Atomic Scale Studies of Spall Behavior in Single Crystal Cu

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Abstract

The micromechanisms related to ductile failure during dynamic loading of single crystal Cu are investigated using large-scale molecular dynamics (MD) simulations. Void nucleation, growth, and coalescence is studied for a single-crystal Cu system under conditions of impact of a shock piston with a velocity of 500 m/s. The compressive shock wave generated reflects from the rear surface as a tensile wave and meets with the tail of the shock wave at the spall plane. The interaction results in a triaxial tensile stress state that nucleates a large number of voids at the spall plane. MD simulations suggest that voids nucleate at intersections of stacking faults generated in the spall plane under the triaxial tensile stress conditions. Two stages of void growth are observed during dynamic failure of single-crystal Cu: Stage I corresponds to fast nucleation and growth of the nucleated voids and Stage II corresponds to coalescence and slow growth of the voids.

Keywords: Dynamic failure; Molecular Dynamics; Voids; Spallation.

1. Introduction

The failure of ductile metals under dynamic loading conditions (spallation) is attributed to the nucleation of microscopic voids that eventually form the fracture surface [1]. Experimentally, the failure behavior is studied using plate impact experiments that impact a flyer plate on to a target plate with a desired velocity [2]. A compressive shock wave is generated in the target plate that proceeds along the length of the sample and reflects back from the rear surface as a tensile wave. A compressive wave is also generated in the flyer plate also reflects back as a tensile wave from the rear surface. These reflected...
tensile waves interact in the sample in the region defined as the spall plane. The interaction of reflected waves produces a triaxial stress state, which results in the simultaneous nucleation of multiple voids in this region. The voids grow and coalesce to form microscopic cracks and failure results in a slab of detached material being ejected from the back surface of the material [3]. Over the last decade, several efforts have been made to understand and predict the material response to dynamic loading conditions. The strain rates achieved during plate impact experiments are typically $10^5 \text{ s}^{-1}$ - $10^6 \text{ s}^{-1}$, [2,4,5,6] whereas, recent advancements using laser induced shocks allow the ability to reach strain rates up to $10^{10} \text{ s}^{-1}$ [7,8,9]. These experiments have focused on the resistance of the material to failure by extracting the spall strength of these metals. The results suggest higher spall strengths of the metal at higher strain rates. The mechanisms of void nucleation in polycrystalline metals are attributed to GB sliding and/or dislocation pileups during impact loading [2]. While the deformation behavior of face-centered-cubic (FCC) metals has been well studied experimentally, the mechanisms of void nucleation, growth, and coalescence are still not completely understood. The lack of understanding can be attributed to the small time scales (picoseconds to micro-seconds) of these processes making it difficult to experimentally identify and characterize these processes.

A better understanding of the micro-mechanisms related to deformation and failure (nucleation, growth, and coalescence of voids) will enhance the ability to design materials capable of resisting damage in conditions subjected to impact/shock. These micro-mechanisms can be investigated by using molecular dynamics (MD) simulations, which can provide the atomic level detail needed for the physical understanding and interpretation of experimental observations. However, there are a few limitations in the application of MD simulations to understand the spall behavior at the macro-scale under experimental conditions. The time scales of these processes can range from picoseconds to micro-seconds and the length scales can range from nanometers to micrometers [10]. The MD simulations typically can study the evolution of the systems for time up to tens of nanoseconds and sizes up to a few hundred nanometers, and therefore, find applicability only to investigate the spatial and temporal evolution of the material microstructures and properties at the scale of the individual phenomena. It is believed, however, that these small length and time scales will not have an effect on the phenomenon of shock wave propagation behaviour and the micromechanisms related to failure. The focus of this paper is to understand the mechanisms of nucleation and growth of voids in single crystal copper. The computational details are presented in Section 2. The shock pressure profile, microstructural evolution and the evolution of the number of voids during failure under shock loading conditions is discussed in Section 3.

2. Computational methods

The spall behavior of Cu [001] is studied using large scale MD simulations at high strain rates using the Voter-Chen (VC) formulation [11] of the Embedded Atom Method (EAM) potential for copper. The VC potential is well suited to describe mechanical properties of nanocrystalline Cu as it provides a good description of the unstable and stable stacking fault energies, as well as the surface and grain boundary energies. The initial single crystal system is created with dimensions of 25 nm x 25 nm x 100 nm. Periodic boundary conditions are used in the X and Y directions and the Z direction is kept periodic. Common neighbor analysis (CNA) and the centrosymmetry parameter (CSP) is used to analyze defects during the deformation simulations. The elements of the atomic-level stress tensor are calculated as

$$\sigma_{ij}(t) = \frac{1}{\Omega} \left[ \frac{1}{2} \sum_j F_{ij}^a r_{ij}^b + M_{ij} v_i^a v_j^b \right]$$  (1)
where $\alpha$ and $\beta$ label the Cartesian components, $\Omega_0$ is the atomic volume, $F_{ij}$ is the force on atom $i$ due to atom $j$, $M_i$ is the mass of atom $i$, and $v_i$ is the velocity of atom $i$. The pressure in the system is calculated as $P = -\frac{1}{3} (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})$, where $\sigma_{xx}$, $\sigma_{yy}$, and $\sigma_{zz}$ are the stresses averaged over the entire system in the X, Y, and Z directions, respectively. The time step for all of the MD simulation runs was chosen to be 2 fs. The temperature was allowed to evolve during the deformation simulations. The MD simulations of impact are carried out by giving a constant inward velocity ($U_p$) to the atoms in the piston along the length of the sample for pulse (square) duration of 10 ps. The inward impact results in a planar shock wave that travels with a velocity ($U_s$) towards the rear surface. A schematic of the simulation setup is shown below in Figure 1.

