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Defect and damage evolution during spallation of single crystal Al: Comparison between molecular dynamics and quasi-coarse-grained dynamics simulations

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ABSTRACT

The links between loading orientation of single crystal Al and the dynamic evolution of defects (dislocations, twins, stacking faults etc.) during spallation are investigated using molecular dynamics (MD) simulations. The microstructural evolution during the shock compression of single crystal Al is observed to be primarily guided by the nucleation and evolution of Shockley partials and twin partials. The shock response and spallation behavior of single crystal Al is observed to be anisotropic and is influenced by the density of various types of dislocations during shock compression and void nucleation at the spall plane. The capability of the "quasi-coarse-grained dynamics" (QCGD) method to reproduce the MD predicted nucleation, interaction and evolution of dislocations during shock compression and spallation of single crystal Al is discussed. The QCGD method retains the relative contribution of different types of dislocations during propagation of shock compression wave, interactions of the wave and spallation of single crystal Al as predicted by MD using a fraction of representative atoms allowing the modeling of of larger sized systems for larger times.

1. Introduction

A critical limitation in the design of next generation blast/impact resistant lightweight metallic materials for armor applications is the understanding of the atomic level mechanisms of deformation during impact loading and spallation failure. In metallic materials, an impact generates a high pressure compressive shock wave which travels through the material leading to the nucleation of multiple defects (dislocations, stacking faults, twins etc.) in the microstructure. The compressive shock wave then interacts with the free surface and reflects as rarefaction wave. The interaction of this rarefaction wave with the initial pressure wave results in the state of high triaxial tensile stress and nucleation of voids in the microstructure. The heterogeneities in the microstructure (grain boundaries, dislocations, stacking faults, twin faults, and their interactions etc.) typically act as the void nucleation sites. These voids coalesce, grow and lead to the fracture (spall failure) of the material [1]. Thus, deformation response of the metal is determined by the nucleation of different types of defects, which are the carriers of plasticity in the microstructure, and their interactions during shock compression and spallation. Hence, a clear understanding of the complex interaction and evolution mechanisms of these defect structures and their role in strengthening/weakening of the microstructure under shock loading conditions is critical to engineer a better impact resistant microstructure.

Experimentally, the shock response of metallic materials is typically studied using either plate impact (strain rates of 10^5–10^7 s^{-1}) [2–9] or laser shock experiments (strain rates of 10^7–10^{10} s^{-1}) [10–16]. The experimental analysis is largely limited to computing shock propagation velocity, peak shock pressures, the Hugoniot elastic limit (HEL), spall strength and strain rates ($\dot{\varepsilon}$) using temporal displacement of the rear surface. The calculated values of the spall strength in these studies indicate a strong dependence on tensile strain rates at $\dot{\varepsilon}$ greater 10^7 s^{-1} [15]. In addition, advancements in the capabilities of laser shock experiments have made it possible to study the wave propagation behavior and shock response of thin films (micron and submicron) of polycrystalline and single crystal Al at ultrahigh strain rates of up to 10^{10} s^{-1} [17–19]. Thus, while the experimental capabilities have broadened the spectrum of strain rates to study spallation of metallic materials, the direct observation of microstructural evolution and deformation mechanisms under conditions of impact loading still remains a significant challenge that needs to be addressed to enable design of impact tolerant materials.

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Molecular dynamics (MD) simulations have been instrumental in interpreting experimental observations by providing atomic level insights into the deformation mechanisms and the dynamic evolution of microstructure at ultrahigh strain rates ($\sim 10^9\ s^{-1}$). Successful applications of MD simulations to understand the evolution of microstructure during shock compression and spallation [20–30] have led to identification of microstructures that render higher spall strengths for FCC metals. For example, coherent twin boundaries in Cu are found to be more resistant to spall failure leading to significant strengthening of the material under shock loading conditions [31]. Similarly, higher values for the spall strength have been found for microstructures that nucleate higher densities of twin partials at the onset of void nucleation for single crystal and nanocrystalline Cu [29]. Such correlations between the deformation twinning and spall strengths are unclear for the case of Al, and hence is a focus of this study. This study aims to gain these insights by quantifying the variations in the nucleation, interactions and evolution of dislocations for various loading orientations subjected to shock compression and spallation. Of particular interest is the investigation of the role of twin dislocations on the spall strength of single crystal Al.

However, the high computational cost limits the capability to use MD simulations to probe the microstructural response at mesoscales. This leads to gaps in the understanding of microstructural evolution at longer length and time scales. The "quasi-coarse-grained dynamics" (QCGD) method [32] scales up the capabilities of MD simulations to the mesoscales using a coarse-grained microstructure and representative atoms (R-atoms). The scaling behavior is attributed to scaled interactions between R-atoms as well as scaled degrees of freedom for the R-atoms. Such a scaling is able to reproduce the microstructural evolution during shock compression as well as spallation of FCC metals [32] as well as HCP metals [33] using reduced number of atoms and larger time-steps. The QCGD method incorporates this capability by modeling the collective evolution of defects rather than modeling individual defects using representative defect structures. This study aims to demonstrate the incorporation of accurate atomic scale characteristics of nucleation and evolution of defect structures in the QCGD simulations as observed in MD simulations for Al. Such a comparison will enable identification of scaling relationships that will allow the prediction of atomic scale dislocation densities in the metal at various stages of the simulation based on coarse-grained microstructures predicted in QCGD simulations.

