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Molecular dynamics studies of the roles of microstructure and thermal effects in spallation of aluminum

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ABSTRACT

Spallation behaviors of nanocrystalline aluminum under shock loading are studied by non-equilibrium molecular dynamics simulations. Simulations on single-crystal aluminum are conducted for comparison. Both classical spallation and micro-spallation are studied. Our simulations show that the shock front structure of the nanocrystalline aluminum sample apparently displays two stages plasticity –– the grain boundary mediated stage and the dislocation mediated stage. The spallation mechanism is dominated by cavitation, i.e., nucleation, growth, and coalescence of voids. It is found that void nucleation mechanism is different in single-crystal aluminum and nanocrystalline aluminum. Void nucleation is induced by dislocation activities in single-crystal aluminum, while is induced by mechanical separation and sliding of grain boundaries in nanocrystalline aluminum. Thermal dissipation during cavitation is studied, and the mutual promotion between cavitation and melting is discovered. Thermal dissipation during cavitation leads to temperature arising in the vicinity of voids and promotes melting around voids. On the other hand, melting of materials leads to dropping of spall strength and thus facilitates the cavitation process. Some quantitative discussions on spall strength and thermal dissipation rate are proposed. The spall strength of single-crystal aluminum first increases and then decreases as shock intensity increases, which is attributed to the competition mechanism between strain rate hardening and temperature softening. Grain boundary effect on spall strength is more remarkable in cases of lower shock intensity. The thermal dissipation rate in void nucleation stage is much larger than in void growth–coalescence stage.

1. Introduction

Spallation is a dynamical fracture phenomenon which results from the tensile stresses generated by superposition of the unloading rarefaction wave and the free surface reflecting rarefaction wave under shock loading. Deep understanding of spall phenomena would provide important viewpoints for constructing dynamical material failure models. The fracture mechanism of spall fracture in ductile metals is dominated by cavitation, i.e., nucleation, growth and coalescence of voids (Antoun et al., 2003; Davison et al., 1977; Molinari and Wright, 2005; Luo et al., 2009). According to whether a solid–liquid phase transformation occurs before cavitation starts, spallation phenomena can be divided into two categories –– classical spallation and micro-spallation. In classical spallation, the main target remains in solid state in the shock compression and the following release stages. Tensile stress leads

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to ejection of solid scabs from the free surface. In micro-spallation, a solid–liquid phase transformation occurs by shock compression or on shock release before spall fracture starts (Xiang et al., 2013a,b; Andriot et al., 1984; Signor et al., 2010; Soulard, 2008; De Rességuier et al., 2010; Chen et al., 2012). In such cases, tensile stress emerges in melted materials and leads to the expansion of a cloud of fine liquid debris from the free surface.

In the past decades, spallation has been widely studied experimentally, theoretically and computationally. In experiments, spallation is induced by using explosively driven flyer plate projectiles or laser-driven shock wave loading (Jarmakani et al., 2010; Lescoute et al., 2010; Wang et al., 2014). For example, Wang et al. (2014) have experimentally observed that the high density high purity aluminum (Al) exhibits higher spall strength than the low-porosity pure aluminum, and found that due to stronger plastic hardening behavior, the spall strength of 2024-T4 aluminum alloy is higher than that of the 7075-T6 aluminum alloy. The most representative theoretical models describing spallation formulation include the Gurson model (Gurson, 1977), the Johnson model (Johnson, 1981) and the Nucleation-And-Growth (NAG) model Curran et al., 1987. These models, which are mainly used to describe classical spallation behavior on macro-scale are essentially empirical and largely rely on unknown parameters established in experiments. On macro-scales, spallation is computationally studied by finite element and meshfree methods with constitutive models related to cumulative damage and fracture criteria (Fahrenthold and Horban, 1999; Benzerga and Leblond, 2010; Ren et al., 2011; Wright and Ramesh, 2008; Czarnota et al., 2008; Campagne et al., 2005; Wang et al., 2013). The response of materials under shock loading is very complex and involves damage creation and propagation, phase transformation, heat generation, heat transfer, etc. The time scales of these processes can range from picoseconds to microseconds and the length scales can range from nanometers to micrometers (Remington et al., 2004). Thus, it is very difficult to construct a theoretical model taking all these aspects into account. Experiments and continuum mechanics are commonly applied to macro-scale analysis of spallation behaviors.

