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MOLECULAR DYNAMICS SIMULATION OF CRACK PROPAGATION IN HCP CRYSTALS

S. Ando[1], H. Tonda[1] and K. Takashima[2]

[1]*Department of Materials Science and Mechanical Engineering, Faculty of Engineering, Kumamoto University, Kumamoto, 860-8555, Japan*
[2]*Precision and Intelligence Laboratory, Tokyo Institute of Technology, Yokohama, 226-0026, Japan*

ABSTRACT

The crack propagation behavior of hcp single crystals has been simulated by molecular dynamics method using Lennard-Jones type potential. A definite dependence of crystallographic orientation on crack propagation behavior was obtained. In a model crystal with initial crack plane and direction were $(10\bar{1}0)$ and $[1\bar{2}10]$, the crack propagated parallel to $(10\bar{1}0)$ $[1\bar{2}10]$ and two sets of prismatic slips were occurred at the crack tip. Therefore, the crack in this crystal is deduced to extend by alternating shear on two intersecting prismatic slip systems. In a model crystal with (0001) $[1\bar{2}10]$ initial crack, the crack propagated parallel to (0001) and small twinning region was occurred in front of the crack. The crack propagation rate in the twin region is lower than those in the matrix region. In the model crystal with $(10\bar{1}0)[0001]$ initial crack, the crack propagate parallel to notch plane with some basal slips and prismatic slips were occurred in front of the crack.

KEYWORDS

HCP, crack propagation, Lenard-Jones potential, molecular dynamics.

INTRODUCTION

Fatigue crack growth in crystalline metals and alloys are fundamentally based on cyclic plastic deformation at the crack tip. The crack growth increment for each cyclic loading (*da/dN*) in such materials often occurs in the range of 10^{-6} to 10^{-3} mm, and this extension is usually smaller than the grain size of such materials. Therefore, it is extremely important to know the fatigue crack growth mechanisms that may occur in singe crystals to promote increased understanding of the intrinsic fatigue crack growth resistance of materials.

Among hcp crystals, α-titanium and its alloys have been applied to aerospace structures and engine components because of their excellent specific strength and corrosion resistance. However, there have been few studies on fatigue crack growth mechanisms in titanium crystals. This may be partly due to the fact that the slip systems of hcp crystals have not yet been identified precisely. In addition, mechanical twinning may occur in hcp crystals. This may make it difficult to clarify fatigue crack growth mechanisms in hcp metals. Therefore, it is important to evaluate the crack propagation mechanism of such materials.

The crack propagation process is subjected to the behavior of atoms near the crack tip. Microscopic analysis using the molecular dynamics has, therefore, advantages over macroscopic analysis. In the present study, the atomic structure at the crack tip in α-titanium single crystals with different orientations has been investigated by method of molecular dynamics simulation.

CALCULATING METHOD

In the present simulation, Lennard-Jones type interatomic potential (Minonishi *et al.*[1], 1981),

$$V(r) = \varepsilon_0\{(d/r)^{12}-2(d/r)^6\} \quad (1)$$

was used, where $\varepsilon_0 = 0.16$ eV, $d = 1.021522a$ (a is the lattice parameter in (0001)) and r is the distance between atoms.

Figure 1 shows the atom arrangement of model crystals used in this study. Every initial crack was set perpendicular to y-axis and its direction was parallel to x-axis. The crystallographic orientations of initial crack plane and direction in the Crystal 1 were $(10\bar{1}0)$ and $[1\bar{2}10]$, those in the Crystal 3 were (0001) and $[10\bar{1}0]$, those in the Crystal 4 were (0001) and $[1\bar{2}10]$ and those in the Crystal 5 were $(10\bar{1}0)$ and [0001], respectively. These models were applied fixed boundary condition along x- and y-axes and periodic boundary condition along z-axis. The number of atoms contained in each model crystals are listed in Table 1. The initial cracks were introduced to the model crystals by terminating interaction between atoms along crack plane. The external load to propagate crack was added on the x- and y- fixed boundary atoms by their displacement, which was estimated by an isotropic elastic field with stress intensity factor K singularity.

