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RESEARCH ARTICLE

INVESTIGATION OF CRACK INITIATION AND PROPAGATION AND ITS INSTABILITY CONDITION USING MOLECULAR DYNAMIC SIMULATION

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ABSTRACT

Modeling and simulation techniques are able to throw new insights in the science and mechanics of materials. Predictability of fracture and failure are becoming more certain and these are now compared with experimental observation. In this work, the authors have investigated the fracture behavior of a single crystal alpha-iron having a mode-I edge crack. Using small-scale Molecular Dynamics Simulation (MDS) and proper choice of interatomic potential and boundary conditions, the authors have shown agreement in the prediction of crack initiation and propagation using Griffith fracture criteria, and crack instability condition from material's fracture resistance in the atomic scale. The simulation shows that the crack does not initiate or propagate until the stress intensity value reaches the stress intensity factor equivalent to Griffith fracture stress for the material. The fracture resistance and crack opening displacement (COD) were measured using the simulated results, similar to that of continuum fracture mechanics. The point of initiation of stable and unstable crack was delineated using the principle of plane stress fracture toughness testing. The results indicated inelastic deformation in the early stage of the application of load when crack propagates.

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INTRODUCTION

In the 1950s, molecular dynamic simulation (MDS) was first introduced by physicists to study the bulk properties of matter. Today the idea of simulation at the atomic or molecular level is applied in physics, chemistry, material science, biology, etc., both in academics and in practice. Using Molecular Dynamics (MD) simulation method the behavior of a variety of molecular systems are studied. These include liquids, solutions, electrolytes, polymers, liquid and solid crystals, etc. Atomistic simulation studies of fracture had addressed both practical problems in materials engineering and in understanding fundamental phenomena in materials science.

Molecular dynamic simulation (MDS) of single and polycrystalline materials have provided new insights in understanding the mechanism of deformation as well as predicting relevant material properties.

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MDS is able to predict the brittle and ductile failure in metals and alloys (Abraham *et al.,* 2002; Buehler *et al.,* 2004; Kotrechko *et al.,* 2006; Abraham, 2001), crack initiation (Abraham *et al.,* 2002), stable and unstable crack propagation (Abraham, 2001; Abraham, 2005; Sieradzki *et al.,* 1988; Beltz *et al.,* 1999; Yang *et al.,* 2014), acceleration and deceleration of crack speed (Guo *et al.,* 2003), intergranular fracture (Farkas *et al.,* 2002), dislocation nucleation, emission, propagation and interaction (Schiotz, 2004; Cleri *et al.,* 1997; Beltz *et al.,* 1999; Zhou *et al.,* 1997b), brittle-ductile transition (Cheung *et al.,* 1990), interaction between a crack and grain boundary/nano-particle/stacking fault (Machova *et al.,* 2009), crack blunting (Beltz *et al.,* 1999), crack tip shielding (Tanguy *et al.,* 2008; Cleri *et al.,* 1997), microstructure evolution (Wu *et al.,* 2012, Kastner *et al.,* 2011), and fracture mechanism (Latapie *et al.,* 2004). Development of simulation techniques and recent progress in the advancement of computational power has thrown new insights in the science and mechanics of materials that can now be compared with experimental observations. However, large scale simulation is not always

necessary to understand the mechanism of deformation and predict mechanical properties of materials.

In molecular dynamic simulation (MDS), with proper choice of interatomic potential and boundary conditions small scale simulation can also predict properties which are comparable to that of experiments.

In this work, with small scale molecular dynamic simulation (MDS) and appropriate boundary conditions, we have demonstrated the prediction of crack initiation and propagation, stable and unstable crack growth and its correlation with Griffith fracture criteria and material's fracture resistance. Fracture resistance curve was drawn with the simulated sample and the point of initiation of stable and unstable crack was delineated using the principle of plane stress fracture toughness testing which are typically used in the continuum scale.

