MODELING AND ANALYSIS OF DYNAMIC CRACK PROPAGATION IN A NANOSCALE BI-LAYER METALLIC COMPOSITE

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Introduction

Mechanics and fracture of nano-metals and alloys have been the subjects of considerable research in recent years. Nanoscale bi-layer metallic composites with mismatch in physical and mechanical properties between two metals across the interfaces are frequently encountered in a broad range of applications of technological importance; for example in micro-electro-mechanical and nano-electro-mechanical systems. Among various atomistic simulation methods, molecular dynamics (MD) has become the method of choice to study dynamic fracture at the atomic/nano scale, as it can provide time-dependent information and allows for the inclusion of strain rate and temperature as meaningful variables in the analysis. In this paper, we present molecular dynamics modeling and analysis of crack propagation under tensile and cyclic loading in a Ni single crystal and a nanoscale composite Ni-Al bi-metallic system, in which a crack initiates and propagates from the Ni surface layer towards the Ni-Al bi-metallic interface.

Methodology

Molecular dynamics simulations using embedded atom method (EAM) inter-atomic potential were conducted to investigate crack propagation under tensile and cyclic loading in both Ni and nanoscale bi-metal composite Ni-Al system. The EAM potential developed by Pun, et al was used to define inter-atomic interactions between the Ni-Ni and Ni-Al atoms.

The schematics and atomistic structures of the simulation geometry used in the present work for the Ni and Ni-Al are shown in fig. 1. An initial crack of roughly 1/5 the layer system length is introduced by partially turning off inter-atomic interactions between atoms in the eight consecutive (001) planes. The two middle planes constitute the upper and lower surfaces of the initial crack. The crack plane is parallel to the *xy* plane. Free boundary conditions were applied in the *x* and *z* directions and periodic boundary condition was applied in the *y* direction (with plane strain condition). Molecular dynamics simulations were conducted using molecular dynamics program, LAMMPS.

For the single crystal Ni, the simulation slab had dimensions of $199a_{Ni}$ x $7\ a_{Ni}$ x $62\ a_{Ni}$ with 349,125 atoms, where a_{Ni} (3.52 A^o) is the lattice parameter of Ni. The Ni-Al bi-layer model was created and assembled from the two semi-infinite perfect crystals of Ni and Al with an orientation relationship of [100] || [100], [010] || [010] and [001] || [001]. The two dimensions in the *y* and *z* directions were not chosen arbitrarily (due to lattice size mismatch of Ni and Al) but determined such that the strains imposed on the Ni and Al semi-infinite perfect crystals is at a minimum.

Results

Mode I Uniform Loading: The crack growth and propagation under uniform loading was studied on a (001) plane for both the Ni and Ni-Al. The strain energy release rate (G) is an important quantity in the analysis of crack propagation. This is the amount of energy per unit area that is supplied by the elastic energy stored in the system. It can be calculated by integrating the stress-strain curve with respect to strain, ε and is given by

$$G = w\int_0^{\varepsilon} \sigma_z(\varepsilon')d\varepsilon' \qquad (1)$$

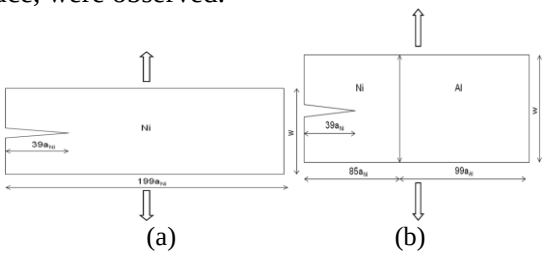
where, w is the width of the strip in the z direction and σ_z is the z component of the stress. The calculated stress-strain curves for Ni, Ni-Al and Al are shown in fig. 2. The maximum reached value of σ_z was found to be 7.56 GPa for Ni, 4.72 GPa for Ni-Al and 3.69 GPa for Al. According to Griffith's criteria, a brittle crack under mode I loading propagates when G corresponding to an applied load is equal or greater than $2\gamma_s$, where γ_s is the surface energy of each plane of the crack. From the stress-strain curve, the calculated critical strain energy release rate at which the crack starts to propagate in Ni (G_{cNi}) is 3.86 J/m^2 and in Ni-Al (G_{cNiAl}) is 2.4 J/m^2. The corresponding given values of the Griffith load from the EAM potential, which is twice the (001) surface energy (γ_s), are given in literature to be 3.756 J/m^2 for Ni (G_{Ni}) and 1.886 J/m^2 for Al (G_{Al}). The value for the critical strain energy release rate in Ni-Al (G_{cNiAl}) from the

present analysis lie appropriately between the Griffith loads for Ni and Al.

