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Shock-induced plasticity in semi-coherent {111} Cu-Ni multilayers

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ABSTRACT

Using atomistic simulations, dislocation dynamics modeling, and continuum elastic-plastic stress wave theory, we present a systematic investigation on shock-induced plasticity in semi-coherent Cu-Ni multilayers. The features of stress wave evolutions in the multilayers, including wave-front stress attenuation and strong interfacial discontinuities, are revealed by atomistic simulations. Continuum models are proposed to explain the shock wave propagation features. The simulations provide insight into microplasticity behaviors including interactions between lattice and misfit dislocations. The formation of hybrid Lomer-Cottrell locks through the attraction and combination of lattice and misfit dislocations is found to be a major mechanism for trapping gliding lattice dislocations at interfaces. The relationship between dislocation activity and dynamic stress wave evolution history is explored. The hybrid Lomer-Cottrell locks can dissociate under shock compression or reverse yielding. This dissociation facilitates slip transmission. The influence of coherent stress causes direction dependency in the slip transmission: a lattice dislocation can transmit more smoothly across an interface from Ni to Cu than from Cu to Ni. The interaction forces between lattice and misfit dislocations are calculated using dislocation dynamics code. Lattice dislocation nucleation from semi-coherent interfaces under shock compression is also reported.

1. Introduction

Nanoscale metallic multilayers have attracted great attention from both academia and industry. The abundance of interfaces in metallic multilayers yields unique mechanical properties, such as high strength and hardness, improved radiation damage resistance, good thermal stability, increased ductility, and improved fracture toughness (Misra et al., 1998; Clemens, 1999; Zheng et al., 2013; Demkowicz et al., 2008a; Zhang et al., 2011; Liu et al., 2011b; Yang and Wang, 2016). Nanoscale metallic multilayers can be fabricated via bottom-up thermodynamic techniques such as physical vapor deposition (Mara et al., 2008) and the electrodeposition of two different metals (Bakonyi and Peter, 2010; Yahalom et al., 1989). In recent years, many have studied the morphologies, interfacial structures, thermal stability, plastic deformation and failure mechanisms of metallic multilayers (Bauer and Jh, 1986; Wan et al., 2012; Misra et al., 2004; Wang et al., 2009; Liu et al., 2013; Wang et al., 2008a, b; Li et al., 2012a; Abdolrahim et al., 2014; Wang and Misra, 2014; Kang et al., 2007; Hansen et al., 2013). These works were recently reviewed by Zhou et al. (2015).

Studies of the shock responses of metallic multilayered materials may be motivated by the potential applicability of such materials in shock-damping devices to attenuate the effects of impacts and blasts. Large differences in the mechanical properties of the component layers induce periodic heterogeneities in multilayer composites that lead to impedance mismatches at the interfaces (Holmes and Tsou, 1972; Johnson et al., 1994; Herbold et al., 2008; Neel and Thadhani, 2011; Specht et al., 2012; Chiu et al., 2013). The interaction of shockwaves with these interfaces can change the propagating wave structure and the attenuation of the

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shockwaves. For this reason, metallic multilayered metals could be applied in structural components that are subjected to strong impact or blast loading, such as high-quality armor and space debris shields in satellites.

