

# MOLECULAR DYNAMICS STUDY ON CRACK GROWTH UNDER CYCLIC LOADING

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The evaluation of mechanical behaviors of materials at a micro scale level has been investigated in recent years. Cracks and grain boundaries are the two major factors determining these properties in metals and alloys. The molecular dynamics method has been applied to examine the fracture of metals including both a crack and a grain boundary in the atomistic scale under monotonic loadings. Nishimura and Miyazaki [1] reported the effect of the grain boundary on the brittle crack propagation in  $\alpha$ -Fe under mode I loading. However, the molecular dynamics simulation is hardly carried out for understanding the fatigue crack propagation in the atomistic scale because fatigue simulation is a time-consuming task.

In this investigation, the mechanical behaviors around a crack tip for a system including both a crack and two tilt grain boundaries under cyclic loading are examined using the molecular dynamics simulation. The grain boundary, whose direction of the axis of misorientation angle is  $\langle 110 \rangle$  and whose plane is  $\{112\}$ , is considered in this simulation. This grain boundary has the lowest grain boundary energy among all tilt grain boundaries. The Johnson potential for  $\alpha$ -Fe is used in the simulation to describe interaction between atoms. The temperature of the system is 300 K and the system includes one million atoms.

As a result, not only a structural transition from bcc to hcp but also emission of edge dislocations is observed around the crack tip during the first loading in order to relax stress concentration. The edge dislocations emitted from the crack tip move to the  $\langle 111 \rangle$  direction on the  $\{112\}$  plane, which correspond to the slip system of  $\alpha$ -Fe. Then, two dislocation pile-ups starting from the grain boundaries are formed after the edge dislocations reach the grain boundaries, because they cannot move beyond the grain boundaries. During the first unloading, the edge dislocations emitted from the crack tip return to the crack tip and disappear in the system. When the loading and unloading are repeated, the emission and absorption of the dislocations at the crack tip observed during the first cycle are repeated. We observe not only the generation of several vacancies around the crack tip but also the crack propagation during cyclic loading. Conclusively, we propose the fatigue crack growth mechanism for the initial phase of the fatigue fracture. That is, the fatigue crack propagates due to coalescence of the crack and the vacancies caused by the emission and absorption of the dislocations at the crack tip.

## References

[1] K. Nishimura, N. Miyazaki, "Molecular Dynamics Simulation of Crack Propagation in Polycrystalline Material," *Computer Modeling in Engineering & Sciences*, v. 2, p. 143-154, 2001.