Dynamic Crack Propagation in a Bi-Metallic Nanolayer

R. Mohan, Y. Purohit

Department of Nanoengineering
Joint School of Nanoscience and Nanoengineering
North Carolina A&T State University
Room 208E, 2907 E Lee Street, Greensboro, NC 27401, USA, rvmohan@ncat.edu

ABSTRACT

Deformation behaviors of nanoscale metallic systems under mechanical loading conditions have received considerable attention in the recent years. Associated with mechanical deformation of the material systems are their fracture and failure. This paper focuses on the computational modeling of the dynamic crack propagation in a bi-metallic nanolayer. In particular, this paper focuses on the dynamic crack propagation in Nickel and Nickel-Aluminum bi-metal nanolayer under tensile and cyclic loading conditions. Atomistic 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. Findings from our study clearly indicate that the crack propagation in such systems is influenced by the interactions and atomic defects at the interfaces, and the associated deformation mechanisms at the nano scale.

Keywords: bi-metallic nanolayers, molecular dynamics, crack propagation

1 INTRODUCTION

Most studies of crack propagation in nano-scale regime have concentrated mainly on the fracture behaviors under tensile loading of either single crystal materials [1-2] or of nano-structures containing grain boundaries and interfaces between similar types of materials [3-4]. Only few studies have considered crack propagation in nano-structures with interfaces between materials of dissimilar types [5-6]. Moreover, very few studies have been performed at atomistic level to investigate material behaviors under cyclic loading [7-8].

Bi-metallic interfaces 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. The mechanical reliability of MEMS/NEMS, in service, depends strongly on their resistance to fracture in the presence of small numbers of cracks formed during their production and operation cycles.

Among various atomistic simulation methods, molecular dynamics (MD) has become the method of choice to study fracture at the atomic 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 work, we used molecular dynamics simulations to investigate crack propagation under cyclic loading in a Ni single crystal and a Ni-Al bi-metallic interface system, in which a crack initiates and propagates from the Ni surface layer towards the Ni-Al bi-metallic interface. This Mode-1 crack growth and propagation were studied under tensile and cyclic loading conditions and are discussed.

2 MODELING METHODOLOGY

Molecular dynamics simulations using embedded atom method (EAM) inter-atomic potential were conducted to investigate crack propagation under cyclic loading in both the Ni and Ni-Al bi-metallic interface system. The selection of the embedded atom method (EAM) for the energy functional in molecular dynamics simulations is a popular choice for the fcc close-packed metals. The EAM potential developed by Pun, et al [9] was used to define inter-atomic interactions between the Ni-Ni and Ni-Al atoms. For the present application, it is critical that the potential reproduces the elastic constants as well as surface energies very accurately and the potential used has been fitted to the elastic constants, surface energies and to other bulk and surface properties of Ni and Al.

2.1 Bi-Metallic Nanolayer

The schematics and atomistic structures of the simulation geometry used in the present work for the Ni and Ni-Al are shown in figure 1. The x, y and z axes are along the [100], [010] and [001] crystallographic directions, respectively. The (001) [100] crack system was studied in both the configurations. For the (001) [100] crack system, the crack-free surfaces are (001) and the crack propagates along the [100] direction. An initial crack of roughly 1/5 the 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 presented in the work were conducted using molecular dynamics program, LAMMPS [10].

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. This molecular system configuration is believed to be large enough to take care of the long-range character of the crack strain fields. 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 minimum and also periodic boundary condition is ensured in the y direction. The total calculated dimensions of 70.015 x 2.464 x 21.87 nm in the three directions in the Ni-Al were found to be comparable with the corresponding three dimensions of 70.048 x 2.464 x 21.824 nm in the Ni single crystal. The energy of the bi-layer was first minimized using conjugate-gradient energy minimization technique. The stresses were than relaxed using MD in NPT ensemble to a pressure of 0 bar and a temperature of 0 ^oK.