MATERIALS AND METHODS

The sample used in the investigation was single crystal alpha-iron with an edge crack. The simulation was two-dimensional. The sample dimension was 100 Å by 31.5 Å, with crack length 11.5 Å. Molecular Dynamic simulation (MDS) was used to simulate the system. Molecular dynamics predicts the motion of atoms, in a sample, governed by their mutual interatomic potentials and requires the numerical integration of Hamilton's classical equations of motion. Figure 1 shows the configuration of the sample, its crystallographic orientation, the orientation of the crack plane and direction and boundary condition for the Molecular Dynamics Simulation (MDS). The vertical boundaries were free surfaces, while five atomic layers along the upper and lower horizontal boundaries were fixed to apply mode-I loading to the system. The boundary conditions were obtained from the continuum theory, equation 1 and 2.

The observation plane was $(10\bar{1})$ and crack direction$\langle 010\rangle$.

$$u_x = (K_I/2\mu).(r/2\pi)^{1/2}.\cos(\theta/2).(2 - 4\nu + 2\sin^2(\theta/2)) \quad \ldots\ldots\ldots\ldots\ldots\ldots(1)$$

$$u_y = (K_I/2\mu).(r/2\pi)^{1/2}.\sin(\theta/2).(4 - 4\nu - 2\cos^2(\theta/2)) \quad \ldots\ldots\ldots\ldots\ldots\ldots(2)$$

Where, K_I is the stress intensity factor (mode I), μ is the shear modulus, ν is the Poison's ratio.

Initially we allocate atoms at the BCC lattice positions and give the velocities of the atoms randomly. The velocities were translated so that the total linear momentum was zero along all the directions. The velocities of the atoms acquired Maxwell distribution after the system attains equilibrium.

Invention of unit systems makes physical laws looks simple and numerical calculation easy. As long as the physics is intact, unit system can be modified to suit the output of the investigation. In our MDS work, we have used a different set of unit system due to very small length and time scale:

Length: Å

Time: τ (=10^{-14} sec)

Mass: amu

Energy: eV (instead of amu. Å$^2/\tau^2$)

Velocity: Å/τ

Acceleration: Å/τ^2

Force: eV/Å (instead of amu. Å/τ^2)

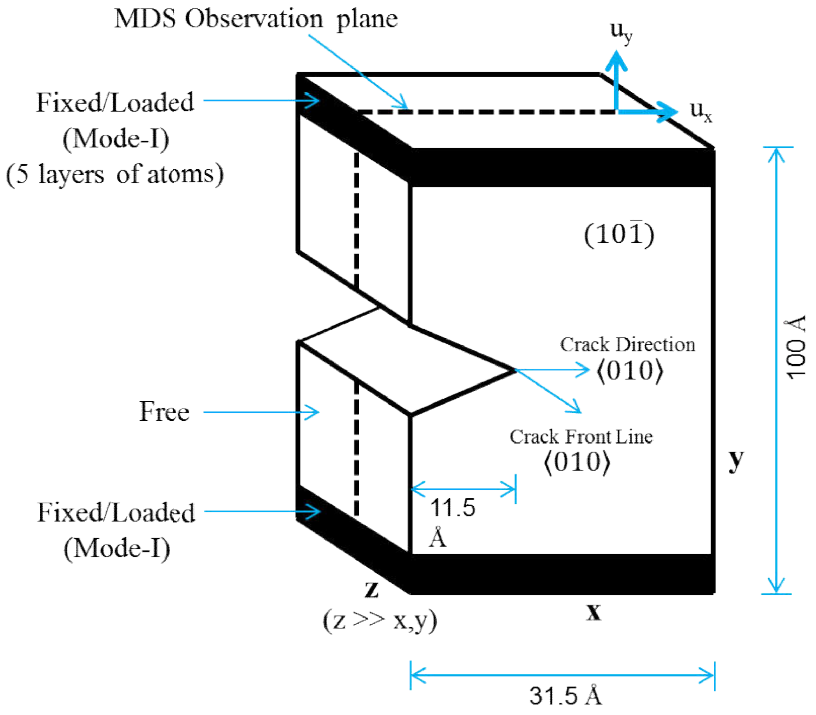

Figure 1. Sample configuration, crystallographic orientation and coordinate system of a crack and plane of simulation

This unit is different than the conventional SI system. Reduced units can also be used (Frenkel *et al.,* 2001).

