Journal of Applied Science and Advanced Technology
Journal Homepage : https://jurnal.umj.ac.id/index.php/JASAT

Molecular Dynamics Approach on Dislocation Emission from Crack Tip Under Stepwise Loading in Aluminum

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ARTICLE INFO

JASAT use only:
Received date : 27 January 2021
Revised date : 21 February 2021
Accepted date : 28 March 2021

Keywords:
Molecular Dynamics
Step wise loading
Aluminum
Dislocation emission

ABSTRACT

Molecular dynamics (MD) simulation is carried out for pure aluminum under stepwise loading condition. This simulation aims to understand the experimental results on impact fracture toughness of aluminum alloys under short pulse loading. The model used in this simulation is featured by an atomistic model with single atom and the [111], [110], and [112] directions, a center-cracked plate model by the atomistic model with 17,402 number of atoms, and the periodic boundary condition in z-axis to postulate the plane strain condition. The obtained results are some dislocations emitted from crack tip, a void nucleation and growth taking place ahead of the crack tip. This micro void was initiated from a dislocation core when the load was kept being constant. This micro void never coalesced with the main crack as the distance between the micro void and the main crack was too far atomically and the micro void growth was stabilized. Energy balance investigation shows kinetic energy of the system was very small and almost constant during the process. The potential energy increased as the external load increased and then became constant when the load became constant. Significant fluctuation of energy was observed during dislocation emission. Some amount of barrier energy must be released for the dislocation emission. The qualitative understanding can be provided by this molecular dynamic simulation.

INTRODUCTION

During the past few decades, fracture mechanics as a scientific discipline has been developed and its basic aspects have already been clarified. However, there are many important problems remaining to be solved. The most notable one is dynamic fracture. Dynamic fracture includes two subjects, a stationary crack subjected to a rapidly applied load, and a rapidly propagating crack under a quasi-static loading. In both cases, the material at the crack tip is strained rapidly and may possess less resistance to fracture than under quasi-static strain rates. In addition, an inertia effect may influence a load history at the crack tip.

Dynamic fracture tests are of interest, because many structural components are subjected to high loading rates in service and must be able to survive during an accident. Thus, these components must be designed against crack initiation under high rate loading or designed to arrest a rapidly running crack.

Furthermore, the fracture resistance of material, under rapid loading, is generally lower than that under static loading. As a consequence, the dynamic fracture toughness value is more conservative than the static one for design criterion [1]. The attempts of extending of static and quasi static fracture criterion were few; suffice to say about well-known experiments by K. Ravi-Chandar, W. Knauss [2]. It was necessary to propose, to discuss, and to test the conditions of dynamic fracture. For that, a material parameter, which defines its dynamic strength are needed. Such a parameter, although not so clearly defined, was proposed by D.A. Shockey et al [3]. The authors associated this parameter with minimal interval needed for preparing of fracture called minimum time (e.g. that a crack becomes unstable when the dynamic stress intensity at the crack tip exceeds a critical value during a certain time defined as the minimum time [4]). The matter is still unclear and not well understood is the

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DOI: https://dx.doi.org/10.24853/JASAT.3.3.97-108

physical meaning of the minimum time, and how it depends on loading parameters (such as when the value of exceeds KID), and how it relates to the time required to develop critical plastic and process zones at the crack tip. N.F. Morozov and Y.V. Petrov [5] proposed the criterion of dynamic brittle fracture with a new parameter called incubation time. The incubation time was defined more accurately, and the method of its determination was developed. Homma et al [6] carried out a series of experiments on cleavage fracture caused by a short stress pulse. According to this work, the cleavage fracture occurs when dislocations emanated from the crack tip pile up at the boundary of the pearlite layer and resultant of the applied stress raised by the crack and the stress caused by the dislocation pile-up exceeds the critical value near the leading edge of the piled dislocation. A dislocation emanated from the crack tip travels to the cleavage fracture nucleation site taking a certain time. If the dislocation travel distance is 30 to 120 μm and the dislocation travel at a speed of 1 m/second, it will take 30 to 120 μ seconds for the dislocation to reach the nucleation site. This means that the cleavage fracture under short pulse loading occurs while some dislocations emanated from the crack tip still are traveling to the nucleation site, namely do not reach their piling up position. Therefore, it is important to carry out a computer simulation to investigate how dislocation behaves and is emitted under short pulse loading and also to understand how the void is developed as reported by the experimental results.

