Title: Shock Response of Cu-Nb Nanolayer Composites

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Intended for: 17th Biennial International Conference of APS Topical Group on Shock Compression of Condensed Matter

June 16-July 1, 2011 Chicago, IL
Shock Response of Cu-Nb Nanolayer Composites

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Large-scale classical molecular dynamics (MD) simulations are used to study the shock response of Cu-Nb nanolayered composites. We describe the development of an interatomic potential which provides an accurate description of deformation twinning in bcc Nb under compression, slip in fcc Cu, and the interface structure of Cu-Nb interfaces with the Kurdjumov-Sachs (KS) orientation relationship. The MD simulations provide insight into the role of atomic Cu-Nb interface structures on the nucleation, transmission, absorption, and storage of dislocations during shock compression, and their role as dislocation sinks upon release. This, together with the effects of confined layer slip and twinning, leads to a greater degree of recovery as compared to either constituent Cu or Nb single crystal for layer thicknesses down to 5 nm, an effect seen both in our simulations and in companion shock experiments.
Shock Response of Cu-Nb Nanolayer Composites
-- Dislocation nucleation and transmission at interface

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Understanding strengthening origin and plasticity mechanism at extreme conditions
Motivation

- Interfaces—a common planar defect in materials, play a crucial role in determining material strength for nanostructured composite materials.

- Prior modeling of Cu/Nb interface has shown that it acts as a very strong barrier to dislocation propagation, transmission across this interface.

Objectives

Dislocation nucleation and transmission at incoherent interface under shock

1. Empirical potentials for bcc-Nb: artifacts vs twin
2. Layer thickness dependence of dislocation nucleation
3. Crystallographic relationship of nucleation and transmission with interface structure
Methodology and Setup of MD simulation

- Nonequilibrium molecular dynamics (NEMD) simulations used the Scalable Parallel short-range molecular dynamics (SPaSM) code with shock waves induced by slamming the sample up against a specularly reflecting wall at piston velocity $u_p$, i.e. the so-called momentum mirror method.

- Large scale Molecular dynamics (MD) simulations were performed with Voter-Chen Cu EAM potential and Ackland FS Nb potentials, to study the interface mediated plasticity of nano-layered CuNb composites with layer thickness of 5nm ($u_p=0.65$km/s, temperature=300K)

Models:

- Nb2.5nm/Cu2.5nm, Nb5nm/Cu5nm, KS type interface
- Nb10nm/Cu10nm, Nb20nm/Cu20nm, KS type interface
Interface structure
Dislocation nucleation at interface
Dislocation transmission at interface
Dislocation nucleation at interface
Dislocation transmission at interface
Dislocation transmission at interface
Interface acts as the source of dislocations and twins (Cu5nm/Nb5nm, 650m/s, SPaSM code) using Combined Voter-Chen Cu potential and Ackland Nb potentials.
Brief Summary and Perspectives

- Interface serve as the source of dislocation nucleation in nanolayered Cu/Nb composite

- Dislocation transmit first from Cu \{111\} slip plane into Nb \{110\} plane, and then into the neighbor Cu \{111\} plane

- Interface pattern controls the dislocation nucleation, and preferred slip system evolve along directions with high linear density of patches

- Crystal orientation is the key factor to control the dislocation transmission, transmission process try to locate at the neighbor slip planes with the smallest angle. Such finding confirms the geometry criterion.
Acknowledgement

Los Alamos National Laboratory and US Department of Energy for financial support.

A. Misra, R. G. Hoagland and M. I. Baskes for valuable discussion, advice and suggestions.

S. N. Medyanik, S. Shao for kind help and valuable suggestions.

S. J. Plimpton, A. Stukowski, J. Li, K. Kadaw for providing some useful code for MD modeling and simulations.

Thanks for your attention!!