The cracked sample was equilibrated before applying load, with time step size of 5 x 10^{-16} sec. The fracture process in the sample was conducted by incrementally loading (mode I) the sample starting from a stress intensity value lower than the Griffith criterion (equation 3) for alpha-iron single crystal. We let the system evolve for a certain number of time steps between each loading to equilibrate, giving an overall simulation time of 340 ps.

$K_{IC} = \sqrt{2\mu G_{IC}/(1-\nu)}$ With $G_{IC}$is twice the surface energy …(3)

In the case of alpha-iron with $G_{IC} = 2*\gamma_S$ = 2*0.089 = 0.178 eV/Å^2, ν = 0.293 andμ = C44 = 0.699 eV/Å^3. We get K_{IC} = 0.6 eV/Å$^{5/2}$ = 0.96 MPa.m$^{1/2}$ (Latapie *et al.,* 2004).Velocity verlet algorithm (Allen *et al.,* 1991) was used for integrating the equations of motion.

At the start of the simulation, an edge crack was introduced to the system, and then it was left to equilibrate. Since no external force was applied to the system, total linear momentum and total energy were conserved. This corresponds to micro canonical (NVE) ensemble.

After the system reaches equilibrium, external load (mode I loading) was applied. The system was again left to equilibrate for a certain number of time steps. With the application of external load, the total energy of the system increases. Since this is related to system temperature, the latter also increases. The increase in temperature depends on the amount of load applied. In applying mechanical loading in fracture simulation, the system temperature can rise to unrealistically high. Hence it is a common practice to control temperature. This corresponds to the canonical (NVT) ensemble.

Many-body semi-empirical potential (such as an embedded atom method, EAM) were used, in the literature, to model the behavior of many metallic materials, particularly those with FCC structure (Farkas, 2002). In this work, pair potential, such as Johnson Potential, was employed to model the fracture behavior of metallic materials, such as alpha-iron (Nishimura, 2004). Johnson Potential was chosen for description of interatomic forces on alpha-iron. Johnson Potential being a pair potential, is a function of a distance between two atoms. It is simple, computationally more efficient and gives accurate simulation results (Nishimura, 2004). The Johnson Potential used in our simulation is the analytic form of three smoothly joined cubic equations and goes to zero with slope at a cutoff distance, existing in the midpoint between the second and third nearest neighbor distances. The Johnson Potential can be written as an equation (4):

$$\Phi(r_{ij}) = -c_1(r_{ij} - c_2)^3 + c_3 r_{ij} - c_4 \quad \text{…….. (4)}$$

Where r_{ij} is the distance between atoms *i* and *j*,c_1 through c_4 are parameters. The values of the parameters are summarized in Table 1, for alpha-iron. Figure 2 shows the interatomic potential plot with distance between atoms in alpha-iron.

To start the simulation, initial positions and velocities were assigned to all particles in the system.

The particle (atom) positions were chosen as per the crystal structure of alpha-iron, that is, BCC structure. Since it's a two-dimensional simulation and the plane of simulation is $(10\bar{1})$, the atoms were placed accordingly. Maxwell-Boltzmann distribution was not used for the velocities initialization. Instead, the velocities of the atoms were given randomly between the limits -0.05 and -0.05 Å/τ. On equilibration the velocities acquire Maxwell-Boltzmann distribution. The fraction of atoms having velocities between v and v+dv is given by the Maxwell distribution function (Haile, 1997), equation (5):

$$f(v_x)\,dv_x = \frac{N(v)\,dv_x}{N} = \sqrt{\frac{m}{2\pi kT}}\,\exp(-\frac{mv_x^2}{2kT})dv_x \quad \text{…….(5)}$$

Where *m* is the mass of one atom; *N* is the total number of atoms, *k* is the Boltzmann's constant; *T* is the temperature in absolute scale, v_x is velocity in the x-direction. Analogous expressions are obtained for the y- and z-components.

During the production stage the data related to the positions, velocities, forces, temperature, energy, crack tip positions and snapshots of the simulation were saved. From these data the properties of the simulation sample were determined.

