surface, which results in the expanding and coalescence of some cold spots. Prominent behavior here is that for the case with $\sigma_{y0} = 20$ GPa, the boundary length $L$ has the largest value. For this case, the value of $\chi$ changes from being slightly positive to being most negative. Combining information about $A$, $L$ and $\chi$, we can know that, with the propagation of compressive wave in the porous material, the number of hot spots with $T > 400$ K quickly increases, but distributes quite scatteredly. After the corresponding compressive wave scanned all of the material body, some scattered cold spots with $T < 400$ K expand and partly coalesce due to the coming in of rarefactive waves. During this procedure, some small hot spots with $T > 400$ K disappear. Therefore, both the high-temperature area $A$ and boundary length $L$ decrease and the Euler characteristic $\chi$ becomes more negative. For other cases, the smaller the boundary length $L$, the flatter the wave front in the temperature map. The material with $\sigma_{y0} = 15$ GPa has the secondary maximum boundary length $L$ and a flatter $\chi(t)$ curve than the material with $\sigma_{y0} = 20$ GPa. This means that the numbers of hot spots and cold spots are not much different. The number of cold spots dominates slightly during the time interval shown in the figure.

In the shock-loading procedure, if we decrease the threshold value $T_{lh}$, the wave fronts in the pixelized temperature map become flatter. Consequently, the values of $L(t)$ are smaller, the $\chi(t)$ values are closer to zero and the curves for $A(t)$ become close to being linear. If we increase the threshold value $T_{lh}$, the pixelized temperature map shows different geometric and topological behavior. Examples are figures 2(b) and (c). $T_{lh} = 500$ K in figure 2(b) and $T_{lh} = 600$ K in figure 2(c). It is clear that the saturation values of $A(t)$ decrease with increasing $T_{lh}$. In the shock-loading
procedure, the material with $\sigma_{Y0} = 12$ MPa has about 20% of material particles that cannot get a temperature higher than 600 K and 5% cannot get a temperature higher than 500 K, and only 1% cannot get a temperature higher than 400 K. For the material with $\sigma_{Y0} = 120$ MPa, in the shock-loading procedure, there is about 15% of material particles that cannot get a temperature higher than 600 K, 4% cannot get a temperature higher than 500 K and only 1% cannot get a temperature higher than 400 K.

When the initial yield is very high, for example, $\sigma_{Y0} = 15$ GPa, the material is very elastic. Consequently, the saturation value $A_S$ of the high-temperature area is small. For example, $A_S = 0.15$ when $T_{th} = 600$ K, which means that 85% of the material particles cannot get a temperature higher than 600 K. For the case with $\sigma_{Y0} = 20$ GPa, $A_S = 0.54$ when $T_{th} = 400$ K, $A_S = 0.11$ when $T_{th} = 500$ K and $A_S = 0.04$ when $T_{th} = 600$ K. For the case with $\sigma_{Y0} = 30$ GPa, only 0.1% of the material particles can get a temperature higher than 600 K in the shock-loading procedure. In the temperature pattern with $T_{th} = 400$ K, the case of $\sigma_{Y0} = 20$ GPa has the largest boundary length. When $T_{th} = 500$ K, the case of $\sigma_{Y0} = 15$ GPa has the largest boundary length. When $T_{th} = 600$ K, the case of $\sigma_{Y0} = 10$ GPa has the largest $L$.

4.2. Effects of the initial shock strength

With decreasing initial shock strength, both the highest and the mean temperatures in the shocked portion decrease. A set of Minkowski measures for the shocking procedure of porous materials with various initial yields is shown in figure 3, where $\Delta = 0.5$ and $T_{th} = 400$ K. The initial impact velocities are different in figures 3(a)–(c). They are 800, 600 and 400 m s$^{-1}$, respectively. The values of initial yields are shown in the legends. Specifically, the initial yields are 12, 120, 1000, 3000, 5000, 8000, 10000, 15000 and 20000 MPa in figure 3(a); in figure 3(b), they are 12, 120, 360, 1000, 3000, 5000, 8000, 10000 and 15000 MPa; in figure 3(c) they are 12, 120, 360, 1000, 3000, 5000, 8000, 10000 and 20000 MPa. Compared with the cases shown in figure 2(a), both the saturation value $A_S$ and the increasing rate $D(T_{th})$ of the high-temperature area decrease when the initial shock becomes weaker. As an example, for the material with $\sigma_{Y0} = 1000$ MPa, when the initial impact velocity is $v_{init} = 1000$ m s$^{-1}$, 99% of material particles arrive at a temperature higher than 400 K in the shock-loading procedure; when $v_{init} = 800$ m s$^{-1}$, the fraction of material particles getting a temperature higher than 400 K is 97%; when $v_{init} = 600$ m s$^{-1}$, the fraction is 89%; when $v_{init} = 400$ m s$^{-1}$, the fraction becomes only 5%.