Many researchers such as Rice [7] have investigated the dislocation nucleation from the crack tip and used linear elasticity to establish the criterion of nucleation of a discrete dislocation and the transition in ductile and brittle fracture. Sinclair and Finnis [8] extended Rice and Thomson analysis to address the problem of whether the presence of one or more emitted dislocation affects the competition between further emission and cleavage. Unfortunately, these analyses are not satisfactory because they used the continuum elasticity for crack tip stress field; invariably have a singularity at the center of dislocation. It is clear that such the singularity does not occur in a real crystal. In addition, when a dislocation is very near the crack tip where the non-linear and atomic lattice effects are significant, the atomic force law needs to be considered. Furthermore, the continuum elastic theory cannot be validly applied to this region and it is essential to analyze the dislocation nucleation and emission from crack tip by atomistic simulation utilizing appropriate inter atomic law and correct crystallographic geometry of the simulated specimen.

Many researchers have carried out molecular dynamics simulation to understand the nature, which occurs near crack tip. Benito deCelis et al [9] developed a 2D molecular dynamics simulation with Johnson and Morse potential to investigate crack tip processes in alpha—iron and copper by using a few numbers of atoms with the fixed boundary and the flexible boundary condition. Kim S. Cheung and Sydney Yip [10] used 2D molecular dynamic simulation with Voter potential, fixed boundary condition, and 2400-3000 numbers of atoms to examine brittle-ductile transition in bcc alpha-iron. Kitagawa and Nakatani [11] used the Finnis and Sinclair potential to calculate the crack tip processes. Several atomistic lattice geometries and crack modes were employed to calculate the nucleation and emission of dislocations. Molecular dynamics simulation of fracture has been performed on the metals Al and Nb, and some intermetallic alloys by Becquart et al [11] with fixed boundary condition. Thijsse et al [14] studied dislocation emission from crack tip in an elastically fcc crystal with 3D molecular dynamic simulation using Lennard-Jones potential. Displacement and stress fields around both nucleating and moving dislocation are compared to the predictions of the Peierls-Nabarro continuum-elastic model by Rice. Kuksin [15] investigated dynamics of edge dislocation and yield stress using molecular dynamics. Zhang et al [13], Chandra et al [16], and Chowdhury et al [17] also used the Molecular Dynamics to investigate fracture mechanics phenomena such as emission of a dislocation and a fast-moving crack tip in aluminum. Even though all of these works showed that molecular dynamic simulation can give precise and detail results to explain such phenomena atomically, but they were only focused on static fracture mechanics, no work was dealt with dynamic fracture mechanics.

The aim of this research is to investigate dislocation movement emitted by crack tip under short pulse loading in pure aluminum based on molecular dynamic simulation. Special attention will be placed on investigating how dislocations are generated near the crack tip and the local phenomena on atomic scale activated at the crack tip, which propagates to extension of the crack and also to determine whether a micro void exists or not after the short pulse loading as shown by the experimental result. The mode I type crack opening process is analyzed for pure aluminum.

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The research methodology employed in this work is simulation based on molecular dynamics algorithm. The results of simulation were compared qualitatively with experimental results of Rizal and Homma [8]. The simulation used some general assumptions that the lattices are face—centered cubic arrangement with an anisotropic properties and stress wave is neglected.

Fundamentals Of Molecular Dynamics

The simplest model of a metallic material at the atomistic scale can be visualized as an array of atoms interconnected with springs. More sophisticated atomistic simulation techniques have now been developed to describe more accurately the atomic interactions in materials. The embedded atom method (EAM) is the most accurate atomic interaction model recently developed and will be used in the simulation technique to describe the atomic interactions in pure aluminum.

The molecular dynamics (MD) approach is used to study fracture mechanics in both a model system and a system with more realistic crystal structures and potentials. The difficulty in simulation of crack tip processes with molecular dynamics is that it is feasible, in most cases, to work with only several hundred discrete particles, and in some cases, up to a few thousand particles, and that this number is not large enough to represent a complete system whose boundaries are sufficiently far away from the crack tip. This makes it necessary to devise methods incorporating the effects of the material outside modeled the region into the simulation by building this region into infinite continuum. Unless the border of the simulation system composed of discrete particles can faithfully transmit the full effects of the outer body, modeled as a continuum, so far as the behaviors of the crack tip is concerned, there is no guarantee that fracture is simulated realistically.