At the atomistic scale, crack tip position or crack extension can be detected either by distance-based method or by energy-based method. In the distance-based method (Lu *et al.,* 2005), if the distance between atoms in front of the crack tip exceeds the critical distance (generally the cutoff distance in the force field computation) crack is considered to be extended. In the energy-based method (Zhou *et al.,* 1997a), potential energy of individual atoms near crack tip is being calculated. In our work, we have used the energy-based method to identify the crack tip, crack initiation and propagation and crack surfaces by plotting the atoms having color based on its individual potential energy value. Crack tip and crack surfaces will have high potential energy (that is, less negative value) and will be visible by color contrast. Atoms with potential energy greater than a certain value are being considered a part of the crack.

Table 1. Parameters for the Johnson interatomic potential for alpha-iron

Range (Å) of 'r_{ij}'	Potential (eV)
1.9 – 2.4	c1 = 2.195976, c2 = 3.097910, c3 = 2.704060, c4 = 7.436448
2.4 – 3.0	c1 = 0.639230, c2 = 3.115829, c3 = 0.477871, c4 = 1.581570
3.0 – 3.44	c1 = 1.115035, c2 = 3.066403, c3 = 0.466892, c4 = 1.547967
> 3.44	c1 = 0.0, c2 = 0.0, c3 = 0.0, c4 = 0.0

RESULTS AND DISCUSSION

The selection of two dimensional simulations were carried out to reduce the simulation time. Two dimensional simulations are satisfactory when one of the lengths of the sample is

comparatively larger than the other two directions. The plane of simulation was $(10\bar{1})$ and a crack front direction was$\langle 010\rangle$, as shown in Figure 1. The slice shown in the figure was the plane of simulation.

Figure 3 shows the initial configuration of the simulated sample just after an edge crack was introduced. The loaded (mode I) region of the sample is in blue and green color.

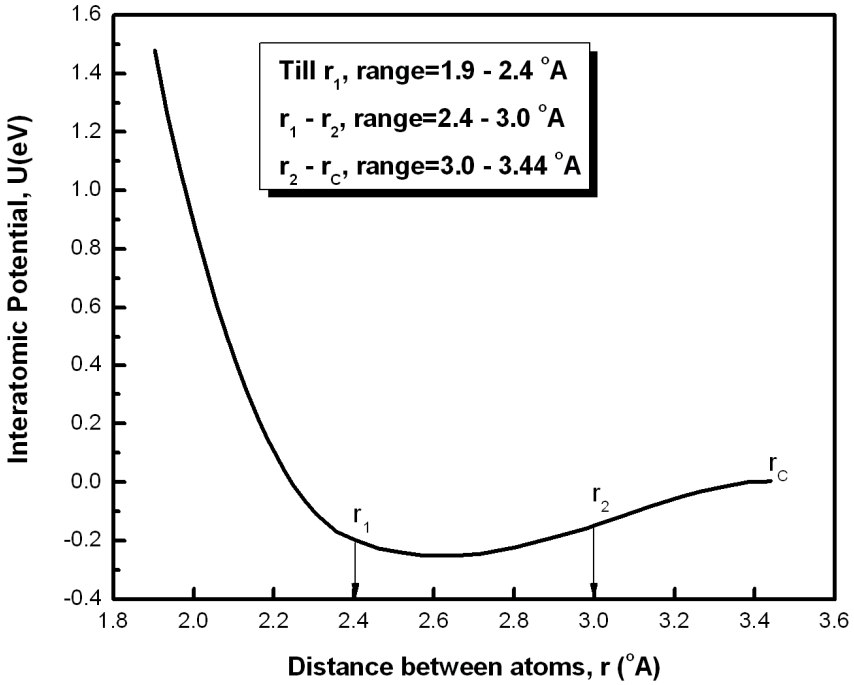

Figure 2. Johnson Interatomic Potential versus distance between atoms, for alpha-iron

