Atomistic simulation of crack propagation along $\gamma$-TiAl lamellar interface

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Abstract. Due to start-up and shut-down operations of engine, TiAl structural components usually undergo not only static but also cyclic mechanical loading. The crack propagation mechanisms of $\gamma$-TiAl under two types of loading are studied in this work to reveal the differences of the mechanisms under constant strain rate and cyclic loading. Since the crack prefers to nucleate at the interface, two types of loadings are applied to a $\gamma$-TiAl interface system with a pre-existing micro-crack at the interface by the means of classical molecular dynamics simulation, the loading direction is along [111] perpendicular to the interface. The evolution of crack tip and dislocation is observed in atomistic scale. The results show that, under both loading types, the crack propagates asymmetrically, Shockley dislocations emit on the ($-11$) slip plane from the right crack tip and slip along $[1-12]$ direction. The dislocations blunt the extension of crack while the left crack tip propagates in a brittle way. During the cyclic loading, different with constant strain rate condition, the crack advances and dislocations slip with increasing loads and retreat during unloading. In addition, the stress decreases and the crack length increases with the increase of the cyclic loading number.

1. Introduction

TiAl intermetallic based alloy has potential for replacing heavier materials in high temperature applications such as automotive and aerospace engine components, due to their remarkable thermomechanical properties and low density. Unfortunately, neither the ductility nor the fracture toughness of TiAl-alloys is particularly high. Thus, it’s of significant importance to study the mechanism of crack propagation in TiAl components.

TiAl alloy formed entirely by lamellar colonies, which is accordingly named “fully lamellar (FL)”, has the most promising mechanical properties over a wide range of temperature[1]. Previous experimental investigations of the influence of lamellar spacing on ductility, creep resistance and fracture toughness show that increasing the number of lamellar interfaces is advantageous[2,3], and enhances the ductility significantly[4–6] while also increasing the creep resistance[7,8]. Meanwhile, micro-cracks prefer to initiate at and propagate along the lamellar interfaces or lamellar colony boundaries[9]. Therefore, investigation of crack propagation in lamellar interface system is of significant importance.

Typical TiAl lamellar microstructures consist of many sharp $\gamma/\gamma$ and few $\gamma/\alpha_2$ interfaces which are all perpendicular to the [111]$\gamma$ or [0001]$\alpha_2$ directions. Different $\gamma/\gamma$ variants can be created by rotating
half of the initial supercell around the [111]γ direction by 60°, taking into three different variants, the pseudo-twin (PT), the rotational-boundary (RB) and the true-twin (TT) by 60°, 120° and 180° respectively[10].

Previous investigations on crack propagation of TiAl intermetallic based alloy mainly using experiment method. Study by experiments are, however, time consuming and costly due to sample fabrication and thus only a limited number of tests per condition can be generally performed. Classical molecular dynamics simulation provides a physical insight into understanding the deformation phenomena in the atomic scale and enables one to predict certain properties of materials. Numerous researches have been done via molecular dynamics to study the crack propagation of various materials, and their studies show that molecular dynamics simulation provides a physical insight into understanding the crack propagation phenomena in the atomic scale[11,12]. In addition, the influences of grain boundary or twin boundary on crack propagation have also been investigated in atomic scale.

In this work, molecular dynamics simulations of crack propagation in a γ/γ interface system under static and cyclic loading have been performed to investigate the different crack extension mechanisms under different loading types.

2. Simulation Details

A semi-empirical embedded atom method (EAM) potential by Zope and Mishin[13] is used to model the interatomic interactions of Ti-Al intermetallic system, using an open code Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)[14]. The simulation box contains about 522240 atoms with a size of 9.8*30*30 nm

3. The simulation box consists of two lamellae with a PT interface and a pre-exist crack, as shown in figure 1(a).

All of the simulations are performed at 0.01 K to avoid the complexity due to the thermal activity of atoms. At first the system is equilibrated through applying NVE ensemble. And then the top and bottom layers are fixed for applying Mode I loading under a uniaxial tensile loading process with a strain rate of 10⁹ s⁻¹. The NVE ensemble is applied during the tensile deformation, and Langevin thermostat is used to control the temperature. Static and cyclic loading is performed in this work respectively, as it is shown in figure 1(b). The periodic boundary condition is assigned in the x and y direction. For the sake of eliminating the stress oscillation resulting from the sudden loading, the loading is applied such that the velocity was linearly distributed along the z-direction. The velocities are maximum positive value and minimum negative value at the top and bottom fixed layers. The time step is chosen to be 0.001 ps.