The most reasonable approach to this problem is to choose the region composed of discrete particles surrounding the crack tip that is large enough to model the important nonlinear effects of the material property, and to consider the outer material as a linear elastic continuum. Since nonlinear effects increase smoothly with stress, the size of the region modeled by molecular dynamics is not immediately apparent. Two types of displacement boundary conditions are considered for the border between the inner and outer regions in molecular dynamics simulations: "fixed boundary " and "flexible boundary". In the first method, the atoms forming the border of the inner system are placed at appropriate positions of the outer region, prior to simulation, and are subsequently fixed as the outer material is removed during the simulation. While this method is the simplest to implement, it is less accurate unless a very large system is used so that the influences of the border on the crack tip are minimized. In the flexible boundary method, the border atoms are surrounded the stationary atoms in the outer region, which move by displacement of the outer region.

As the inner region modeled by molecular dynamics is still attached to the outer continuum, relaxes during the simulation, forces are generated on the atoms in the border region. These forces are relieved in an iterative fashion through the use of a Green's function derived from the linear elasticity theory applied to the outer region. Thus, in this method, the border region is not quite rigid, but its flexibility is still limited by the action of the outer region.

Molecular dynamics simulation computes the motions of individual molecules in a model of solid, liquid, and gas. The key idea is motion, which describes how positions, velocities, and orientations change with time. Molecular dynamics is a powerful method for exploring the structure of solids, liquids and gases. The idea is a simple one: calculate the forces acting on the atoms in a molecular system and analyze their motions. When enough information on the motion of the individual atom has been gathered, it is possible to condense it all using the methods of statistical mechanics to deduce the bulk properties of the material. These properties include the structure (e.g. crystal structure, predicted x-ray and neutron diffraction patterns), thermodynamics (e.g. enthalpy, temperature, pressure) and transport properties (e.g. thermal conductivity, viscosity, diffusion). In addition, molecular dynamics can be used to investigate the detailed atomistic mechanisms underlying these properties and compare them with theory. It is a valuable bridge between an experiment and a theory. In molecular dynamics, the forces between molecules are calculated explicitly and the motion of the molecules is computed with a suitable numerical integration method on a computer [18]. This is nothing more than solving Newton's equations of motion for the constituent atoms. The starting conditions are the positions of the atoms (taken, for example, from a known crystal structure) and their velocities (generated from random numbers and scaled to the desired temperature) [20]. Following Newton's prescription, based on the initial positions, velocities and forces, it is possible to calculate the positions and the velocities of the

atoms at a small time interval (a time step). From the new positions, the forces are recalculated and then the next time step is made. The cycle has to be repeated many times in the course of a full simulation, usually for many thousands of time steps. It is worth noting that a single time step is usually of the order of 1 femto second (10^{-15} second!).

Equation of Motion

The Langrarian formulation of classical mechanics provides a general basis for dealing with these more advanced problems [19], and we begin with a brief summary of the relevant results. There are of course other ways of approaching the subject, and we will also make passing reference to Hamilton's equations. The starting point is Hamilton's varitional principle, which concisely summarizes most of classical mechanics into statement that phase-space trajectory followed by a mechanical system is the one for which the time integral ζ dt is an extremum, where ζ is the Langrarian. A given set of **N** independent generalized coordinates and velocities {r_i, dr_i/dt} that describe the state of a conservative system (one in which all forces are derived from some potential energy function ϕ), so that ζ =ζ ({r_i}, {dr_i/dt}, t), then can be shown to satisfy the Langrange equations.

$$\frac{d}{dt}\left(\frac{d\xi}{dr}\right) - \frac{d\xi}{dr_i} = 0, \qquad i = 1, \dots, N \tag{1}$$

This equation forms the starting point for many of the subsequent developments. Newton's second law is a simple consequence of this result, where if r_i denotes a component of the Cartesian coordinates for one atom (assuming identical mass m):

$$\xi = \tfrac{1}{2} m \Sigma_i \dot{r}_i^{\,2} - \phi(\{r_i\}) \tag{2}$$

Then, equation (2) becomes

$$m\frac{d^2 r_i}{dt^2} = F_i = -\frac{\partial \Phi}{\partial r_i} \tag{3}$$

Where m is the mass of an atom and r_i is position of atom i and ϕ is interatomic potential, which will be described later. Position vector r_i that locates atom i and a system are described in Fig. 1. In differential calculus, the acceleration is related to the velocity, and the velocity is related to the position through the mathematical process of integration. Many of what is called analytical mechanics are concerned with this integration process. In molecular dynamics, it is performed numerically using an integration algorithm.

Inter-atomic Interaction

The modeling techniques have been improved to such an extent that the major remaining deficiency is the inaccuracy of the interatomic potential to be used. It is then essential to construct reliable interatomic forces that can reproduce experimental data.