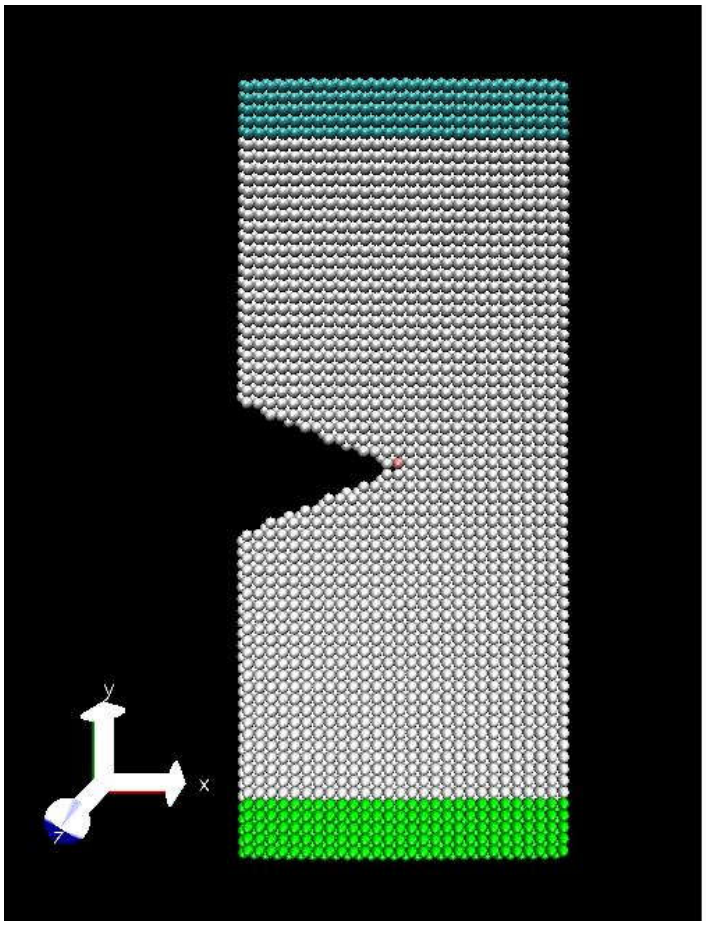

Figure 3. Initial configuration of the simulated sample just after an edge crack is introduced. The loaded (mode I) region of the sample is in blue and green color. Red color atom in front of the crack shows the crack tip. Energy-based method is used to identify the crack tip