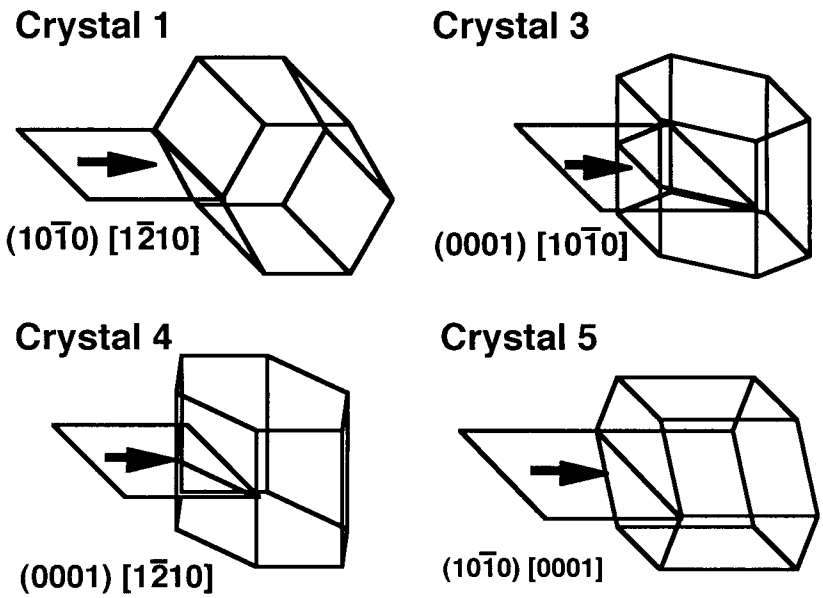

Figure 1: Model hcp crystals and initial crack orientation.

TABLE 1
Size of model crystals.

	X atoms	Y atoms	Z atoms	Total
Specimen-1	44	48	2	4224
Specimen-3	26	50	2	2600
Specimen-4	42	50	2	4200
Specimen-5	54	24	2	2592

The magnitude of time step used in integration of the equation of motion was $2x10^{-16}$ s and the increment in external field is K = 0.01MPam$^{1/2}$ every 5000 time steps. The initial temperature of the crystals were set to 293K.

RESULTS AND DISCUSSION

All of the crystals consist from two atomic layers. The atoms of each layer are represented by circles and squares, respectively. Figure 2 shows the atomic structure at the crack tip in Crystal 1. The arrows in the figure show the y-component of relative displacement between atoms according to Vitek's method (Vitek *et al.*[2], 1970). Crack propagation in Crystal 1 was occurred at K = 0.56 MPam$^{1/2}$, and the dislocations were emitted upward and downward of the crack. Each directions of emitting dislocations were inclined 60 degree to the initial crack plane. This indicates that two intersecting prismatic slip systems ($(1\bar{1}00)$ $[11\bar{2}0]$ and $(01\bar{1}0)$ $[\bar{2}110]$) were activated at the crack tip. As a result, the crack in Crystal 1 was propagated parallel to $(10\bar{1}0)$ $[1\bar{2}10]$ initial crack.

In the fatigue crack growth in real titanium single crystals (Mine *et al.*[3], 1998), many slip trace of prismatic slips were observed near crack surfaces. The result of Crystal 1 is similar to that of real titanium single crystals. Therefore, as shown in Fig. 3, the slip-off model of crack propagation in titanium single crystals is deduced from present simulation result.