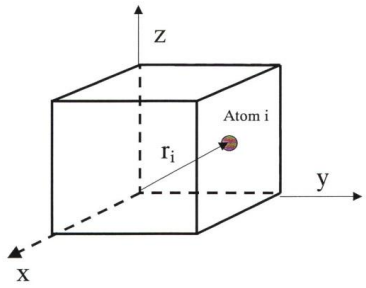

Fig. 1. A Cartesian fixed reference frame {X, Y, Z}

The simplest model at the atomistic scale can be visualized as an array of atoms interconnected with springs. More sophisticated atomistic simulation techniques have now been developed to describe more accurately to the atomic interactions in materials.

The Embedded Atom Method (EAM) is a recent approach used to simulate the interaction between atoms in metal and inter-metallic compounds. It is states that the energy contribution of an atom on its surrounding neighbors is a function of the local electron density due to all the surrounding atoms.

This approach becomes particularly important when point defects such as vacancy clusters, free surfaces, grain boundaries or dislocation cores are introduced and the density in the material is changed. Based on the EAM approach, the interaction energies of the atoms are composed of two potential functions. A classical pair interaction potential, V (Morse function), describes the attractive and repulsive electrostatic interaction between two atoms. An embedding function F takes into account the interaction energy of each atom with the local electron density associated with the neighboring atoms. Consequently, the total energy of the system is written as:

$$E = \tfrac{1}{2}\Sigma_{i,j} v(r_{ij}) + \Sigma_i F(\bar{\rho}_i) \tag{4}$$

With: $\bar{\rho}_i = \Sigma_i \rho(r_{ij})$

Where ρ is the electronic density function, $\bar{\rho}_i$ is the density at atom i due to all its neighbors,

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and r_{ij} is the inter-atomic distance between the atoms i and j. The interaction energies are however only taken into account within a selected cutoff distance (usually a second closest neighbor distance) and considered as zero outside of this region. The embedding function F(ρ) is determined by assuming that the crystal obeys Rose's equation of state, which scales the cohesive energy of most metals.

The embedding functions and the pair interaction potentials are generally designed to fit various physical properties and the pair interaction potentials are generally designed to fit various physical properties of a system such as lattice constants, elastic constants, or formation energies of diverse defects. In pure metal, such as Al, three function are required to describe the system. $V_{Al\text{-}Al}$, F_{Al}, and ρ_{Al} describes the properties of the pure Al. knowing the values of these variables described above, the potential energy of the considered system is then calculated using Equation 4.

The embedded atom method is however constrained to several types of limitations. Due to an angular dependence of the electron density that is not considered, the EAM technique fails to describe the interactions between covalent materials such as Si and Ge. The method is also limited in some cases where Cauchy pressure, defined as

P =1/2. (C12 - C44)

(C12 and C44 being elastic constants), is negative. In this case, the elastic constants determined by EAM do not fit the properties of the materials.

EXPERIMENTAL METHOD

Material Model

Aluminum has a face-centered cubic (fcc) crystal structure. The eight corner octants contribute totally in one atom, and the six face-centered atoms contribute in total atoms per a unit cell. In a metal, the lattice constant a is related to the atomic radius **R** by:

$$(a_{fcc})_{metal} = \frac{4R}{\sqrt{2}} \quad (5)$$

The packing factor for an fcc metal is 0.74, which is greater than 0.68 for a bcc metal. This is quite logical since each atom in a bcc metal has only eight neighbors, whereas each atom in an fcc metal has 12 neighbors. This is verified in Fig. 2.a-c, it is observed that the front face-centered atom has four adjacent neighbors, four neighbors in contact on the backside, and four comparable neighbors sitting in front.

A sphere model illustrating this crystal structure is shown in fig. 2.c whereas Fig. 2.a is a hard sphere model representation of an fcc unit cell, and Figure 2.b is a reduced-sphere model representation of the same unit cell.