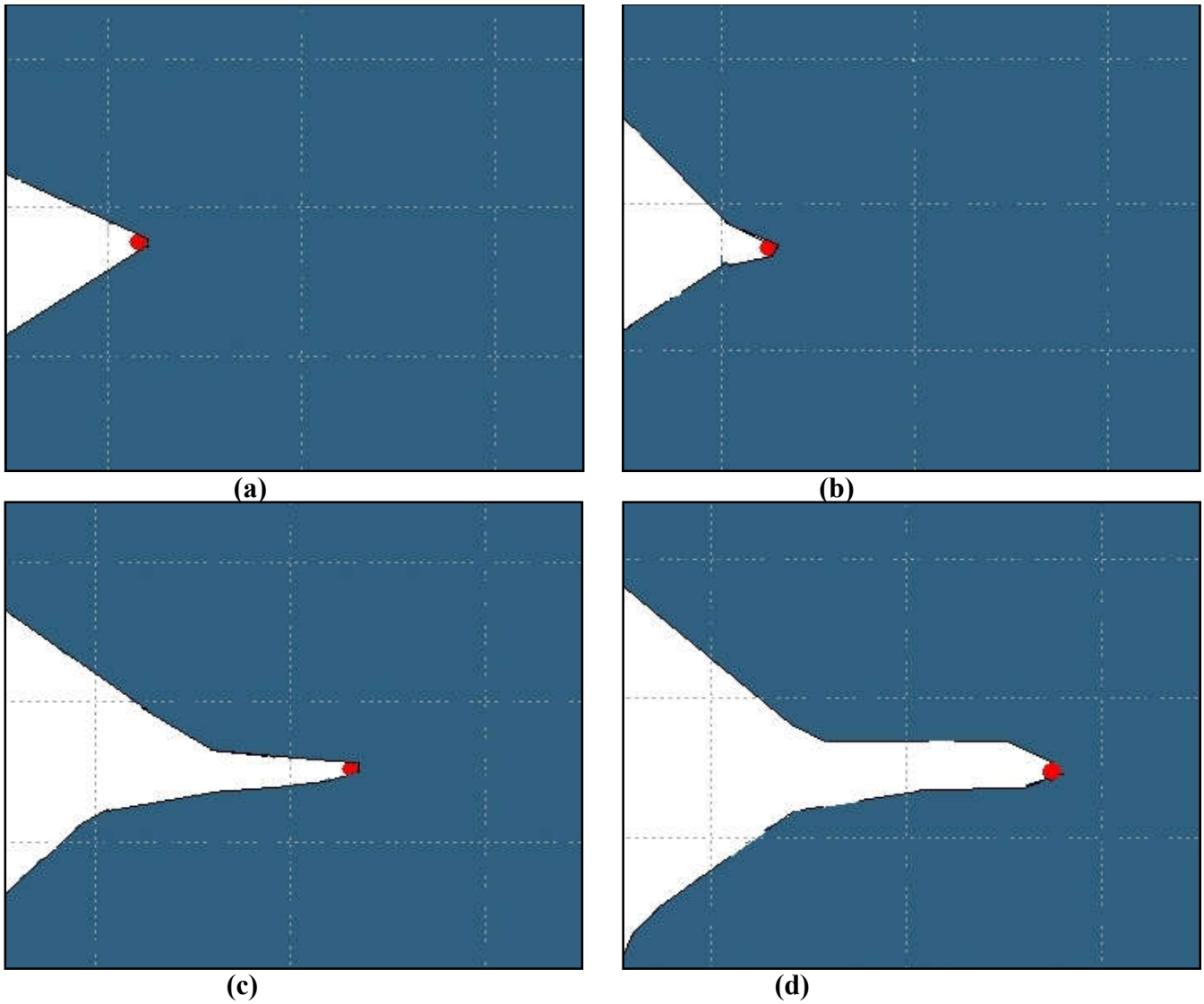

Figure 4. (a) – (d): Various configuration of the sample at various stages of the simulation. Only the region near the crack tip is shown here. Red circle shows the crack tip position. The figures show there is no crack deviation and it propagates in mode-I configuration

The validation of the algorithm can be checked by few of the results obtained during the start of the simulation. Energy conservation: Energy conservation is one of the most important considerations. The energy conservation was satisfied. It also indicates that the time step chosen for the simulation was appropriate. If the time step would be of higher value, energy conservation (in the absence of external force) would be violated. The choice of the interatomic potential was appropriate in the sense that earlier work (Nishimura, 2004) was done successfully using the Johnson potential to calculate the interatomic forces.

Crack Initiation and Propagation

An edge crack sample was simulated using MDS. The sample was loaded in mode-I configuration. The simulation was started at a stress intensity value of 0.40 eV/Å$^{5/2}$. The load was increased after every few time steps.

Until the value reaches about 0.60 eV/Å$^{5/2}$, there is no indication of crack initiation or propagation. The stress intensity factor equivalent to Griffith fracture stress (SIFEGFS) for single crystal alpha-iron is 0.6 eV/Å$^{5/2}$ (0.96 MPa.m$^{1/2}$). As the simulation was carried on with higher stress intensity value the crack initiates and then propagates. The simulation was carried out until the stress intensity value reaches about four times the SIFEGFS value. The snapshot of the simulation was captured.

Figure 4 shows various stages of the simulation. Only the region near the crack tip is shown in the figures. The crack shows there is no crack deviation and it propagates in mode-I configuration.

Crack Opening Displacement (COD) Measurement

The crack opening displacement (COD) measurement was done to study how the crack opens with increasing load or the magnitude of the stress intensity factor. The measurements weremade at two places in the simulated sample – near topmost left and near the mouth (Figure 5).