3 RESULTS AND DISCUSSIONS

3.1 Mode I Uniform Loading

The crack growth and propagation 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 data with respect to strain, ε. In the present molecular strip system, this 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 stress for each atom is due to its interaction with all other atoms in the system (within the force cut-off). Atomistic per atom stresses, a stress x volume formulation, as implemented in LAMMPS were calculated and summed over all the atoms of the system to get σ_z component of the stress. σ_z increases with strain to a certain value and then decreases for all the three systems. 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 propagate 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. The calculated critical strain energy release rate from the stress-strain curve 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 3.756 J/m^2 for Ni (G_{Ni}) and 1.886 J/m^2 for Al (G_{Al}) [11]. 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. 2. The atoms are colored as described above with yellow for dislocations, brown for stacking faults, and green for surface atoms. 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 Ni-Al bimetal system as discussed above, 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 they start traveling away from the interface towards the bulk Al. 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 beyond the Ni-Al interface. However, the system continues to dissipate elastic energy through continued creation and motion of dislocations in Al. The snapshots in fig. 2(b) for Ni-Al also show formation and evolution of stacking faults associated with nucleation of dislocations from the interfacial bi-layer. The stacking faults, which in this case start at the interfacial layer, are bounded by the dislocation loops (colored in yellow). Further discussions and details are presented in [12].

3.2 Cyclic Loading

The cyclic loading was applied in a strain-controlled manner at a strain rate of 2.29×10^9 s^{-1}. To simulate fatigue failure in a small number of cycles the structures were

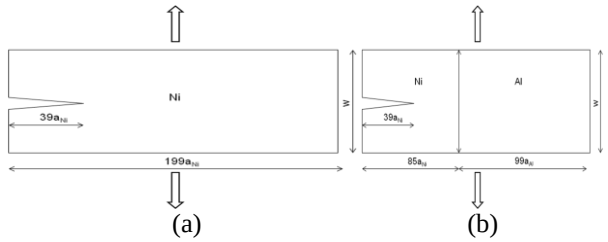
subjected to maximum strains (e_{max}) larger than those required for initiating crack propagation in Ni and Ni-Al. The loading pattern applied to the two systems with a load ratio of 0.85, and two different maximum applied strains (e_{max}) of 0.046 is shown in fig. 3. A high value of load ratio (e_{min} / e_{max} = 0.85) was used to prevent the inner faces of the crack from contacting each other during unloading. Before applying cyclic load the two systems were subjected to initial tensile strains of 0.039 for e_{max} of 0.046.

The slabs were initialized at zero temperature and the outward strain rate of $2.29x10^9$ s^{-1} was imposed on the outer most columns of atoms defining the upper free surfaces of the slab in the z direction. A linear velocity gradient was applied across the slab resulting in an increased outward strain with time in the z direction. After loading to a given maximum strain (e_{max}) the directions of the velocities and the velocity gradient were reversed unloading the system to reach the minimum strain (e_{min}). The atom velocities were initiated in the required direction at the beginning of each loading and unloading half cycle to alleviate the stress wave overlap that could arise from the high rate of deformation. The loading and unloading cycles lead to the crack growth and propagation and eventual structural failure of the materials. In order to compare crack growth under cyclic loading with that of crack growth under tensile loading, MD simulations under mode I tensile loading (at a strain rate of $2.29x10^9$ s^{-1}) were also conducted for both the Ni and Ni-Al.

The crack growth and propagation were studied on the (001) plane for the two systems. Illustrative pictures after various loading cycles (and e_{max}) showing mechanisms of crack propagation for both Ni and Ni-Al are shown in fig. 4. In all of the figures discussed, 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. In all of the images, atoms with a centrosymmetry parameter close to zero are removed to facilitate easier viewing of the defects inside the structures. The visible atoms are associated with crack surfaces, exterior slab surfaces (only three surfaces are shown), Ni-Al bi-interfacial layer and other defects created during crack propagation. The atoms are colored with yellow for dislocations, brown for stacking faults, and green for surface atoms. The yellow and brown are also associated with atoms with crystallinity other than the fcc.

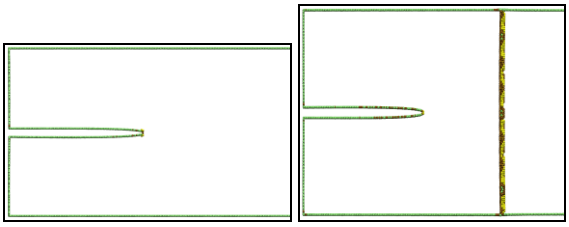
Case 1: Maximum Strain (e_{max}) = 0.046

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 at lower e_{max} move in a straight line with fatigue cleavage of atomic bonds in the crack plane. The crack growth in Ni however, stops 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 reach the interface during the 3rd fatigue cycle. When crack reach 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.



