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Regular Article

Shock-induced time-dependent strength behavior in amorphous alloys from a microscopic view

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ABSTRACT

Shock-induced strength behavior and the corresponding microstructural evolution have remained unclear for decades. We propose a viscous-solid model from a microscopic view implied by simulations with non-equilibrium molecular dynamics. The model describes the shocked microstructure very well and shows time-dependent strength behavior upon shock-induced yielding in amorphous alloys. For the first time, we find that the Kohlrausch-Williams-Watts equation [$\varphi(t) = e^{-(t/)^{\beta}}$] is quantitatively applicable in the modelling of time-dependent strength behavior at the non-equilibrium shockwave front. The parameters in the Kohlrausch-Williams-Watts equation are found to agree well with several experimental facts.

Over recent decades, the responses of various materials to shock loading have been extensively investigated, but they remain largely unclear in the literature. The shock loading generates high temperatures, a high strain rate, and extremely high pressure [1], which can influence a material's solid-solid phase transformation [2,3], instability [4,5], and other shock phenomena [1]. The shock-induced flow stress or strength of materials can be defined as the stress deviator, $\sigma_s = (\sigma_z - \sigma_y)/2$, with z in the direction of the shock. In parallel with the experimental facts, we use a dynamic strength concept: it reaches the shock yielding strength (σ_Y) immediately when the shockwave arrives and quickly relaxes to a finite value (σ_f) at the Hugoniot state behind the shockwave front. σ_f, the flow strength of material at the Hugoniot state, has been measured for a variety of materials shocked to no more than 55 GPa [6–9]. If the shock pressure is not high, reloading and unloading measurements can be used to obtain σ_Y, which corresponds to the yield strength at the Hugoniot state. These limited data imply a reduction from σ_Y to σ_f during shock loading [6,8]; however, the non-equilibrium and ultrafast nature have inhibited a thorough investigation of this subject. The time-dependent strength relaxation or σ_Y-to-σ_f relaxation can only be inferred from a numerical analysis of the measured particle velocity profile [6–9] or transmission x-ray diffraction spectrum [10,11]. The shock-induced relaxation mechanism, its effect on other phenomena, and the corresponding material microstructural evolution have remained quite unclear for decades.

In this article, we describe the time-dependent strength behavior in shocked amorphous alloys by developing a material model based on non-equilibrium molecular dynamics (NEMD) simulations. We chose amorphous alloys for their intrinsic homogeneous structure and deformation beyond nanometers, and the weak interactions between defects in these materials [12–16] greatly reduced the size effects in the NEMD simulations, which enabled a direct comparison between data from the simulations and those from future experiments.

NEMD simulations were carried out with LAMMPS [17]. A cube of amorphous $Cu_{46}Zr_{46}Al_8$ alloy that comprised 8000 atoms was prepared with a standard quenching procedure (1.25×10^{10} K/s). It was further periodically replicated to create a sample for shock simulation. The atomic interactions in all of the simulations were described using the potential developed by Cheng et al. [18]. Shock waves were generated with the piston method at 10 K [19,20]. The details of the model and data analysis are provided in the supplementary materials.

In this study, elastic shockwaves at low particle velocities (u_p) and two-wave structured shockwaves at high particle velocities were confirmed in the $Cu_{46}Zr_{46}Al_8$ alloy by means of spatial wave profile analysis, as experimentally revealed in amorphous alloys shocked by gas gun [6] or pulsed thermal spray (PTS) [21]. A best-fit algorithm was developed to evaluate the shockwave velocity (D) in our simulations. The D-u_p relationships are shown in Fig. 1. Three linear D-u_p relationships with different slopes are shown in Fig. 1, corresponding to three different Hugoniot relationships: SI (u_p = 625, 750, 875, and 1000 m/s), SII

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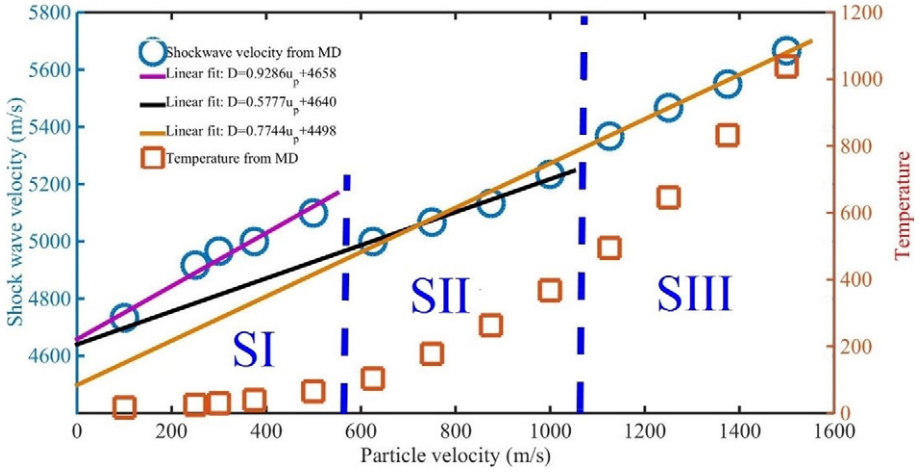

Fig. 1. Steady shockwave velocity versus particle velocity relationship (circles), shock temperature versus particle velocity relationship (square), and fitted Hugoniot relationship in three regions as indicated (solid lines).