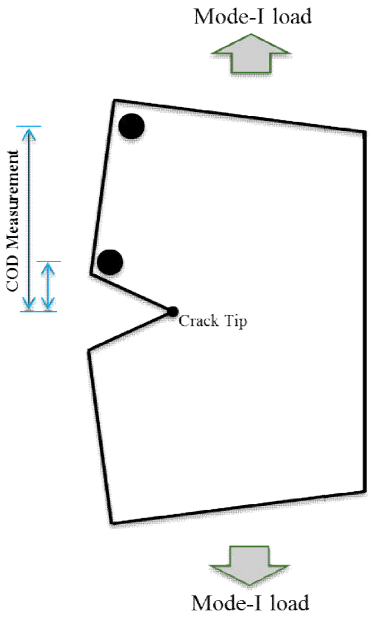

Figure 5. Sample configuration to calculate crack opening displacement (COD) measurement

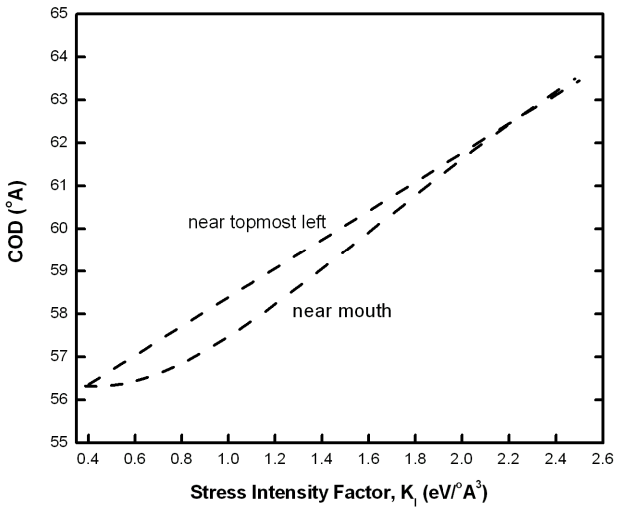

Figure 6. Stress intensity factor versus crack opening displacement (COD). The gap between the two curves shows there is some sort of non-elastic deformation

Figure 6 shows the result. The average value was considered in the graph, as there were fewer fluctuations in the results. The fluctuations are primarily due to atomic vibrations. The gap between the two curves shows there is some sort of non-elastic deformation. Plastic deformation cannot be totally ruled out, as the effect of dislocations are not been considered in the investigation.

Crack Growth Phenomena

Parameters derived from the quantitative characterization of the simulation data can be compared with those obtained from experiment. One such important quantity is fracture resistance. Figure 7(a) shows the crack resistance curve obtained from simulation, such as are used in continuum fracture mechanics. This curve gives information on how the crack advances as increasingly higher loading is applied. The solid line was drawn considering the average value of the simulated data. Figure 7(b) shows the crack instability condition. Crack instability occurs when the rate of change in the elastic energy-release rate $\partial G/\partial a$ equals the rate of change in the material's resistance to such crack growth $\partial R/\partial a$. Crack instability occurs as a stress intensity factor of about 2.2 eV/Å$^{5/2}$. The *G* curve is drawn from the relation, equation (6):

$$G = \frac{K_I^{\,2}}{E}(1-\nu^2) \qquad \ldots\ldots\ldots\ldots\ldots\ldots 6)$$

Where, *G* is the strain energy release rate, *E* is the Young's modulus, ν is the Poison's ration, K_I isthe stress intensity factor in mode-I load. Till the stress intensity factor value reaches 0.6 eV/Å$^{5/2}$, there is no sign of crack movement. With increasing displacement in the boundaries of the simulated sample the crack initiates and propagates. Stable crack growth occurs till the value of stress intensity factor reaches 2.2 eV/Å$^{5/2}$. Thereafter unstable crack growth occurs.