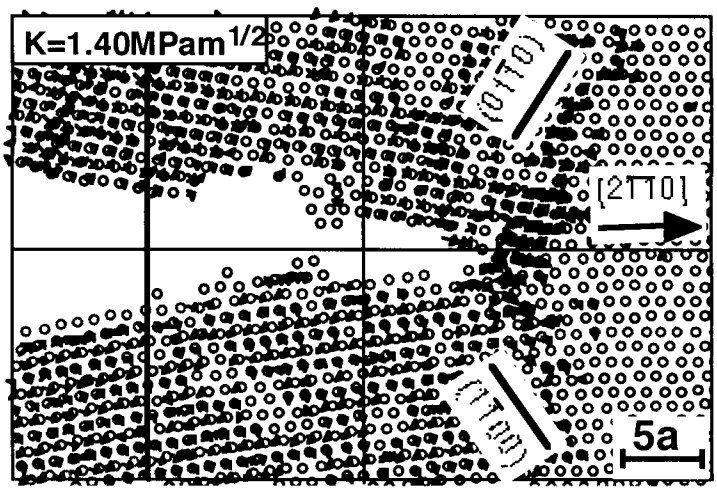

Figure 2: Atomistic structure of crack tip results in Crystal 1 at K = 1.40MPam$^{1/2}$.

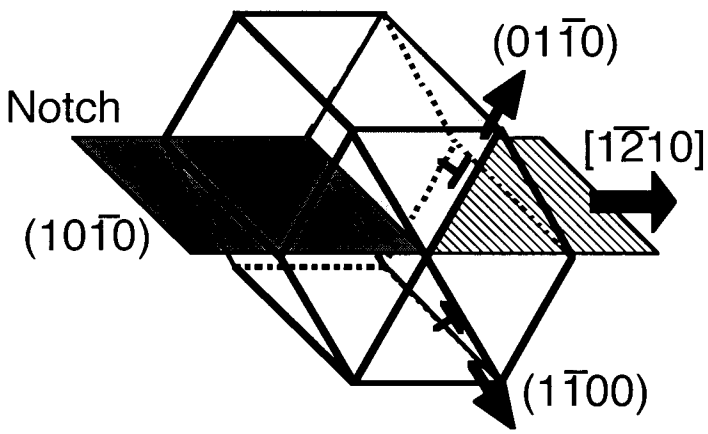

Figure 3: Slip-off model activated in Crystal 1.

In the case of Crystal 3, the initial crack started to propagate at K = 0.50 MPam$^{1/2}$ and, as shown in Fig. 4 by solid lines, $\{10\bar{1}1\}$ twins occurred at the crack tip with increasing K. In the case of Crystal 4, the initial crack propagated parallel to (0001) with increasing K as brittle manner. In this crystal, as shown in Fig. 5, a region which shows different atomic orientation to the matrix was developed. Since the atomic orientation of that region corresponds to (0001) plane, it can be seen that $\{10\bar{1}2\}$ deformation twin occurred in front of the crack tip at K=1.03 MPam$^{1/2}$. After that, the crack was propagated through this twin region.

Figure 6 shows a crack tip structure in Crystal 5. The initial crack started to propagate at K = 0.67 MPam$^{1/2}$, and the crack became blunt with emittion of many partial dislocations parallel to the basal planes from the crack tip.

Figure 7 shows relationships between the crack growth length and the stress intensity factor in each model crystals. A slope of the curve for Crystal 4 is larger than that of Crystal 1 and Crystal 3 below K = 1.1 MPam$^{1/2}$. This indicates that the crack parallel to (0001) plane propagates easily than in the case of Crystal 1 and Crystal 3. The crack in Crystal 3 propagated through $\{10\bar{1}2\}$ twin region above K = 1.1 MPam$^{1/2}$, then the slope of the curve in Fig. 7 becomes small. This indicates that the crack growth rate in the twin region is low than that of the matrix. In real titanium single crystals with a crack parallel to (0001), fatigue cracks were propagated with many $\{10\bar{1}2\}$ twins and fatigue crack propagation resistance on (0001) crack is higher than the case of crack propagation with alternating shear of prismatic slips[3]. From above simulation results, it is suggested that because of the crack growth rate is low in the $\{10\bar{1}2\}$ twin occurred in front of the crack, fatigue crack propagation resistance with respect to (0001) crack in titanium single crystal becomes high.