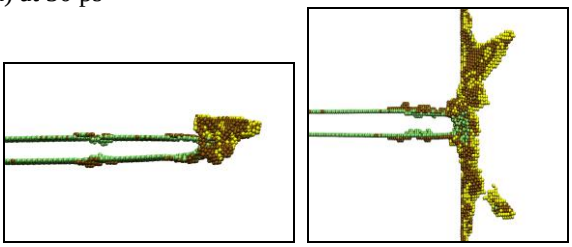
(a) (b)

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



Nickel Ni - Al

(a) at 50 ps



Nickel Ni – Al

(b) at 70 ps

Figure 2: Snapshots of crack propagation in Ni and Ni-Al Bi-metallic nanolayer

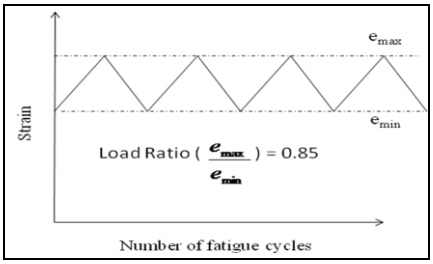
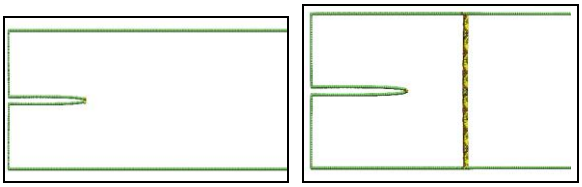
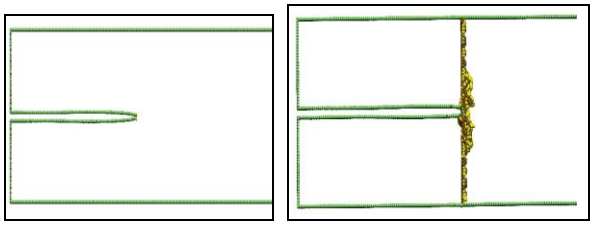


Figure 3: Strain controlled loading pattern applied to Ni and Ni-Al nanolayer



Ni Ni – Al

(a) After 1 fatigue cycle



Ni Ni - Al

(b) After 3 fatigue cycles

Figure 4: Crack propagation in Ni and Ni-Al metallic nanolayer

4 CONCLUDING REMARKS

Molecular dynamics simulations under tensile, cyclic mode I fracture loading were conducted to study crack propagation in a nano-scale Ni single crystal and a bi-metallic Ni-Al system with a crack initiating and propagating from Ni towards the Ni-Al interface. Our results for Ni single crystal are in agreement with predictions given by Abraham, et al [6] for fcc solids with 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. Our 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. As the propagating crack approaches the interface, a small bud called the 'process zone' at the crack tip start interacting with interfacial defects that eventually blunts the crack tip and ceases further crack growth.

The embedded atom method inter-atomic potential was used to investigate behavior of the (001) [100] crack system under strain controlled cyclic loading in both the systems. A cyclic loading with constant amplitude of maximum strains was applied at a high load ratio (0.85) to the two systems. Depending on the value of the maximum strain e_{max}, the crack propagates either by fatigue cleavage of the atomic bonds in the crack plane or by void nucleation in the regions near the crack tip. In Ni-Al, as crack approaches the bi-metallic interface, dislocations start emanating from the interfacial bi-layer. The presence of interface in the Ni-Al prohibit crack from propagating beyond the interface. The creation of voids slows down crack growth in both the Ni and Ni-Al at higher value of e_{max} during cyclic loading. Plastic deformation dominates crack propagation during tensile loading that result in slower crack growth, when compared to the crack growth under cyclic loading. The earlier nucleation of dislocations at the crack tip in Ni-Al prevents crack from reaching the interface during tensile loading. Future work will focus on investigating crack propagation under cyclic loading for material systems with more complicated crystallographic orientations and also at higher temperatures.

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