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Molecular dynamics studies on energy dissipation and void collapse in graded nanoporous nickel under shock compression

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ABSTRACT

We present systematic investigations on energy dissipation and void collapse in graded nanoporous nickel by non-equilibrium molecular dynamics simulations. It is found that void size gradient influences the time history path of the energy dissipation. Under strong shock loading conditions, when the voids are completely collapsed, the total energy dissipation is dependent only on the porosity, and is independent of the void size gradient in the shock direction. The total energy dissipation increases with the increase of porosity. However, when the porosity increases to a critical value of 6%, the total energy dissipation reaches an upper limit. Increasing the porosity beyond this critical value would not result in further increase in energy dissipation. The simulations show that voids collapse is attributed to the combined effect of transverse and longitudinal plasticity flow of void wall. Two mechanisms of voids collapse are revealed: the plasticity mechanism and internal jetting mechanism. Under relatively weaker shocks, the plasticity mechanism, which leads to transverse collapse of voids, prevails; while at the stronger shock strengths, the internal jetting mechanism, which leads to longitudinal flow, plays a more significant role. The earliest appearing dislocations in a void may either nucleate at the front half surface or on the back half surface, depending on the position of the void in the sample and the void size gradient. Moreover, the simulations provide quantitative descriptions about the effects of loading intensity on energy dissipation rate and void collapse rate. We show that the energy dissipation rate can be well represented by a quadratic polynomial function of the shock loading velocity, and the void collapse rate is a linear function of the shock loading velocity.

1. Introduction

The porous materials, in particular metallic nanoporous foams, have attracted considerable attention with regard to shock response (Erhart and Bringa, 2005). When shock waves propagate through nanoporous materials, the energy associated with shock and blast loading could be attenuated and dissipated. Such particular characteristics are widely used in various engineering applications such as the design of safety shells for protection from explosions and porous structures for noise reduction in high speed railway tunnels (M.W. M.W. Seitz and Skews, 2006; Evans and Hutchinson, 1998). For these applications, it is important to understand the thermo-mechanical behaviors of metallic nanoporous materials under shock loading (M.Z. Xiang et al., 2013).

Several researchers have investigated the dynamics response of porous materials at macroscale experimentally (Butcher et al., 1974; Carroll and Holt, 1972; Bonnan et al., 1998; Héreil et al., 1997; Powell, 2003; Yasuhara et al., 1996; Zeng et al., 2010; Kitagawa et al., 2006; Kazemikamyab et al., 2011; M.W. M.W. Seitz and Skews, 2006), theoretically (Singh et al., 2010; Nield and Bejan, 2006; Fellah and Depollier, 2000; Madeo and Gavrilyuk, 2010; Polenov and Chigarev, 2010; Bruck, 2000) and by numerical simulation (Roschning and Huber, 2016; Ruan et al., 2003; Liu et al., 2012; Fan et al., 2013). For example, Butcher et al. (1974) have used quartz pressure sensor to study the shock compression characteristics of powder metallurgically-foamed aluminum with 22% porosity, and verified the validity of model developed by Carroll and Holt (1972) by comparing predicted steady-wave rise times with measured stress-wave profile data. Bonnan et al. (1998) and Héreil et al. (1997) have used polyvinylidene fluoride (PVDF) piezoelectric gages and velocity interferometer system for any reflector to record the stress history and particle velocity

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history, respectively, and obtained the shock adiabatic curves of foamed aluminum with 9% and 17% porosity. Powell (Powell, 2003) has experimentally investigated the energy absorption rate of aluminum foam-filled braided tubes. His results have shown that the energy absorbed by unit volume foam aluminum is proportional to the density.

Yasuhara et al. (1996) have analyzed the influence of porosity and internal structure in polyurethane foam on the distal stress of impacted samples. Zeng et al. (2010) have performed a series of experiments to test the influence of density gradient on the impact behavior of functionally graded cellular materials. It is found that the gradient profile plays an important role in both the energy absorption and the transmitted force when the equilibrium state is not reached, nevertheless, the density gradient profile has a rather limited effect on the energy absorption capacity when the equilibrium state can be reached rather quickly. Kitagawa et al. (2006) have observed the shock wave attenuation in the polyurethane foam. Their experimental results have indicated that the change of momentum loss in the material depends on the structure and quantity of voids, and the inertia of material has no effect on the pressure recovery. Kazemikamyab et al. (2011) have obtained the shock dynamics response of porous aluminum via the modified Hopkinson Bar. They have decomposed the stress signal into two parts: high frequency and low frequency. Such a decomposition can distinguish between the effect of gas pressure in the pore and that of stress in the matrix material. Furthermore, it has been found that the wave interaction in the lower porosity material could lead to the oscillation of stress signal. M.W. Seitz and Skews (2006) have presented the semiempirical formulas on permeability and tortuosity of typical foam materials and provided a large amount of valuable experimental data for setting up the quantitative relationship between the properties (permeability, tortuosity, stiffness and cell morphology) of foam materials and pressure amplification factor under shock loading condition.