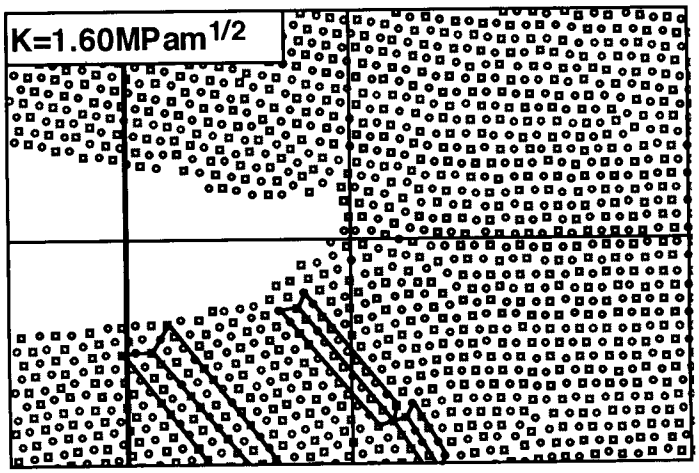

Figure 4: Atomistic structure of crack tip results in Crystal 3 at K = 1.60MPam$^{1/2}$.

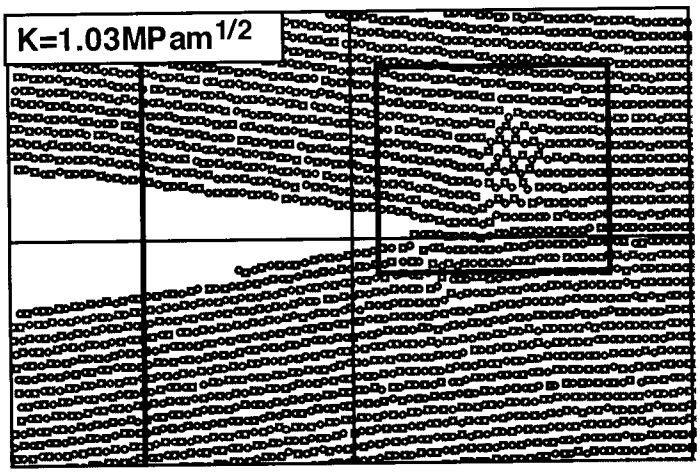

Figure 5: Atomistic structure of crack tip results in Crystal 4 at K = 1.03MPam$^{1/2}$.

In the case of Crystal 5 with crack propagates [0001], the threshold value of stress intensity factor for crack propagation is higher than other three crystals and the curve of crack growth rate is lowest. In the case of titanium single crystal, a fatigue crack normal to (0001) propagates to [0001] when high stress intensity factor range is applied (Yamada *et al.*[4], 1999). This shows that crack propagation resistance with respect to [0001] is heigest and this is agreement with the simulation result in Crystal 5. It was also reported that the fatigue crack normal to (0001) inclined (0001) and propagated at low stress intensity factor range[4]. In Crystal 5, it was not seen such a behavior at low stress intensity factor. We need more investigation about this point.

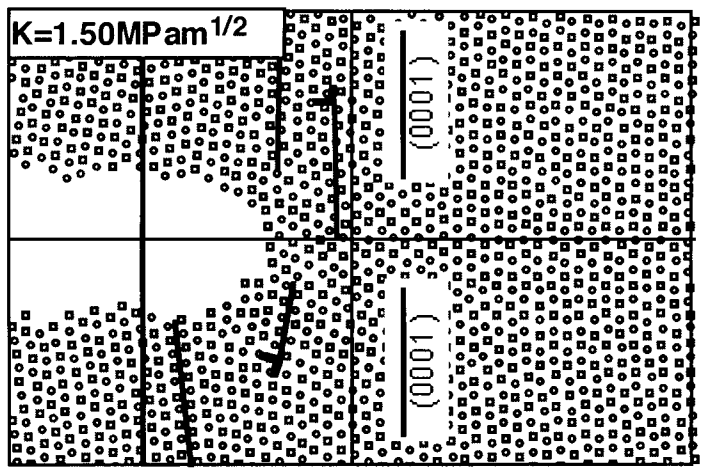

Figure 6: Atomistic structure of crack tip results in Crystal 5 at K = 1.50MPam$^{1/2}$.

