Elastic-plastic collapse of super-elastic shock waves in face-centered-cubic solids

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Abstract. Shock waves in the [110] and [111] directions of single-crystal Al samples were studied using molecular dynamics (MD) simulations. Piston-driven simulations were performed to investigate the split shock-wave regime. At low piston velocities, the material is compressed initially to a metastable over-compressed elastic state leading to a super-elastic single shock wave. This metastable elastic state later collapses to a plastic state resulting in the formation of a two-wave structure consisting of an elastic precursor followed by a slower plastic wave. The single two-zone elastic-plastic shock-wave regime appearing at higher piston velocities was studied using moving window MD. The plastic wave attains the same average speed as the elastic precursor to form a single two-zone shock wave. In this case, repeated collapse of the highly over-compressed elastic state near the plastic shock front produces ultrashort triangle pulses that provide the pressure support for the leading elastic precursor.

1. Introduction

Shock-induced high-strain-rate phenomena in materials can result in a wide range of responses such as elastic-plastic transformations [1–7], structural phase transitions [8, 9], orientation-dependent stress-induced “cold” melting [10, 11], and spallation [12, 13]. Because of the complexities of the processes involved and difficulties in conducting experiments at high pressures and temperatures, the underlying processes have long been investigated using molecular dynamics (MD) simulations.

Recently the fine structure of steady plastic shock waves (SW’s) in aluminum has been studied using the Moving Window - Molecular Dynamics (MW-MD) method, which yields highly accurate structure maps and profiles of material flow across the shock-wave front in the regime where the elastic and plastic fronts maintain a constant average separation [6]. It was discovered that a plastic SW with a Rayleigh line above the Hugoniot Elastic Limit (HEL) can have a spatially nonuniform two-zone structure. This two-zone structure is made up of a leading elastic zone consisting of an elastic front with following uniaxially compressed solid, and a plastic zone consisting of a plastic front with following plastically deformed material. The solid in the leading zone exists in a metastable elastic state lying on the extension of elastic branch of the Hugoniot beyond the HEL. It was also pointed out that dynamic deformations within the plastic front result in emission of ultrashort triangle-shaped elastic pulses that support the high pressure in the elastic zone and synchronize the speeds of the elastic and plastic fronts resulting in a constant average elastic zone length.
Herein, we address the specific mechanism of elastic-plastic relaxation and associated phenomena that were only touched upon in reference [6]. In particular, we detail the mechanism of elastic-plastic collapse in Al that leads either to split shock waves or a single shock wave with a two zone structure depending on the final state pressure. The same mechanism works in all simulated fcc solids including nickel, copper, and Lennard-Jonesium.

2. Simulation techniques
For simulation of shock-wave propagation in the split shock-wave regime, where the elastic and plastic fronts separate at a constant rate, the standard piston-driven MD approach was used. This is a straightforward simulation technique where the material sample is compressed by a piston in the same fashion as in experiment. Such an approach is limited only by available computer power. It works well if enough atoms can be treated for long enough times that the elastic and plastic shock waves moving at different but constant velocities have both stabilized. Split SW’s were simulated in an Al sample with pre-existing vacancies uniformly distributed with a concentration of \(10^{-3}\) vacancies per atom. The sample had a large longitudinal length \(L_x = 1 \mu \text{m}\), and lateral dimensions \(L_y = 24.1 \text{ nm}\) and \(L_z = 11.9 \text{ nm}\) with periodic boundary conditions imposed in the lateral directions. The density of the sample was 2.683 g/cc, corresponding to an equilibrium Al crystal at zero pressure and 300 K temperature. To generate a SW in the piston simulations, the sample moved freely with a prescribed speed toward a piston at rest. The piston was modeled by a quadratic potential wall \(a(x - x_0)^2\), where \(x_0\) is the fixed position of the piston in the MD box and the coefficient \(a\) determines the rigidity of the wall. Before collision with the piston, the sample had about 10 ps to equilibrate with the help of a Langevin thermostat.

In studying two-zone shock waves we used the MW-MD technique that simulates the SW in the reference frame of the front [6, 10, 14–16]. Like standard piston-driven simulations, the MW method assumes a simulation cell with periodic boundary conditions imposed in directions lateral to the direction of shock-wave propagation. Unlike piston simulations, however, crystalline material is fed into a MW simulation upstream from the shock wave and removed self-consistently downstream. Thus, the MW-MD method efficiently decouples simulation time from sample length. This method has significant advantages over the piston-driven approach in simulating complicated shock front structures with a steady but large length behind the leading edge of the shock wave. In particular, a substantial suppression of non-physical fluctuations of macroscopic physical quantities can be achieved by MW-MD due to long-time averaging. Again, the longitudinal dimension of the moving MD box must be larger than shock front length. Further details of the MW-MD simulation setup are given elsewhere [6,10]. The stress-matched embedded atom Al potential used is identical to the one used in those works [6,10].