The aim of this paper, therefore, is two-fold: The first aim is to identify the links between crystal orientation, dislocation evolution and spall strength in Al microstructures. This is investigated by comparing dislocation density evolution during shock compression and spallation of single crystal Al along ⟨0 0 1⟩, ⟨1 1 0⟩ and ⟨1 1 1⟩ orientations. The second aim is to accurately describe the collective evolution of MD-predicted dislocation densities during shock compression and spallation in QCGD simulations. Of particular importance is the capability to reproduce the collective nucleation, interactions and reactions between dislocations. The details of the computational setup and algorithms are provided in Section 2, the MD simulations investigating the role of loading orientation on shock compression and spallation behavior of single crystal Al are discussed in Section 3, and the QCGD predicted collective evolution of defect structures is discussed in Section 4.

2. Computational details

The MD simulations are performed using LAMMPS [34] with the interactions between the atoms defined using the EAM potential for Al [35] that reproduces energetics of defect structures as observed experimentally. The single crystal Al system comprises of ~38 million atoms with dimension of 50 nm along lateral directions (X-axis and Y-axis) and dimension of 250 nm along the Z-axis (shock). The lateral dimensions are set to be periodic, whereas the system is free in the Z direction. The initial as-created systems are equilibrated at room temperature and zero pressure. The shock simulations are carried out for three loading orientations of single crystal Al along the Z axis (⟨0 0 1⟩, ⟨1 1 0⟩ and ⟨1 1 1⟩). The shock wave propagation behavior and spall strengths are analyzed by sectioning the system along the sample length as discussed in [29]. The shock in the MD simulations is induced using a rigid piston at left end of the sample (3 nm region at bottom Z coordinates) that is driven with an constant inward velocity (Z direction) U_p of 1 km/s (impact velocity) for a fixed time (square pulse).

The microstructural characterization of voids uses the "centro-symmetry parameter" (CSP) [36] algorithm and that of stacking/twin faults uses "common neighbor analysis" (CNA) [37] algorithm. In addition, the lengths of various types of dislocations such as Perfect dislocations (1/2⟨1 1 0⟩), Shockley partials (1/6⟨1 1 2⟩), Frank partials (1/3⟨1 1 1⟩), Hirth locks (1/3⟨0 0 1⟩) and Stair-rods (1/6⟨1 1 0⟩) are quantified based on the "dislocation extraction algorithm" (DXA) [38,39] implemented in the "crystal analysis tool" (CAT) [40]. The lengths of twin partials [29] are quantified and used as a validation of the QCGD method to reproduce the MD predicted nucleation, interaction and evolution of dislocations. A time-step of 2 fs is chosen for all the MD simulations and the QCGD simulation.

3. Defect/damage evolution using MD simulations

The piston impact along the ⟨0 0 1⟩ orientation with a velocity of 1000 m/s results in a planar shock wave with a two wave (elastic-plastic) structure traveling towards the rear end of the sample. The variation of compressive pressure and dislocation density (all types listed above) along sample length in the shock loading direction at a time corresponding to the end of shock pulse (t = 20 ps) is shown in Fig. 1(a). The elastic front is characterized by a sharp peak in the value of pressure, referred to as upper "Hugoniot elastic limit" (HEL), followed by a dip in the pressure value, referred to as lower HEL. The lower HEL marks the transition from elastically compressed region to plastically compressed region as seen by a rise in dislocation density behind lower HEL. The shock compression along ⟨0 0 1⟩ direction results in a peak pressure of 18.6 GPa and plasticity is primarily governed by the nucleation of Shockley partials and twin partials within the plastic front with significantly less contributions from the other types of dislocations.

The entire process of shock compression and spallation of single crystal Al can be analyzed in four stages i.e. shock compression stage (SI), shock propagation stage (SII), shock wave reflection and interaction stage leading to void nucleation (SIII), void growth and coalescence stage (SIV). Fig. 1(b) and (c) shows the pressure profile and dislocation densities during the four stages of impact loading along ⟨0 0 1⟩ orientation. The shock compression of single crystal Al along ⟨0 0 1⟩ orientation results in the propagation of the high pressure compressive wave (denoted by red[1] region) to the rear end of the sample as shown in Fig. 1(b). This compressive wave results in nucleation of dislocations in the single crystal Al microstructure as it travels through the material as seen by a sharp rise in the Shockley partial and twin dislocation densities during SI and SII in Fig. 1(c). The compressive wave reflects from the rear surface at the beginning of SIII resulting in the relaxation of compressive pressure which leads to a sharp drop in the density of twin

[1] For interpretation of color in Fig. 1, the reader is referred to the web version of this article.