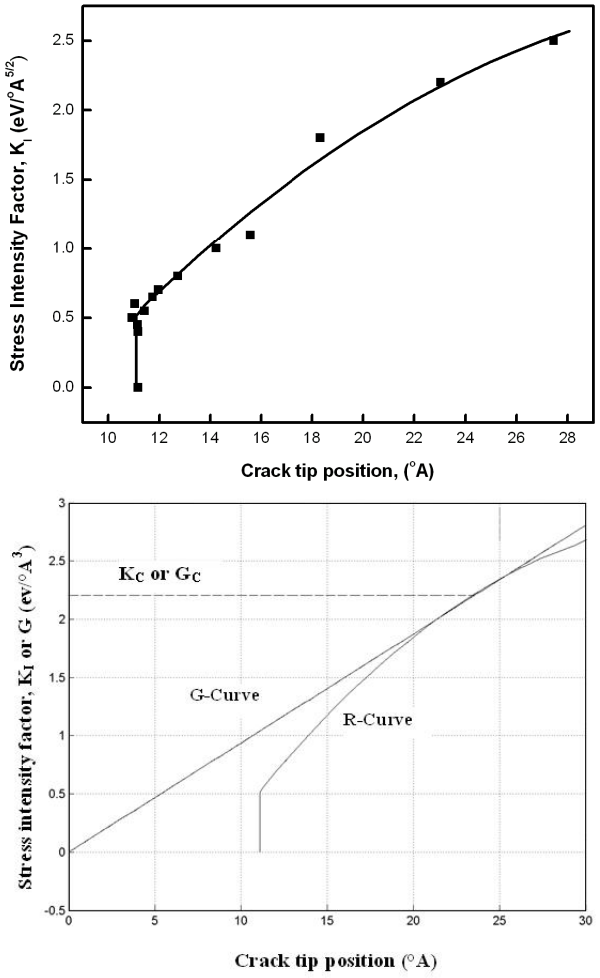

Figure 7. (a) Fracture resistance curve, obtained from simulation. This curve gives information on how the crack advances as increasingly higher loading is applied. (b) Crack instability condition. Till the stress intensity factor value reaches 0.6 eV/Å$^{5/2}$, there is no sign of crack movement. With increasing displacement in the boundaries of the simulated sample the crack initiates and propagates. Stable crack growth occurs till the value of stress intensity factor reaches 2.2 eV/Å$^{5/2}$. Thereafter unstable crack growth occurs

For validation of the results, few of the issues were considered which showed the validation of the results. (1) The quality of the theory or model: The type of equations of motion used in the simulation were very well used in various places successfully (Buehler *et al.,* 2004; Lu *et al.,* 2005; Park *et al.,* 2005; Dienes *et al.,* 1987). The boundary conditionswere chosen from the solution of the displacement field of a semi-infinite crack in an isotropic medium (Sih *et al.,* 1968). The Johnson potential was used, which was used earlier to give many successful results (Nishimura *et al.,* 2004). (2) The simulation was carried out for a long time to relax the sample at every load or stress intensity value. This was done to equilibrate the sample before the higher load was applied. (3) The computer program was written in C language. And the validation of the algorithm has already been discussed in this section. (4) Results were compared with theory and it shows satisfactory correlation.

Conclusions

In this work, molecular dynamic simulation technique was used to investigate the fracture behavior of single crystal alpha-iron having a mode-I edge crack. The temperature of simulation was kept at about 2K. Two dimensional simulation was carried out and this is sufficient if one dimension is sufficiently large compared to the other two dimensions. The fracture behavior is studied at the atomic scale by incrementally loading the simulated sample in mode I configuration to higher stress intensities.

1. Using small scale molecular dynamic simulation and proper choice of interatomic potential and boundary conditons, we have demonstrated the prediction of crack initiation and propagation using Griffith fracture criteria. The sample was stressed by increasing displacement mode on the boundaries and this applied displacement corresponds to a stress intensity factor. The simulation was started at a stress intensity factor value below that of stress intensity factor equivalent to Griffith fracture stress (SIFEGFS) for the simulated sample. There is no sign of crack initiation or propagation till the value of stress intensity factor reaches the SIFEGFS, thereafter crack initiates and propagates.
2. Fracture resistance curve was drawn using the simulated results. The stable crack growth phenomenon and the crack instability condition are depicted on the fracture resistance curve.
3. The edge crack in the sample propagates in mode-I configuration. This is determined from the simulated results by direct observation of the crack tip position using the energy-based method.
4. The crack opening displacement (COD) measurement was done to study how the crack opens with increasing load or the magnitude of the stress intensity factor. The measurements were done near the top left corner of the sample and near the mouth of the crack. The estimated values of COD show that there is some inelastic deformation. Plastic deformation cannot be totally ruled out, as the effect of dislocations are not considered in the investigation.

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