In addition, some scholars have established corresponding mathematical model for the propagation of one-dimensional stress wave in the ideal porous medium (Singh et al., 2010; Nield and Bejan, 2006; Fellah and Depollier, 2000; Madeo and Gavrilyuk, 2010; Polenov and Chigarev, 2010; Bruck, 2000). For instance, Bruck (2000) has formulated a one-dimensional wave propagation model in porous functionally graded materials (PFGMs) to investigate the stress peak and the time delay in PFGMs. It is concluded that the optimal architecture for attenuating stress waves in PFGMs will depend greatly upon the design stress for the reflected wave. These mathematical models have reference value for studying the propagation characteristics of stress wave in the porous medium, but it is difficult to use them in practice.

Numerical simulation software based on continuum mechanics, such as LS-DYNA and ABAQUS, are widely used for investigating dynamic behaviors of porous materials. Roschning and Huber (2016) have set up the quantitative relationship between structural disorder and macroscopic mechanical properties (elasticity modulus, Poisson's ratio and yield strength) in the nano-porous gold by means of finite element method. Ruan et al. (2003) researched the dynamic behavior of hexagonal aluminum honeycombs by means of finite element simulation using ABAQUS. It is shown that the deformation modes of honeycombs under dynamic loading are related to impact velocity. Three different types of deformation modes, i.e., “*X*”, “*V*” and “*I*” shaped modes, are observed under low, moderate and high impact velocity, respectively. Liu et al. (2012)) and Fan et al. (2013) have established the density graded material models with the metal hollow sphere via LS-DYNA, respectively. The density graded distribution of models can be controlled by changing the geometric size of cell. It has been indicated that putting the higher density foam layer on the impact end, and lower density foam layer on the protected end can effectively increase the energy absorption of materials.

In general, shock experiments on foams are challenging, because of the technical difficulties associated with low densities and pronounced structural inhomogeneities in such materials. In shock experiments, it is difficult to capture the evolution process of various microstructures in detail, and in the macro numerical simulations, the evolutions of microstructures are reflected into several internal variables of constitutive relation by the statistics, homogenization and other artificial means. These methods cannot visualize and embody the entire physical process of materials. On the other hand, thanks to the continuous increase in computing power, molecular dynamics simulations have become a powerful tool in the study of the high-strain rate response of materials and served as a useful complement to experimental research and macro simulations.

In the literatures, molecular dynamics simulation has been used to study the responses of porous materials under impact loading. Erhart and Bringa (2005) have found that the localized massive plastic deformation induced by the existing voids leads to the formation of nanograins. In addition, it has been investigated that compared with perfectly crystalline samples, the particle velocity in the nanoporous copper has shown the temporal delay, and this delay increases with porosity. Zhu et al. (2007) have proposed a two-dimensional stress model to explain the anisotropic plasticity. They found that the loading direction changes the distribution of the resolved shear stress along the slip plane around the void and induces different dislocation emission mechanisms. Bhatia and Solanki (2013) have investigated single nanovoid growth in aluminum using molecular dynamics simulation. Their simulations have revealed the dependence of nanovoid growth on the void size, strain rate, crystallographic loading orientation and initial nanovoid volume fraction. Davila et al. (2005) have investigated the micro-structural changes in ductile porous metals during high strain rate loading by means of atomistic simulations. It has been concluded that the local massive plastic deformation surrounding the voids can lead to the formation of nano-grains; and a temporal delay of the particle velocity in the porous materials increases with the porosity. Wu and Carey (2013) have adopted molecular dynamics simulation to discuss the effect of microstructures (void shape and distribution) in the high porosity nano-foam materials on the dynamics response of materials. It has been found that the arrangement and aspect ratio of voids play a significant role in the void collapse, and formation and evolution of free surface jetting. Jian et al. (2015) have constructed open-cell nanoporous Cu via the kinetic Monte Carlo method and studied the influence of porosity and specific surface area on the compression curve to elucidate the relationship between shock wave velocity and particle velocity, and shock melting. Their results have indicated that the porosity is a dominant factor of shock response, but the effects of specific surface area at nanoscales can be considerable. In addition, the quantitative relationship among melting temperature, porosity and specific surface area was also presented in their studies. Zhao et al. (2015) have investigated the effects of porosity on shock melting in the honeycomb nanocopper foam materials by means of molecular dynamics simulation. Their results have shown that there are alternating high and low pressure stripes in the compacted region due to the influence of reflected wave disturbance forming on the void surface. Furthermore, in the shock compression region, the internal jetting caused by voids collapse can lead to the local hotspots forming at the voids wall. Soulard et al. (2015) have systematically investigated the influence of shock strength, void size and gas filled in the voids on the shock melting. They found that the melting of materials surrounding the voids was a result of plastic work induced by the voids collapse, and the gas filled in the voids has a strong inhibitory effect on the collapse of voids and melting of materials. The molecular dynamics simulations performed by Al-Qananwah et al. (2013) have indicated that the porous material protective layer can effectively reduce the peak value of stress wave and impact kinetic energy by about 30%.

Although there have been some studies on the shock response of nanoporous materials by molecular dynamics simulations, the reports on the effect of voids distributions on the energy dissipation are still scarce. Therefore, it is desirable to gain a more detailed picture of the mechanism of void compaction, based on more realistic models and