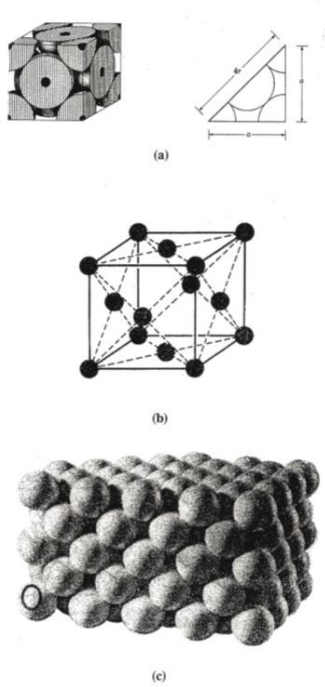

Fig. 2. An fcc atomic representation

Simulation Model

This work investigated only a small area near crack tip in a very large continuum elastic material under mode I opening crack load. Because the atomistic area is very small namely in angstrom scale compared to the crack length, this problem can be classified to small scale yielding (SSY) as described in Fig. 3. When a load is applied to this model, the atoms will behave nonlinearly. The dash line is the boundary between the atomistic area and the continuum elastic material, during the simulation it will follow the elastic solution for an un-isotropic material as written in the following equation 6:

$$U_x = K_I(2r)^{1/2} Re\left[\frac{1}{S_1 - S_2}\{S_1 p_2 (cos\theta + S_2 sin\theta)^{1/2} - S_2 p_1 (cos\theta + S_1 sin\theta)^{1/2}\}\right]$$

$$U_y = K_I(2r)^{1/2} Re\left[\frac{1}{S_1 - S_2}\{S_1 q_2 (cos\theta + S_2 sin\theta)^{1/2} - S_2 p_1 (cos\theta + S_1 sin\theta)^{1/2}\}\right]$$

Where r and θ are the polar coordinate of the atom for which displacement is calculated and the origin is located at the crack tip. K_{IG} is the stress intensity factor given by

$$K_{IG} = \sqrt{2\gamma}\left\{\left(\frac{S_{11}S_{22}}{2}\right)^{1/2}\left[\left(\frac{S_{22}}{S_{11}}\right)^{1/2} + \left(\frac{2S_{12}+S_{66}}{2S_{11}}\right)^{1/2}\right]\right\}^{-1/2} \quad (7)$$

Where σ is the applied load and a is the length of the crack. The variable S1 and S2 are the roots of the characteristic equation:

$$S_{11}S_i^4 - S_{16}S_i^3 + (2S_{12} + S_{66}).S_i^2 - 2S_{26}.S_i + S_{22} = 0 \quad (8)$$

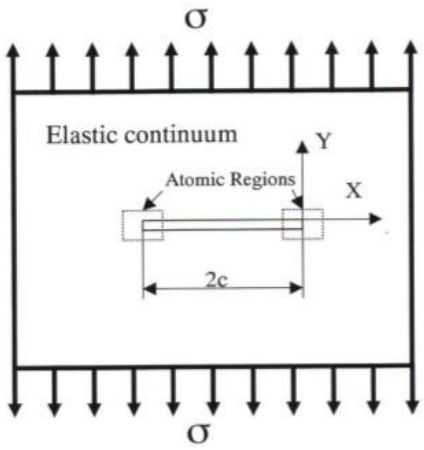

Fig. 3. Atomic region in continuum material

Where S_{ij} the compliance coefficients corrected for plain strain conditions. Equation (6) has the four complex roots S_1, S_2, $S_3 = S_1^*$, $S_4 = S_2^*$. The values of p_1, p_2, q_1, and q_2 from Equation (6) are obtained from the following equations:

$$p_1 = S_{11}S_1^2 + S_{12} - S_{16}S_1$$

$$p_2 = S_{11}S_2^2 + S_{12} - S_{16}S_2$$

$$q_1 = \frac{S_{12}S_1^2 + S_{22} - S_{26}S_1}{S_1} \quad (9)$$

$$q_2 = \frac{S_{12}S_2^2 + S_{22} - S_{26}S_2}{S_2}$$

The simulation model used here is derived from a single atom configuration, which depends on an atomic orientation as described in Fig. 2. The design of the atomic configuration based on the fcc slip system described above is shown in Fig. 2. The x-axis is set up as [110] direction because it is expected that dislocations will move along this axis and y and z-axis are set up as [111] and [112] directions respectively.

Because of computer processing limitation, it is only 17,407 atoms were used in this simulation with atomic size (30 x 30 x 4.5).a_0, where a_0 is the lattice constant of aluminum (a_0 = 4.04 A°). Two kinds of boundary conditions are used here, namely fixed boundary condition that is applied to x and y axis and the periodic boundary condition is applied to z axis to accommodate the plane strain condition to the model.

Loading Condition

The loading condition in this simulation is approached from one-point bend experiment. The behaviors of a material under rapid loading can differ significantly from those under a static or quasi-static condition. In rigid dynamics, it is assumed that, when a force is applied to any point on a body, the resultant stresses set every other point in motion instantaneously, and the force can be considered as producing linear acceleration of the whole body, together with an angular acceleration about its center of gravity. In the theory of elasticity, on the other hand, the body is considered in equilibrium under the action of applied forces, and it is assumed that the elastic deformation reaches its static value. These treatments are sufficiently accurate for the problem in which the time for the application the force and for setting up of effective equilibrium are short compared with the time in which the observations are made.