(u_p = 625, 750, 875, and 1000 m/s) and SIII (u_p = 1125, 1250, 1375, and 1500 m/s), separately. The shock-induced temperature increases are also presented in Fig. 1. For SI, insignificant temperature increases and a bulk sound velocity at zero pressure that was close to the longitudinal sound velocity were signatures of an elastic shockwave. No significant strength loss was observed at the shock front for SI as shown in Fig. 2(c). For SII and SIII, two-wave structured shockwaves and significant temperature increases indicated a transition from elastic to plastic deformation at the shock front, followed by time-dependent strength behavior, as shown in Fig. 2(d) and (e). When u_p = 875 m/s and u_p = 1250 m/s, the strength gradually relaxed to σ_f with a finite value after immediately reaching σ_Y when the shockwave arrived. Due to their ability to sustain flow strength, the solid structures in the $Cu_{46}Zr_{46}Al_8$ alloy were sustained in our simulation time scales for both SII and SIII even though they slightly differed in Hugoniot relationships, which may have resulted from high-pressure consolidation. The finite flow strength also explained the difference between the equation of the state directly from the molecular dynamics (MD) simulation and that calculated from the Hugoniot relationship, as shown in Fig. 2(f).

As in Fig. 2, time-dependent σ_Y-to-σ_f relaxations were evident for SII and SIII. Other NEMD studies suggested that such relaxations in crystal metals were manifested by the dynamics of the dislocations created upon yielding [22]. In this study, the $Cu_{46}Zr_{46}Al_8$ alloy was yielded via formation of shear localized regions (SLRs) as in previous studies of

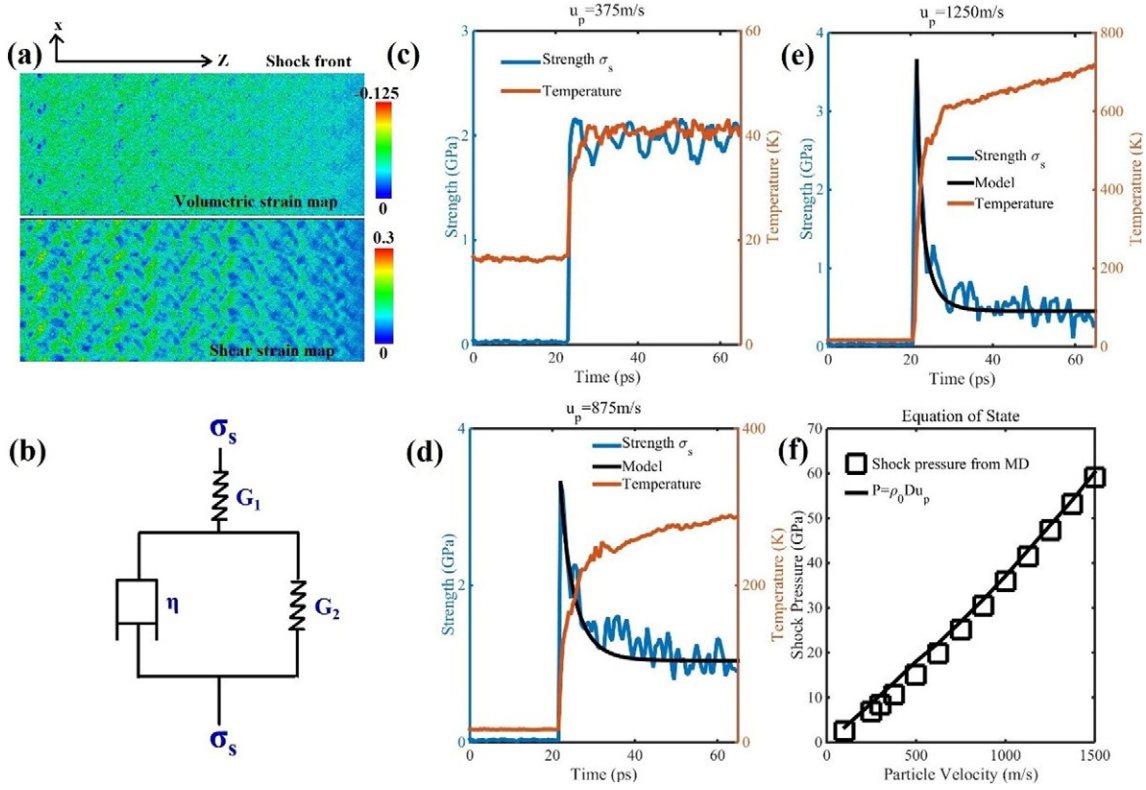

Fig. 2. (a): Illustration of atomic volumetric strain map and shear strain map at shock front (u_p = 875 m/s) colored by strain magnitude. (b): Illustration of viscous-solid model. (c), (d), and (e): Time-dependent strength behavior (purple lines), fitted non-exponential strength relaxation (black lines), and temperature increases (red lines) in a fixed 1-nm-thick slice at z = 120 nm. (f): Equation of state obtained from MD (square) and calculation (solid line).