The snapshot pictures showing an enlarged and a close-up view of the defect structures formed at the crack tip after initiation of plastic deformation at 50 and 70 ps in Ni and Ni-Al are shown in fig. 3. The snapshots at 70 ps show formation and evolution of stacking faults associated with nucleation of dislocations from the crack tip. The stacking faults are bounded by dislocation loops, which start at the crack tip. The appearance of dislocations at the crack tip suggests a dynamic brittle-to-ductile transition which leads to a crack arrest in the Ni. When the surfaces of the crack began to roughen atomically, the crack attains a velocity of approximately one third of the Rayleigh wave speed.

In nanoscale bi-metal composite Ni-Al system, the crack surfaces initially grow brittle with crack surfaces getting roughened at around one-third of the Rayleigh wave speed. As the crack growth approaches the bi-metal interface, dislocations start emanating from the interfacial bi-layer and start traveling away from the interface towards the larger Al region. As the crack nears the bi-metal interface, the 'process zone' at the crack tip start interacting with defects at the interface that eventually blunts the crack tip and ceases further crack growth ultimately prohibiting crack from propagating.

Cyclic Loading: The cyclic loading was applied in a strain-controlled manner at a strain rate of $2.29 \times 10^{9}\ s^{-1}$. To simulate fatigue failure in a small number of cycles the structures were subjected to maximum strains (e_{max}) larger than those required for initiating crack propagation in Ni and Ni-Al. Cyclic loading with a load ratio of 0.85, and maximum applied strain (e_{max}) of 0.046 was employed. The crack growth and propagation were studied on the (001) plane for the two systems. Illustrative pictures after various loading cycles showing mechanisms of crack propagation for both Ni and Ni-Al are shown in fig. 4. In all of the figures the atoms are colored according to the centro-symmetry parameter, which is a scalar quantity designed to identify defects such as interfaces, stacking faults and dislocations. For the maximum applied strain e_{max} of 0.046, the snapshot sequence of the crack propagation during fatigue cycles 1 and 3 for Ni and Ni-Al (fig. 4(a) and 4(b)) show that the crack in both systems move in a straight line with fatigue cleavage of atomic bonds in the crack plane. The crack growth in Ni however was noticed to stop after 9 cycles and crack length fluctuates at around 645 angstroms for the next 20 fatigue cycles. The dislocations nucleate from the crack tip during the 29th fatigue cycle. For Ni-Al the propagating crack reaches the interface during the 3rd fatigue cycle. When crack reaches the interface, dislocations start emanating from the interfacial bi-layer (fig 4(b)). With continued cyclic loading, little changes in the defect structures that form, when crack hit the interface, were observed.



(a) (b)

Fig. 1: (a) Schematic of geometry for Ni; (b) Schematic of geometry for Ni-Al bi-layer nanoscale metallic composite

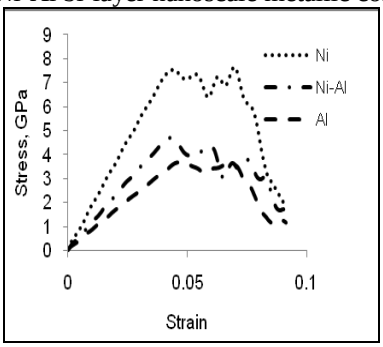
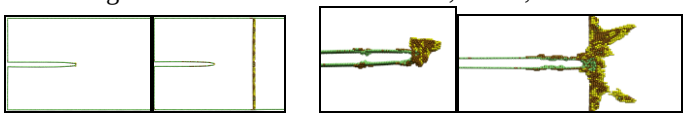


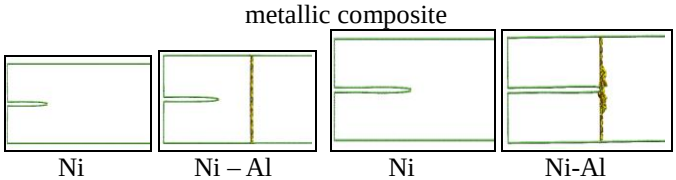
Fig. 2: Stress-Strain Curves for Ni, Ni-Al, and Al



Ni Ni – Al Ni Ni-Al

(a) at 50 ps (b) at 70 ps

Fig. 3: Snapshots of crack propagation in Ni and Ni-Al Bi-metallic composite



Ni Ni – Al Ni Ni-Al

(a) After 1 fatigue cycle (b) After 3 fatigue cycles

Fig 4: Crack propagation in nanoscale Ni and Ni-Al metallic composite

Concluding Remarks

MD modeling analysis of crack propagation in Ni single crystal indicate the crack initially growing brittle and eventually undergoing a dynamic brittle-to-ductile transition with a spontaneous proliferation of dislocations from the crack tip following a roughening of the crack surfaces. Results for Ni-Al also showed an initial brittle crack propagation with planar cleavage of bonds between the two neighboring (001) planes defined by the initial seed crack and crack surfaces getting roughened when the crack propagation speed is about one-third of the Rayleigh wave speed for the case of uniform loading.