However, when forces are applied for only very short periods of time, or changed rapidly, the effects must be considered in terms of propagation of stress wave. In this case, when the deformation is imparted from the outside at very high velocity, it is seen that one portion of the body is stressed while the other portion does not experience this stress yet. In other words, stresses (associated with deformation, strain) have to travel through the body at specified velocities.

Dynamic fracture occurs under a rapidly load, which is produced by impact or by explosive detonation. But in contrast to quasi-static loading, dynamic condition involves loading rates that are greater than those encountered in conventional tensile test or fracture toughness test. Thus, the material at the crack tip is strained very fast.

In addition, the features of dynamic fracture distinguishing from quasistatic behavior are the presence of stress waves, vibrations, and inertia effects. All these factors have made the measurement and analysis of fracture behavior under a high loading rate is more complex, and moreover results obtained from dynamic fracture test could be difficult to interpret.

Since dynamic fracture mechanics can be in some extend considered as a logical extension of static fracture mechanics, dynamic fracture behavior tends to be treated semi-empirically on basis of static fracture behavior. For instances, crack tip stress intensity is also used as a dynamic fracture parameter to explain a crack instability criterion under rapid loading.

The conditions necessary for the crack initiation and propagation under stress wave

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impingement are not well understood. Neither standard testing procedures nor a rigorous crack instability criterion are well established. Despite of this fact, some researchers have proposed some criterions for crack instability in structural materials under short pulse loading.

One of the proposed criterion is based on classical static fracture mechanics, that crack become unstable when the maximum dynamic stress intensity exceeds its critical value, KDyn,max . The dynamic fracture toughness was determined from the critical crack size, the amplitude of the tensile pulse, and the static fracture mechanics formula, $K = \sigma \ f(a/w)$. Thus, in this criterion, the instability parameters are only crack length and stress level.

Later it was discovered by Kalthoff and Shockley [4] that the criterion described above could not explain experimental data of crack instability in an epoxy plate by short tensile stress pulses. Moreover, the experimental results by Homma et al (Fig. 4) show that the maximum value of dynamic stress intensity $K_{Dyn,Max}$, produced by critical stress pulse for crack initiation cannot be regarded as dynamic fracture toughness, KID. Fig. 4 shows that $K_{Dyn,Max}$ varies with crack length for a material and hence it cannot be taken as a material property. From the experimental result shown above, it is approached to a step wise step function as described in Fig. 5. The load increase until certain amplitude and the load is kept constant.

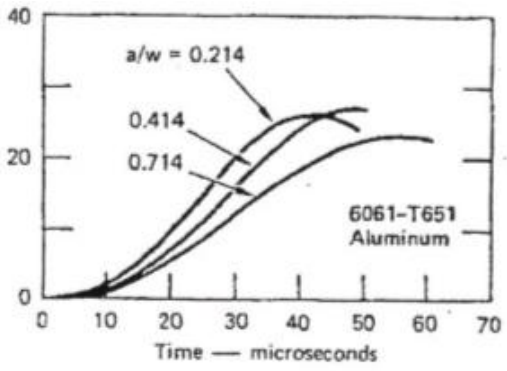

Fig. 4. Experimental Loading

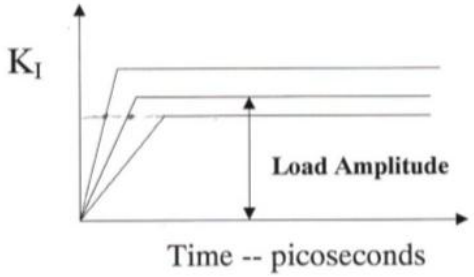

Fig. 5. Step Wise Loading

Time Step Selection

Time-step size is correlated to stability of computation and the system. The stability of system here means how the system conserves the energy during the simulation. Numerically, the shorter time step is used in a simulation, the more precise the result is, but the other problem is the time scale of the simulation because if too short time step is huge computation time is necessary to obtain the result in a certain time scale. The optimum time step is obtained through trial and error from the simulation. In practice the total system energy will fluctuate, particularly at the first 10 or more steps of a simulation namely before the high order time derivatives have had a chance to be initialized during the integration process. It is needed to judge what amount of fluctuation is tolerable. The past fluctuation of about one 5000th of the total system energy per twenty times step has been allowed. It is useful to plot the value of the total energy versus time step to gauge the system instability. Therefore, we have to choose an optimum time step in this molecular dynamics simulation.