![Figure 1: Schematic of the MD system showing the setup of the impact simulation. The piston (black region) corresponds to the impactor plate and the green colored region corresponds to the target plate.](image)

### 3. Spall Behavior of Single-Crystal Copper

To understand the temporal response of the metal to the shock wave propagation, the system is divided into sections along the $Z$ axis and the values of pressure and velocity are averaged for all the atoms in each section. A contour plot of the evolution of pressure ($P$) and velocity ($V$), as a function of time along the sample in the shock direction, is shown in Figure 1(a), and 1(b), respectively. A positive value of pressure corresponds to compressive pressure and a negative value corresponds to tensile pressure. The peak shock wave pressure for an impact velocity of 500 m/s is calculated to be $\sim 12$ GPa. A tail of the pressure wave is observed at the end of the shock pulse ($\sim 10$ ps). Figure 2(b) shows that the piston velocity of 0.5 km/s results in the material flow velocity of $\sim 0.5$ km/s. The shock wave reaches the rear surface at $\sim 20$ ps, thus resulting in a shock wave with a velocity of $\sim 5$ km/s. The reflected tensile wave interacts with the tail of the initial pressure wave as shown by the intersecting white arrows as shown in Figure 2 and results in a triaxial tensile stress state occurs at a time of $\sim 28$ ps to produce a state of high triaxial tensile. As will be discussed later, voids nucleate and grow in the region (spall plane) experiencing the triaxial tensile stress. The triaxial state of stress drives the tensile pressure to a peak value of 10.6 GPa that results in the nucleation of multiple voids at the grain boundary junctions. This peak value of the tensile pressure is defined as the spall strength of the material.

The rear surface velocity (in the shock direction) is plotted as a function of time in Figure 3(a). Point A corresponds to the time of the arrival of the first shock wave to the rear surface. This shock wave accelerates the material to approximately twice the velocity of the particles behind the shock front, as shown by point B. The acceleration causes the material to go into tension as a result of which the rear surface decelerates as shown by the curve after point B. Triaxial tensile stresses develop that cause the voids to nucleate at the spall plane at point C. The nucleation of voids results in a second shock wave that results in the acceleration of the rear surface after point D. The strain rate is calculated from the rear surface velocity profile to be $6.8 \times 10^9$ s$^{-1}$. 
To understand the evolution of voids, number, a three-dimensional grid of cubic cells is superimposed over the atomic configuration, and clusters of two or more contiguous empty cells are identified as voids [12]. The cell size (0.36 nm) is chosen so as to have at least several atoms in the cell for the case without any voids. The evolution of the number of voids ($N_V$) in the system as a function of time for various
impact velocities is shown in Figure 3(b). It can be seen that the number of voids increases very fast till a time corresponding to point D, after which, the number of voids decreases slowly. It can be seen that the evolution of the number of voids ($N_V$) can be described in two stages for all impact velocities. The first stage (I) corresponds to the nucleation of voids randomly at stacking fault intersections. The first stage of void growth is very fast till the voids meet and begin to coalesce. The coalescence of voids to form larger void clusters leads to the onset of the second stage (II) of void growth.

![Figure 4: Evolution of the microstructure as a function of time during spall of single crystal copper at a time of (a) 38 ps, (b) 42 ps, (c) 46 ps, (d) 50 ps, and (e) 54 ps.](image)

To understand the micro-mechanisms of void nucleation and growth, intermediate snapshots of the system at intermediate times are illustrated in Figure 4 with the atoms colored according to the CNA analysis. The contour for the atoms colored according to their CNA analysis is as follows: the red colored atoms represent local hexagonal close-packed order (stacking faults), the green atoms represent bulk fcc stacking, the light blue atoms represent a coordination greater than 12, and the blue colored atoms represent a coordination of less than 12. Voids are observed to nucleate at stacking fault intersections in the spall region. The atoms on the void surface are represented by blue atoms. The creation of the voids is accommodated by the shearing of nearby atoms leading to the formation of a disordered shell of atoms.
around the void. These disordered atoms have a coordination of less than 12 and hence are blue in color as well. Continued deformation under the triaxial state of tensile stress increases the size of this shell of disordered atoms around the voids as seen by the increased number of blue atoms and decreased number of green atoms around each void as shown in Figure 4(a)-(e). The disordered atoms, however, begin to recrystallize back to the FCC structure as shown by the transformation of several blue atoms to green atoms in Figure 4(d)-(e). This recrystallization is attributed to the increased temperature of the system due to the nucleation and growth of the voids [13]. These results suggest that MD simulations can be used to investigate the ductile failure micromechanisms in metals as observed experimentally.

4. Conclusions

Molecular dynamics simulations are carried out to understand the micromechanisms (nucleation, growth, and coalescence of voids) related to dynamic failure in single crystal Cu. At an impact velocity of 500 m/s. The spall strength calculated for nanocrystalline copper compares very well with that observed experimentally for single crystal Cu. Voids are observed to nucleate at stacking fault intersections in the spall region. The growth of the voids occurs along the grain boundaries pushing more and more atoms into the surrounding grains. The evolution of voids shows two distinct stages: The first stage (I) corresponds to the fast nucleation of voids followed by the second stage (II) of coalescence of voids. The information obtained from these simulations suggests the development of an analytical model to predict the evolution of voids during dynamic failure of FCC metals. However, more simulations are needed to understand the effect of grain size as well as strain rate on the nucleation, growth, and coalescence of voids during dynamic failure.

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References