The shock responses of composites are generally studied from a macroscopic perspective using experiments and continuum elastic-plastic wave theory. Earlier studies focused on the Hugoniot curves of composites. Using plate impact experiments, Holmes and Tsou studied the Hugoniot curves of unidirectional fiber-reinforced composites (Holmes and Tsou, 1972). Both the shock-wave velocity and the free-surface velocity were measured by optical techniques; the shock front in the composite was found to be steady. Garg and Kirsch utilized concepts from the theory of interacting continua to derive a generalized set of conservation equations (i.e., the Hugoniot relations) across a steadily propagating disturbance in composites (Garg and Kirsch, 1971). Herbold et al. investigated the shock response of polytetrafluoroethylene-Al-W granular composites by experiments and numerical simulations (Herbold et al., 2008). They found that shock loading of this granular composite induced redistribution of internal energy between components. Such energy redistribution can be tailored by manipulating the particle sizes of the rigid components; higher fractions of thermal energy are transferred to soft and light components as the heavy and rigid components are increased in size. Neel and Thadhani (2011) studied the shock-compression Hugoniot curves of several tetrafluoroethylene-hexafluoropropylene-vinylidene fluoride (THV)-alumina particle composites with varying porosities through plate-impact experiments. The experimental results were correlated to the model predictions by adjusting the “effective” Grüneisen parameter. Kelly and Thadhani (2016) later studied the shock-compression response of highly reactive Ni-Al multilayered thin foils using laser-accelerated thin-foil plate-impact experiments. They also performed mesoscale shock simulations in the CTH programming environment using real imported microstructures of the cross-sections of multilayered Ni-Al foils to compute and correlate the Hugoniot response with the experimentally determined equation of state. At particle velocities below 150 m/s, the experimentally determined equation of state matched the CTH-predicted inert response and showed consistency with the observed unreacted state of the Ni-Al target foils recovered from this velocity regime. At higher particle velocities, the experimentally determined equation of state deviated from the CTH-predicted inert response. Chiu et al. (2013) conducted thick-walled cylinder experiments and simulations of the dynamic collapse of Ni-Al concentric laminate cylinders. They demonstrated the phenomenon of cooperative buckling originating in the innermost layers. The instability of all layers was dictated by the buckling mode of the inner layers. Specht et al. (2012) investigated the wave propagation response of cold-rolled Ni and Al multilayered laminated composites with various orientations by using finite-volume simulations. They found that the layer orientation of dissimilar materials in the multilayered laminated composite greatly affected the dissipation and dispersion of shockwaves. . It is found that orientation of the layers of dissimilar materials in a multilayered, laminated composite can greatly affect the dissipation and dispersion of shock waves. Specht et al. (2017) also measured the Hugoniot curves of NiAl multilayers by plate-on-plate impact experiments. The experimental Hugoniot curve agreed with the finite-volume simulation. Han et al. (2011) studied the shock-induced plasticity behaviors of Cu-Nb multilayers. Comparative study of the shock-induced plastic deformation of the pure Cu and Nb versus that of the Cu-Nb nanolaminates emphasized the importance of the heterogeneous phase interfaces in determining the dynamic deformation behaviors of multilayer materials. Han et al. (2014) also studied the deformation and failure of bulk Cu-Nb nanocomposites under planar shock loading. They found that voids generally nucleated within the Cu phase, which has a higher impedance and lower spall strength than Nb, rather than along the Cu-Nb interfaces or in the Nb phase. This finding contradicted the general theory of failure initiation at interfaces, and indicated that the Cu-Nb interfaces were stable under dynamic loading. Germann et al. (2009) used laser-launched flyer plate experiments and large-scale molecular dynamics (MD) simulations to study the shock responses of Cu-Nb nanoscale multilayered (nanolayered) composites. They observed a strengthening effect at the interfaces under dynamic shock loading, in both MD simulations and post-mortem examinations of shock-recovered samples subjected to 20-GPa shock loading. The MD simulations provided insight into the dislocation nucleation and transmission processes occurring under compression, as well as the subsequent annihilation of said dislocations upon release. Molinari and Ravichandran (2006) analyzed the steady plastic shocks generated by planar impact on metal-polymer laminate composites in the framework of gradient plasticity theory. The following experimental features were well reproduced by gradient plasticity modeling: shock width was proportional to the cell size; the strain rate magnitude was inversely proportional to cell size; and strain rate increase followed a power-law relationship with the applied stress amplitude. While these results were equally well described by first- and second-order gradient plasticity theories, the first-order gradient plasticity approach was favored in comparing the theoretically predicted structure of the shock front to the experimental data.

Studying details of the thermomechanical behaviors of metallic multilayers under shock loading is experimentally challenging, because the reflection and transmission of shockwaves at metallic multilayer interfaces create very complex thermodynamic paths. A complete temporal record of stress, velocity, and temperature is necessary to properly characterize the material state during shock loading. However, such kinetic behavioral information is not readily obtained from current shock experiments. In addition, complex processes triggered by the interactions between shockwaves and interfaces cannot be observed directly or easily by current experimental techniques. MD simulations are an important alternative approach for studying the dynamic behaviors of materials under shock loading (Xiang et al., 2013a, b, 2017). MD simulations can provide details of atomic-scale mechanisms, which cannot be directly observed in experiments.

Much recent MD simulation-based research has addressed the strengthening effects of interfaces and the underlying micromechanisms (Shao and Medyanik, 2010; Shao et al., 2015; Mitchell, 2002; Rao and Hazzledine, 2000; Wang et al. 2008b, a; Ghosh and Arroyo, 2013; Peng and Wei, 2016; Zhu et al., 2015; Salehinia et al., 2014; Li et al., 2012b; Zbib et al., 2011; Wang et al., 2014). However, studies using MD simulations to understand the atomic-scale details of interactions between shockwaves and interfaces have been infrequent. Recently, Zhang et al. (2013) utilized non-equilibrium MD simulations to reveal the dislocation processes underlying the effects of bimetal interfacial structures on the plastic responses of Cu-Nb nanolayered composites to shock compression. Critical shock pressures for the nucleation and transmission of dislocations across atomically flat interfaces were shown to be substantially higher than those from faceted interfaces. In the present work, using 111 Cu-Ni multilayers as an example, we