![Figure 1](image)

**Figure 1.** Schematic of the (a) simulation model and (b) two types of loading regimes.
The visualization of the simulation results is performed by OVITO[15]. Dislocation extraction algorithm (DXA) and common neighbor analysis (CNA) are used to identify the structure and dislocations[16].

3. Result and Discussion

Figure 2 lists the stress-strain curve and snapshots of the microstructure at different loading stages under static loading. Imagines are colored according to CNA analysis. Green and red atoms represent the perfect FCC and HCP (interface or stacking faults here) structures respectively, and the dark blue atoms are of the other structure (crack boundary and dislocation core here).

![Figure 2. PT interface system under static tensile loading along z direction: (a) stress-strain curve and (b)-(f) snapshots of microstructure evolution around the micro-crack.](image)

There are three major competing deformation modes in $\gamma$-TiAl with L1$_0$ structure: $1/2\langle 110 \rangle$ ordinary dislocation, $\langle 101 \rangle$ superlattice dislocation and $\{ 111 \} < 11\bar{2} >$ true twin which serves the chemical order of $\gamma$ phase. And the dominant slip system is $\langle -1-11 \rangle < -1-1-2 \rangle$ under loading along $< 111 >$ direction according to the Schmid factor analysis. According to the DXA analysis which is used to compute the Burger vectors of dislocations, it can be found that the Shockley dislocation with Burger’s vector=$1/6[ -1-1-2 ]$ emits from the right crack tip and slip on the $(-1-1)$ plane at 25 ps (figure 2 (c)). Thus, the simulation result agrees well with the Schmid factor analysis. And the propagation of the right crack tip is blunted by the slip plane (figure 2 (d)).

The L1$_0$ intermetallic TiAl alloy has an asymmetric structure, which makes only one type of slip system can be found under loading along $< 111 >$ direction. In the upper TiAl lamella, the preferred slip system is not parallel to the crack tip due to the twist angle of 60°. Therefore, the upper lamella requires more energy for dislocation nucleating from the crack tip than the lower lamella. In the lower TiAl lamella, the relative angles between the preferred slip plane and the interface plane are $\theta_L$ and $\theta_R$ respectively (figure 2 (c)). The left crack tip with a larger angle requires a larger amount of energy to nucleate and propagate dislocation away from the crack tip[17]. Therefore, only one slip system can be found at the right crack tip, and the crack propagates in a brittle way along -$y$ while in a ductile way along $y$.

Under cyclic loading along z direction, as it shown in Figure 1 (b), the crack propagation under loading before 35ps is similar to it under static loading. Figure 3 (a) lists the snapshots of the crack evolution in the first cyclic loading. At the beginning of the unloading process (40ps), the crack is still growing along -$y$ due to the high stress. And then the left crack tip and the slip system at the right
crack tip retreat (60ps). In addition, at the end of the unloading (70ps), the left crack tip returns to its initial state while the dislocation emitted from the right crack tip doesn’t disappear.

![Figure 3.](image)

*Figure 3.* (a) the snapshots of crack propagation; (b) stress-strain curves of the three loading cycles; (c) cracks at the longest stages in the three loading cycles under cyclic loading

It can be observed from the stress-strain curves of the 3 cycles (figure 3 (b)) that the stresses decrease as the cyclic loading number increase. According to the simulation result, the crack length propagates to the longest at 50ps, 120ps and 190ps in three cycles respectively. Figure 3 (c) lists the longest cracks in the three cycles. It can be speculated that the maximum of the crack length is longer as the increase of the cyclic loading number.

4. Conclusion
In summary, crack propagation in a γ-TiAl intermetallic lamellar system with a PT interface is investigated by classical molecular dynamics under static and cyclic loading. The following conclusions can be drawn:
(1) Due to the different energy required to nucleate dislocation of the two crack tip, the crack propagates asymmetrically along the PT interface of γ-TiAl under high strain rate.
(2) Under cyclic loading, the stress decreases and the crack length increases with the increase of the cyclic loading number.

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