In figure 3(c), the case of $\sigma_{Y0} = 3000$ MPa has the maximum high-temperature area $A$, boundary length $L$ and Euler characteristic $\chi$. In this figure, after the high-temperature area $A$ reaches the maximum value, it begins to decrease, which means that, under such a shock strength, most material particles cannot get a temperature higher than 400 K; the threshold value 400 K has been very close to the highest temperature in this system. To understand better why the maximum high-temperature area occurs at about $t = 2000$ ns, we show the configurations with a condensed temperature map in figure 4, where the three snapshots are for the times $t = 1500$, 2000 and 2500 ns, respectively. The areas with temperatures higher than 400 K are shown in yellow; the other areas are shown in blue. One can find that the high-temperature area at time $t = 2000$ ns is the largest among the three snapshots. From the heights of the upper free surface, one can find that the one for $t = 2000$ ns is the lowest, which means that the shock-loading procedure

Figure 2. Minkowski measurements for cases with various initial yields, where $\Delta = 0.5$ and $v_{init} = 1000$ m s$^{-1}$. The values of $\sigma_{Y0}$ are shown in the legend in units of MPa. $T_{th} = 400$ K in (a), $T_{th} = 500$ K in (b) and $T_{th} = 600$ K in (c).
finishes at about that time. When the unloading procedure starts, the area with high temperature decreases. From figure 4 one can also find that the high-temperature regimes for $T_{th} = 400$ K have been very dispersed. This is consistent with the large value of boundary length and is consistent with the above observation that only a small portion of the material particles gets a temperature higher than 400 K under such a shock strength.

4.3. $(\sigma_{Y0}, T_{th})$ pairs for the same $A(t)$ behavior

As mentioned above, among the three Minkowski functionals, the high-temperature area $A(t)$ is the only one that is monotonic when the threshold value $T_{th}$ decreases and/or as the shock-loading procedure goes on. It is natural to check if $A(t)$ shows the same behavior when using appropriate $(\sigma_{Y0}, T_{th})$ pairs. Figure 5 shows such examples for the case with initial impact velocity $v_{init} = 1000$ m s$^{-1}$. In figure 5, the temperature threshold for the reference material, aluminum, is 420 K. From figure 5 we can find that in materials with different initial yields, if we choose an appropriate $T_{th}$ to observe, the high-temperature area $A(t)$ shows the same behavior in the shock-loading procedure. Such a property can be understood better by observing figures 1 and 4. From figures 1 and 4, it is also clear that, for a fixed shock strength, with the increasing of the initial yield, the wave front becomes wider, the high-temperature regimes become more scattered and more low-temperature domains are embedded in the compressed portion. This morphological behavior is manifested by larger boundary lengths and more negative Euler characteristics in figure 5.

If we use the $(\sigma_{Y0}, T_{th})$ pairs in figure 5 as the coordinates, we get the curve labeled $'V_{init} = 1000$ m s$^{-1}$' and 'Al: 120' in figure 6(a). For the shock strength $v_{init} = 1000$ m s$^{-1}$, the material with $\sigma_{Y0} = 5$ GPa has the maximum $T_{th}$, which is about 590 K. In this case, the shock contributes the maximum plastic work and the system has the highest temperature. If we increase the temperature threshold $T_{th}$ to 460, 540 and 570 K, we have the other three curves. Along each of them, $A(t)$ shows the same behavior in the shock-loading procedure. If we decrease the shock strength to $v_{init} = 800$, 600 and 400 m s$^{-1}$, we get the other three plots of figure 6. The maximum value point $\sigma_{Y0M}$ moves towards the lower value of
become smaller and $\chi(t)$ becomes close to zero; the curves for $A(t)$ become close to linear.

5. Conclusion

Shock wave reaction results in various characteristic regimes in porous materials. The properties of these regimes are highly important in practical applications. Based on the material-point simulation and morphological characterization, we investigate how the initial yield influences the behavior of high-temperature regimes in shocked porous materials. It is found that, under fixed shock strength, the total fractional area $A$ of high-temperature regimes $(T > T_{th})$ and its saturation value first increase and then decrease when initial yield $\sigma_{Y0}$ becomes higher. In the shock-loading procedure the fractional area $A(t)$ may show the same behavior under various choices of $T_{th}$ and $\sigma_{Y0}$. For the same $A(t)$ behavior, $T_{th}$ first increases and then decreases when $\sigma_{Y0}$ becomes higher. At the maximum point $\sigma_{YM}$, the plastic work by the shock reaches the maximum value. Among $\sigma_{YM}$, two materials with different mechanical properties may share the same $A(t)$ behavior even for the same threshold $T_{th}$. The high-temperature regimes in the material with the higher initial yield $\sigma_{Y0}$ are more dispersed. Other kinds of characteristic regimes, for example, those with high pressure, high particle speed, etc, can be studied in the same way.

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