3. Elastic-plastic collapse in the leading elastic wave
When a crystal lattice is compressed uniaxially by a perfectly flat piston, plastic deformation cannot begin immediately, even if the applied stress exceeds the dynamical strength of lattice. MD simulations indicate that the delay of the elastic-plastic transformation varies over a wide range, depending on the piston speed and roughness, existence of defects, and other aspects of the sample [1, 2, 4, 17]. Hence, the initially generated elastic SW can propagate a significant distance into the lattice and produce an over-compressed elastic state above of the conventional Hugoniot elastic limit (HEL).

To resolve the elastic-plastic transformation in further detail in this case, it is necessary for the initial delay for the onset of the elastic-plastic transformation exceed about 20 ps. On the other hand, this delay must be limited by approximately one-half the length of sample used in the MD simulation, which gives about 50 ps for a micrometer-sized Al sample. By adjusting the speed of the piston, we ran several test simulations to obtain an appropriate delay time. It was
Figure 1. Elastic-plastic collapse of an Al crystal (with vacancy concentration $10^{-3}$) over compressed uniaxially along the [111] direction by a super-elastic SW generated by a piston with speed 0.84 km/s. (a) The collapse started from homogeneous dislocation nucleation at 30.5 ps, which later developed to a cloud of dislocation loops shown by the $Q_4$ map at 33.9 ps. As a result, the longitudinal stress $P_{xx}$ and shear stress $\tau$ relaxed in a zone with plastic deformation, as illustrated on the lower panel with stress profiles. (b) Stress and density profiles during collapse. The sharp drop in pressure generates two rarefaction waves (RW’s) propagating in the forward and backward directions. Each RW moving with the local sound speed is followed by a slower plastic front (PF). Two diverging RW cause opposite material flows resulting in increase of density in PF’s. Also see P-V diagram of discussed processes in figure 2.

found that for the piston speed of 0.84 km/s the delay time is 30.5 ps. This is long enough to resolve details of plastic deformation and material flow evolution in the Al sample.

Figure 1 shows the stress and density profiles after the elastic-plastic collapse of the Al crystal uniaxially over-compressed in the [111] direction by a high-speed super-elastic SW. (As an aside, similar collapses have been observed in MD simulations of Lennard-Jones crystals [3] and cyclotrimethylene trinitramine [5].) The corresponding evolution of elastic and plastic states in the P-V plane are presented in figure 2, where the plotted elastic and plastic branches of shock Hugoniot for the simulated Al crystal were calculated in reference [6]. Because of a lack of pre-existing dislocations, only homogeneous dislocation nucleation can initiate the elastic-plastic transformation. Indeed, at 30.5 ps a small dislocation loop appeared at –420 nm. It triggered an avalanche of dislocation multiplications resulting in the formation of a cloud of dislocation loops shown in the map of the local atomic order parameter $Q_4$ in the lower color panel of figure 1(a). The nearly isochoric process of dislocation accumulation in this small region of the crystal lasts until the shear stress drops sufficiently to stop further increase of the dislocation number at about 0.5 ps. We term such a fast elastic-plastic relaxation associated with a sharp decrease of the longitudinal stress (in this case 3.3 GPa) an elastic-plastic collapse.

The sudden pressure drop localized just after the collapse within a region about 10 nm wide leads to formation of a spherical rarefaction wave that transforms quickly into two plane waves in the narrow sample with the periodic boundary conditions used in our piston-driven simulation. These two elastic rarefaction waves (RW’s) propagate with the local longitudinal sound speed in the elastically compressed crystal in the forward and backward directions. See profiles in figure 1. While these RW’s do not initiate plastic deformation, the two following plastic fronts (PF’s) generate plasticity via propagation/penetration of dislocations situated in the front toward the elastically compressed solid with high shear stress. Homogeneous dislocation nucleation plays no role in the PF propagation, as the leading RW’s reduce the shear stress ahead of the PF.

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Although the two elastic RW’s diverge from the initial location of the elastic-plastic collapse, opposite pressure gradients in the RW’s generate converging material flows directed to this location. As a result, there is an increase of density around this location in figure 1(b) and corresponding decrease of specific volume on the P-V diagram along the collapse pathway in figure 2. This increase of density is associated with an increase of pressure around the collapse until the pressure reaches a final state on the plastic branch of Hugoniot. Concurrently, the longitudinal stress $P_{xx}$ at the end of RW decreases during such a densification process, because the pressure gradient in the PF is not large enough to halt the converging material flows produced by the RW’s. Hence, the jump of pressure on the PF increases with time, finally reaching a value large enough to decelerate the incoming flow and stop further densification around the collapse. After that moment, which is nearly 40 ps in the simulation (see green line in figure 1), a plateau in the density profile is formed, and the pressure at the end of RW ceases to decrease, so that the PF gains its maximal amplitude and becomes a final plastic SW shown in figure 2.