On the other hand, molecular dynamics (MD) simulation is an important alternative for studying spallation. Although computational capabilities limit MD simulations to sub-micron length scales and sub-nanosecond time-scales, they serve as important complements to shock wave experiments. One of the advantages of MD is that it directly reveals atomistic scale damage processes, which are helpful for our understanding of damage mechanisms. Moreover, in MD simulations, it is convenient to directly measure distribution of concerned physical quantities such as mass density, stress and temperature. MD simulations have been widely used to explore micro-mechanisms of classical spallation (Krivtsov, 1999; Dávila et al., 2005; Oleynik et al., 2005; Indeitsev et al., 2006; Zhao et al., 2007; Luo et al., 2009; Srinivasan et al., 2007) and micro-spallation (Xiang et al., 2013a,b; Soulard, 2008). For example, Krivtsov (1999) has indicated that spall strength of material first increases and then decreases with mesoparticle velocity dispersion in classical spallation via MD simulation. Luo et al. (2009) have investigated spall damage of single crystal Cu under square and Taylor shock wave loading with MD simulations. These simulations indicate that Taylor wave loading results in higher spall strength than the square shock loading at the same shock velocities. Srinivasan et al. (2007) have investigated that microstructural features generated by shock wave have influences on spallation strength and the nucleation site. By MD simulations on micro-spallation of Pb, Xiang et al. (2013a,b) have observed that in micro-spallation, nucleation sites are scattered and the number of nucleation sites is much larger than that in classical spallation, and the amount of ejecta increases as the shock intensity increases, which is consistent with experimental observations (Andriot et al., 1984; De Rességuier et al., 2010). The micro-spallation of Cu has been studied by Soulard (2008) via MD simulations. And it has been shown that a finite size quasi-solid region exits behind the shock front because the melting is slower than compression.

Dynamic mechanical responses, including damage and fracture induced by shock loading, are strongly dependent on microstructures. Nanocrystalline metals have some appealing characteristics including ultrahigh yield and fracture strengths, decreased elongation and toughness, superior wear resistance, etc (Kumar et al., 2003). Some shock experiments and MD simulations have been conducted to study microstructure effects on spall damage. Kuksin et al. (2010) have studied the influence of the material microstructure (GBs, and nanosize pores) on failure mechanisms in Al sample by MD simulations. It is found that the width of the amorphous liquid-like layer at GBs increases when material approaches the melting curve, and the formed liquid layer decreases the critical stress for microcrack propagation along GBs. Chen et al. (2006) have experimentally studied spallation behavior of Al with varying microstructures. It is shown that grain size effects on spall strength are obvious at lower stresses, but are indistinguishable at higher stresses. Dongare et al. (2010) have simulated the classical spallation behavior of nanocrystalline Cu by means of MD. They confirmed that higher shock intensities result in higher strain rates and higher values of spall strengths for the metal as well as nucleation of larger number of voids in shorter time. They also confirmed that for the same shock intensity, the spall strength of the nanocrystalline copper is lower than that of single crystal copper. Luo et al. (2010) have studied spall damage of Cu with particular microstructures, such as hexagonal prisms shape grain by MD simulation. It is found that GBs serve as the nucleation sites for crystal plasticity and voids, due to the weakening effect of GBs and stress concentrations. The mechanisms of void nucleation, growth and coalescence for nanocrystalline metal under shock loading are still not completely understood, which is attributed to the small time scales of these processes and the heterogeneous nature of these materials, which makes it difficult to experimentally identify and characterize these processes.

Under dynamical loadings, the temperature of materials may vary dramatically during deformation and fracture processes. Thus, thermal effect is an inevitable problem when constructing spallation models, though it was not