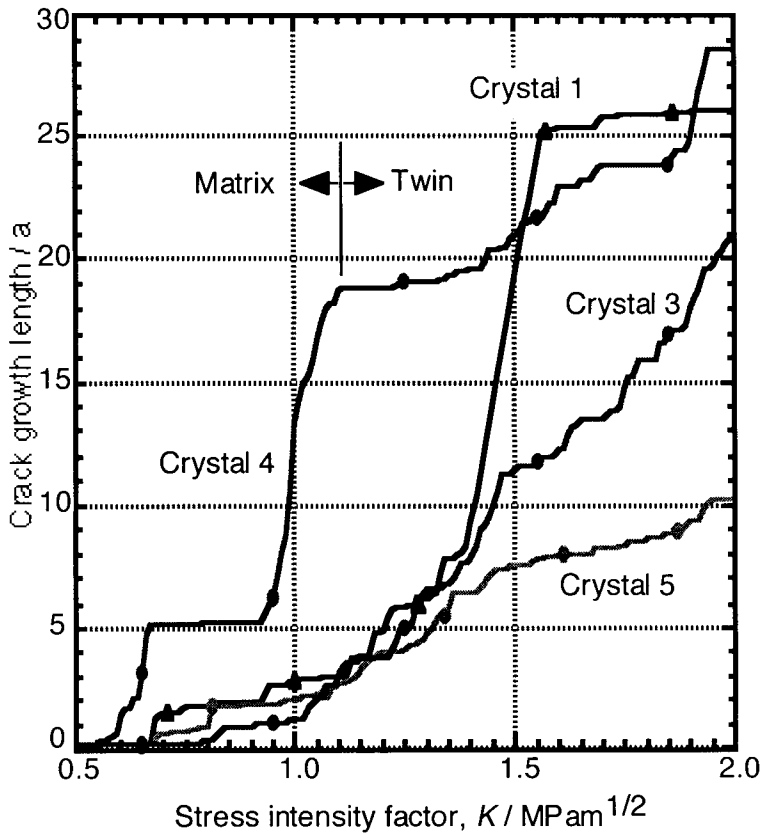

Figure 7: Relationship between crack grwoth length vs. stress intensity factor.

CONCLUSION

The crack growth behavior of a-titanium single crystals has been investigated by molecular dynamics simulation using Lennard-Jones type potential. Results are summarized as follows:

1. In the model crystals with the initial crack plane and direction were $(10\bar{1}0)$ and $[1\bar{2}10]$, a crack propagated parallel to $(10\bar{1}0)[1\bar{2}10]$ by alternating shear on two intersecting prismatic slip systems. This behaviors are similar to those of real α-titanium single crystals. From this result, the slip-off model consist of two intersecting prismatic slip systems was proposed.

2. In the model crystals with the initial crack plane and direction were (0001) and $[10\bar{1}0]$, $\{10\bar{1}1\}$ twins occured at the crack tip.

3. In the model crystals with the initial crack plane and direction were (0001) and $[1\bar{2}10]$, a brittle crack propagated and$\{10\bar{1}2\}$twin occurred in front of the crack. The crack growth rate in the twin region was lower than in the matrix.

4. In the model crystals with the initial crack plane and direction were $(10\bar{1}0)$ and [0001], a crack propagated to [0001] with many partial dislocations. The crack growth rate is lowest than other three crystals.

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