The RW propagating in forward direction will reach the leading super-elastic SW and attenuate it along the elastic branch of Hugoniot to a pressure level at the RW end. This causes gradual deceleration of elastic precursor as shown by a green arrow in figure 2. After propagation of about 1.5 $\mu$m the “final” split-wave regime with an elastic precursor followed by a slower plastic shock wave is established. However, with increasing elastic zone length the probability of elastic-plastic collapse somewhere in elastic precursor could also increase. Hence, the process could repeat many times driving the HEL to lower and lower values at longer and longer times to the point that this behavior is no longer accessible in MD simulations.

Our MD simulations of overdriven two-zone single shock waves in fcc metals also indicates that a similar process of elastic-plastic collapse can happen from time to time inside the elastic zone [18]. However, in this case the collapse leads only to an ephemeral attenuation of elastic wave that later recovers due to supporting elastic pulses emitted by a following plastic front.

### 4. Mechanism for emission of supporting elastic pulses in the two-zone regime

For a Rayleigh line above the HEL, it is known that emission of supporting elastic pulses by a plastic shock front plays a key role in formation of the single two-zone single shock wave. This two-zone shock wave consists of separated elastic and plastic fronts moving with the same speed [6]. Below we show that the emission of these supporting pluses is generated by elastic-plastic collapse of the uniaxially over-compressed crystal impinging on the plastic front.

MW-MD simulation was carried out of a two-zone SW moving at $8.59$ km/s in the [110] direction of an Al single crystal with dimensions $800$ nm $\times 12$ nm $\times 11.9$ nm. This shock velocity corresponds to a piston velocity of $2.31$ km/s. The sample contained vacancies at a concentration.
Figure 3. Elastic-plastic collapse at the end of elastic zone of a two-zone single SW moving with velocity 8.59 km/s along the [110] direction in an Al crystal. After about 10 ps of accumulation of elastic solid and stress build-up, a highly over compressed elastic shoulder is formed at the edge of the plastic front. See section of blue line between -135 and -120 nm. Then, the collapse is initiated roughly in the middle of this shoulder. The pressure drop by 10 GPa lasts about 6 ps, and high-speed triangle-shaped elastic pulse (green line) is finally detached from the plastic front. The red line shows the beginning of new accumulation of elastic solid in the next cycle of elastic pulse emission. During propagation the amplitude of the elastic pulse becomes smaller due to attenuation by a rarefaction tail of the pulse. See arrows in panel (a).

of $10^{-3}$ vacancies per atom. After a delay, a two-zone elastic-plastic single SW was formed with a steady average elastic zone width of $\sim 280$ nm. See flow profiles in figure 3. In these snapshots the stress profiles in the elastic zone is not flat, but rather contains several triangle-shaped elastic pulses propagating from the plastic front toward the leading elastic front.

The mechanism of elastic pulse emission can be described as a stress build-up followed by an elastic-plastic collapse. At the first stage a layer of elastic solid approaches the pressure jump at the plastic front. Because the elastic-plastic transformation cannot occur instantaneously, the crystal decelerates and accumulates at the edge of plastic front without plastic deformation. In this region it is over compressed uniaxially by about 10 GPa above the average longitudinal stress in the elastic zone. See the blue line in figure 3(a). Owing to the smaller compressibility of the crystal in [110] direction, the leading front of the resultant super-elastic shoulder moves faster than following plastic front. The increase of shear stress and amount of metastable material in the super-elastic shoulder significantly reduce the waiting time for elastic-plastic collapse. In the given simulation the stress-build up before collapse lasts from 5 to 15 ps.

The second stage of the emission process involves elastic-plastic collapse, introduced in the previous section. Homogeneous dislocation nucleation happens at the left edge of the super-elastic shoulder, where the material exists in a much over-compressed state. This collapse initiates an avalanche of dislocation loop multiplications within the dark sports shown in the panels of figure 3 depicting maps of $Q_4$ and shear stress $\tau$. As a result, the shear stress relaxes and the longitudinal stress drops by about 10 GPa in just 5.7 ps after the onset of collapse. See the green lines in figure 3. The shown collapse is completed during 9.5 ps, and gives way to the stress build-up stage for the next cycle of emission. A small stress shoulder along the red line in figure 3 at the edge of plastic front illustrates the beginning of next stress build-up. As a result of the elastic-plastic collapse, two rarefaction waves are generated at the end of the super-elastic shoulder. The right-moving rarefaction wave together with shoulder forms a triangle-shaped
elastic pulse, which moves faster than both the plastic front and the leading elastic front.

This study so far of elastic-plastic collapse in the two-zone case uses relatively narrow samples with periodic boundary conditions imposed in the lateral directions allowing the evolution of 1D waves to be traced. In wider samples, many local elastic-plastic collapses can occur almost simultaneously at the edge of plastic front, resulting in emission of the spherical elastic pulses, as shown in figure 4. The evolution of the wave pattern is then more complicated. However, as they approach the leading elastic front, these spherical waves merge into planar elastic pulses (see figure 4) that provide the pressure support allowing the elastic front to remain high on the elastic Hugoniot above the HEL. Without such a supporting mechanism, the leading elastic wave would attenuate with time, decelerate, and be overridden by the plastic front.

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