RESULTS AND DISCUSSION

In this study, a single atom lattice with a slit crack was investigated. The simulation set up are as follows:

Material: Aluminum, Number of atoms: 17,407, Temperature: 300 K, Pressure: 0 Pa, Inter-atomic Potential: EAM Potential proposed by Diana Farkas et al., Integrator: Finite different method, Time step (At): 10-15 second, Boundary condition: fixed and periodic boundary condition, KIG (based on Equation 3.3): 0.2219 MPa

After the boundary condition and the loading conditions were imposed on the initial model, it was found that some phenomenon took place after the equilibrium process. They were dislocation emission from crack tip, void growth, loading rate effect on void growth, and energy change in the simulation system during the process.

 ISSN : 2622-6553 (Online)

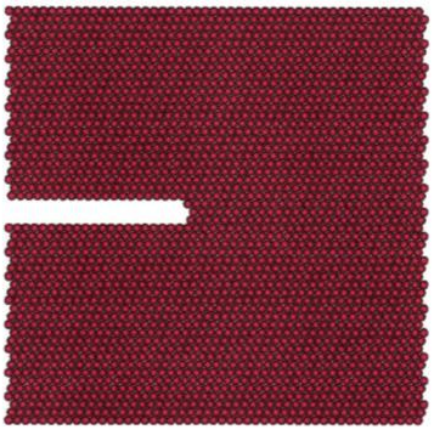

Fig. 6. Initial condition

Using molecular dynamics, the atom movement process in each model was computed under a given loading condition. Since the molecular dynamics technique follows the actual forces on the atoms as they migrate, the microscopic fracture and plastic mechanism can be identified by direct observation, without any priori assumptions. As the simulation progresses, and the stress intensity factor is increased up to three times the Griffith value, the crack begins to advance. The load is stated in term of Griffith value to easily imagine how high the load is applied in this simulation.

Dislocation

Edge dislocations were emitted from the crack tip during the simulation. Based on the observation, the first edge dislocation was emitted when the load was 1.2 KIG, and then this dislocation moved away along the slip plane with the Burgers vector a0/2<110>, when the load reached 3 KIG two edge dislocations were emitted from the crack tip, one is in the upper part and the other is in the lower part. The dislocation continued to move as the load increased and when the dislocation reached the boundary condition, the dislocation was blocked by the boundary layer, then it could not move anymore. The process of dislocation emission is shown in Fig 7.

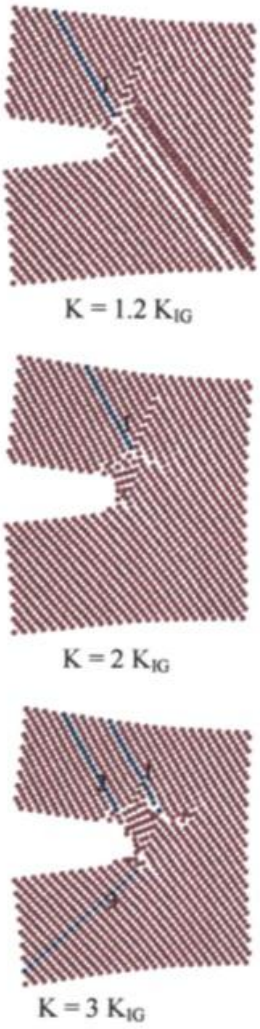

Fig. 7. Emission of edge dislocation

Void Growth

When the load reaches a certain level as shown in Fig. 7, the load was kept constant for a long period. During this period, a void was initiated ahead of the crack tip and grew. The first dislocation described in section 4.1 becomes a core of a micro void ahead of the crack tip (around 15° inclined from the x axis) at time 6 ps. While the second dislocation moved away from the crack tip to pile up the micro void, the third dislocation (in the lower part) coalesce with the main crack. At time 9.5 ps, the fourth dislocation was emitted and the void continued to grow. Finally, the void growth is saturated after 20 ps. The evolution of this void growth is plotted in the Fig. 8 where the starting point is the time when an edge dislocation became a micro void core.

