Atomistic Simulation of Slip, Twinning and Phase Transitions in Shocked Metals and Nanocomposites

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Summary: Employing nonequilibrium molecular dynamics simulations, we characterize the defect substructures induced in nanolayered Cu/Nb composites by shock compression, and their manifestation on macroscopic observables such as pressure, shear stress and temperature. We find that atomic interface structures directly influence the nucleation, transmission, absorption, and storage of dislocations, thus impacting the response of such nanocomposites to shock compression and release.

Introduction

Molecular dynamics (MD) simulations have provided unique insight into the atomic-scale mechanisms of shock-induced plasticity and phase transformations, revealing detailed information about pathways and their dependence on crystallographic loading direction. Embedded atom method (EAM) potentials provide a reasonable description of many fcc and bcc metals, including Cu, Al, Ni, Ce, Fe, Ta, and Nb, and are efficient enough that large-scale simulations with billions of atoms are computationally tractable, particularly for the short (sub-ns) timescales required for the transit of a shock wave through a micron sample length. For the metals just mentioned, such simulations have exhibited shock-induced dislocation slip, deformation twinning, and solid-solid phase transformations. Even less explored is shock-induced plasticity in hetero-nanocomposites; the complexity and difficulty of modeling of hetero-phase interfaces adds to the interatomic potential challenge. Here we present a simulation study of the shock response of Cu/Nb nanolaminates, including the interrelationship between the interface-mediated defect structure that is generated during shock compression, e.g., dislocation nucleation and transmission, and macroscopic quantities such as pressure, shear stress and temperature.

Results and Discussion

Our large-scale nonequilibrium molecular dynamics (NEMD) simulations utilize the SPaSM (Scalable Parallel Short-range Molecular dynamics) code. A Cu/Nb bilayer with the experimentally observed Cu/Nb incoherent interface structure is created by periodically joining a (111) slab of perfect fcc Cu with an (110) slab of perfect bcc Nb, with a Kurdjumov-Sachs (KS) epitaxial orientation so that z = [111]Cu || [110]Nb is the direction normal to the interface planes, and x = [1-10]Cu || [-111]Nb and y = [11-2]Cu || [1-12]Nb are the transverse directions, in which periodic boundary conditions are used. This interface is then relaxed to achieve an equilibrium structure. We utilize a recently developed embedded atom method interatomic potential for Cu/Nb which combines a Voter-Chen Cu potential with an Ackland-Thetford Nb one, chosen based upon a recent study where we compared the high-pressure response of several Nb potentials [1]. The initial results presented here are for Cu and Nb layers each 5 nm thick, with a multilayer sample consisting of 12 bilayers leading to a total sample length ~120 nm. Following relaxation and equilibration, a planar shock wave is introduced in the z direction by impacting the sample into a specularly reflecting “momentum mirror”.

For a 5 nm Cu / 5 nm Nb multilayer, we find a purely elastic response until the piston speed up reaches a critical threshold up ~ 650 m/s. At this shock strength, plastic deformation initiates with the emission of a Shockley partial dislocation loop into a Cu layer from the Cu/Nb KS interface (circled event at 6 ps in Fig. 1). The elastic limit for a perfect Cu single crystal shocked in the [111] direction is up ~ 750 m/s, indicating that heterogeneous nucleation from the interface can serve as the source of plasticity during shock loading. The interface structure and layer thickness (or interface density) can thus play key roles in determining the modes of plasticity (and the corresponding Hugoniot elastic limit) of multilayered nanocomposites due to both the preexisting defect content contained in the interfaces, as well as confinement effects of lattice dislocations within the individual layers.

As the shock loading process continues, additional Cu lattice dislocation nucleation events from an interface (including emission of a second Shockley partial to form a perfect dislocation loop) are observed (a few examples are circled in blue in Figure 1), as well as dislocation transmission from Cu to Nb and Nb to Cu layers (yellow circles in Fig. 1). As a result of such processes, full lattice dislocations are produced inside both Cu and Nb layers [2].

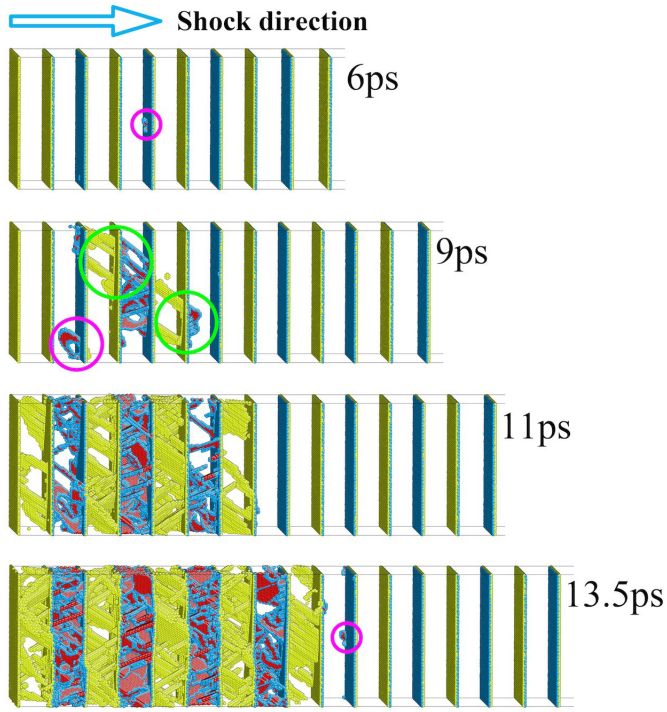

Figure 1. Snapshots of shock-induced defective structures in a 5 nm Cu / 5 nm Nb multilayer. The shock is propagating from left to right, and the initial (leftmost) layer is Nb. Atoms in ideal fcc or bcc sites are omitted, showing only surface and defect atoms. Times are relative to initial impact, and only layers behind the (elastic) shock front are shown at each time. A few dislocation nucleation (transmission) events are circled in blue (yellow).

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[1] R.F. Zhang, J. Wang, I.J. Beyerlein, and T.C. Germann, “Twinning in bcc metals under shock loading: a challenge to empirical potentials,” *Phil. Mag. Lett.* (in press, 2011).

[2] R.F. Zhang, J. Wang, X.Y. Liu, I.J. Beyerlein, and T.C. Germann, “Nonequilibrium molecular dynamics simulations of shock wave propagation in nanolayered Cu/Nb nanocomposites,” in Shock Compression of Condensed Matter – 2011, eds. M.L. Elert, W.T. Buttler, J.P. Borg, J.L. Jordan, and T.J. Vogler (*American Institute of Physics*, 2011), in press.

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