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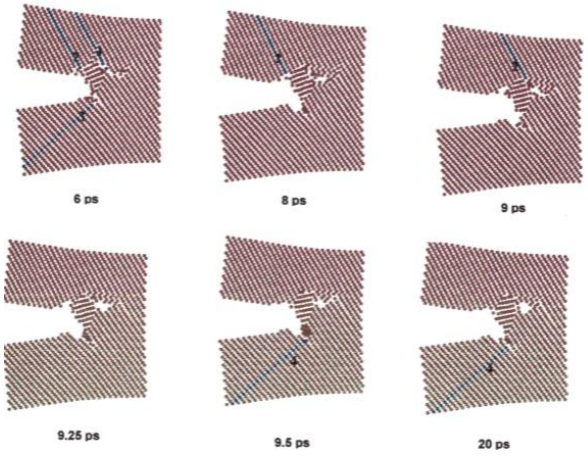

Fig. 8. Evolution of void growth

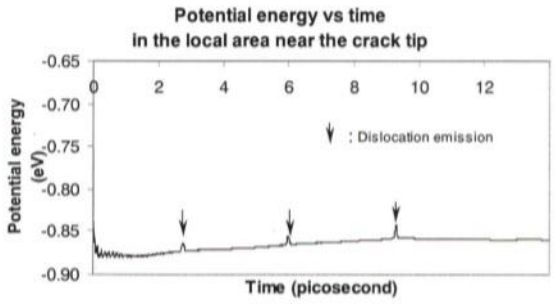

Fig. 9. Potential Energy Change

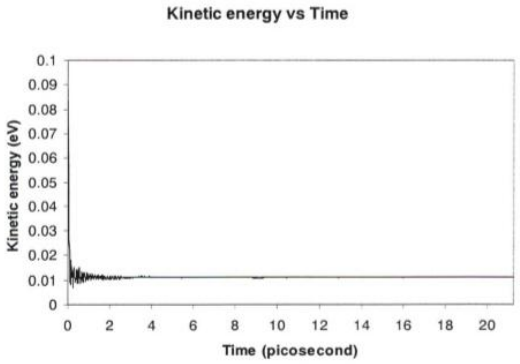

Fig. 10. Potential Energy Change

Loading Rate

Three kinds of loading rates are applied to the model. The loading rates are 0.08876 MPa.m0.5/ps, 0.11095 MPa.m0.5/ps, and 0.14793 MPa.m0.5/ps. It can be investigated that the higher the loading rate, the smaller the void grows. It is in a good agreement with plastic theory that when a load is applied to a material at a very high loading rate, there is no enough time for material to undergo plastic deformation this is why the void size became smaller under the higher loading rate.

Energy change

During the simulation, energy change of system is also investigated in terms of potential energy and kinetic energy as shown in Fig. 9 and 10. The kinetic energy is very small compared with potential energy because the mobility of atoms is very small in solid. During the simulation process, the value of kinetic energy is constant but potential energy increases as the external load increases and when the load is kept constant after reaching the plateau load it also remained constant. It can be investigated that there is significant change in energy at the moment when a dislocation is emitted from the crack tip. It means that the system released some amount of energy to emit a dislocation. The energy change is an energy barrier to emit a dislocation.

CONCLUSION

In this study, computer simulation techniques were used to explore the fracture and deformation behavior in pure aluminum. The simulation process was carried out using Molecular Dynamics for single atom aluminum under stepwise loading conditions. Molecular dynamics simulation of crack tip plasticity can provide several insights of dislocation emission and void growth as reported by experiment. The obtained results are summarized as follows:

a. Some dislocations were emitted from crack tip. For instance, four edge dislocations were emitted from the crack tip after the application of stepwise loading for 20 picoseconds. These dislocations moved along the slip system with Burgers vector a0/2[110]. The emission rate depends on the rising speed of the stepwise loading.
b. A void nucleation and growth took place ahead of the crack tip. This micro void was initiated from a dislocation core while the load was kept constant. This micro void never coalesced with the main crack as the

micro void and the main crack tip was separated too far atomically and the micro void growth was saturated.

c. Kinetic energy of the system was very small and almost constant during the process. The potential energy increased as the external load increased and then became constant when the load became constant. Significant fluctuation of energy was observed during the dislocation emission. Some amount of barrier energy must be overwhelmed for the dislocation emission. The qualitative understanding can be provided by this molecular dynamic analysis.

d. The use of Molecular Dynamics was motivated by the ability of the technique to reproduce the physical behavior of the system. Since the MD technique follows the actual forces on atoms as they migrate, the fracture mechanism can be identified by direct observation, without any priori assumptions. However, it is important to emphasize that the accuracy of this technique depends on the potential used.

ACKNOWLEDGMENT

Financial support from the Japanese Ministry of Education, Culture, Sports, Science and Technology (Monbukagakusho) is gratefully acknowledged.

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