MOLECULAR DYNAMICS SIMULATION STUDIES
IN FRACTURE MECHANICS

by

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ABSTRACT

Molecular Dynamics (MD) simulation has been applied to the
study of fracture mechanics in real materials. The simulation
system was composed of an atomic crack tip embedded in an infor-
finite continuum medium under an external tensile stress (mode-I
fracture). The structure and properties of the crack tip have
been analyzed for semibrittle materials (\(\alpha\)-iron) and ductile
materials (Cu) which were characterized by appropriate potential
functions.

A computer program has been developed which can be applied
to any system of classical crystalline solids under a wide range
of boundary conditions: periodic, free, fixed and flexible
boundaries. In particular, a new boundary method has been
developed for the treatment of the crack tip. With the use of
this method the problems of previous boundary conditions have
been resolved, namely, large deviations from Griffith theory in
the case of brittle materials and constraints against the emis-
sion of dislocations in the case of ductile behavior. The method
has allowed a realistic simulation of real materials: confirma-
tion of Griffith theory by MD simulation, the observation of the
correct cleavage plane during crack propagation in \(\alpha\)-iron, and
the nucleation of dislocations in copper along the directions of
minimum shear stress.

Atomic effects around the crack tip region, up to twenty
interatomic distances away from the crack tip, were studied. The
technique provided a unique way of observing nucleation of
dislocations from the crack tip, an effect that is ultimately re-
sponsible for the ductile behavior of a material. Also it has
allowed the detailed analysis of the atomic structure and
non-linear stress field surrounding the crack tip.

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1. Introduction
1. Introduction

In modeling a defect in a solid there are two aspects of the problem to consider. First, the method can be based on a continuum theory or utilize a discrete model such as is done with a molecular dynamics or lattice statics approach. Second, if a discrete method is employed, some potential must be used to describe the interatomic interactions. The discrete approach introduces additional computational complexities in contrast to a continuum model. However, it offers the possibility of an understanding of material properties on a more fundamental level.

There are specific cases where in order to study the structure and behavior of a defect one cannot apply a continuum linear solution. In these cases the behavior of the defect is determined by a region that is only a few interatomic distances in extent and where high concentration of stress can occur. There, atomic processes and non-linear forces must not be ignored. This is the case of modeling crack tip behavior, dislocation cores and determination of Peierls barrier. In such cases molecular dynamics (MD) simulation can be a very useful technique for studying the static configuration of the defect as well as its dynamic properties.

When a MD simulation is applied the fundamental terms in which the mechanical properties of materials are understood are basically two: atomic structure and interatomic forces. MD is a numerical simulation technique where given the structure and interatomic forces of a certain material one can simulate its
equilibrium and dynamical properties (1-4). The method consists of calculating the classical trajectories of several hundred particles interacting through a known potential function, by numerical integration of the Newton's equations of motion.

The equations of motion that govern the time evolution of the atomic coordinates are a set of coupled, non-linear ordinary differential equations. The time evolution of the phase coordinates is called the trajectory, and the MD technique consists of numerically integrating the equations of motion to solve for the trajectory at discrete time points.

In this work our goal is to apply MD simulation to the study of fracture mechanics in real materials. The first studies of this type were carried out in a discrete lattice with very simple models in one or two dimensions and highly idealized interatomic force laws (5). These simplified models, however, contributed greatly to the understanding of fracture properties in terms of microscopic physical parameters, such as lattice structure and interatomic force law.

Subsequent studies using computer simulation were concerned with systems of larger number of particles and more realistic interatomic force laws, such as the calculations for α-iron by Gehlen and Kanninen (6) and for silicon by Sinclair and Lawn (7).

The main difficulty with these computer simulations has been the specifications of the external boundary conditions. Periodic boundary condition is a simple and accurate way of simulating the properties of an infinite homogeneous system. However, when the system contains a defect and is acting under the
effect of an external force, a different procedure must be used. One alternative is to apply an uniform external stress directly over the free surfaces of the system. The other consists of matching the solution at the boundary to a continuum elastic solution. Of the two alternatives, only the second simulates realistically the behavior of a macroscopic crack surrounded by a sufficient amount of material under the action of an exterior stress applied far from the crack and it alone will be used in our simulations.

Our study of the properties of fracture mechanics by MD simulation consists of simulating the crack tip behavior in a three-dimensional atomic system, introduced in an infinite continuum medium under the action of an external stress (mode-I fracture). Two types of materials have been studied, α-iron and copper, which were characterized by appropriate potential functions.

A new boundary method has been developed to resolve the problems of previous simulations. The continuum theory has been applied to the boundary of the system but instead of fixing the position of the particles at the boundary according to the displacements given by this solution, the continuum linear stresses were applied and kept fixed during the simulation. The boundary particles were free to move. The method has allowed a realistic simulation of real materials: confirmation of Griffith theory by MD simulation, the observation of the correct cleavage plane during crack propagation in α-iron, and the nucleation of dislocation from the crack tip in ductile materials, Cu.
The new method applied to the boundary jointly with the standard methods of MD are summarized in chapter two, where a description of the problems associated with the different types of boundaries is included.

Chapter three summarizes several important concepts in continuum theory of fracture pertinent to this work, namely, the Griffith theory of brittle materials and the criteria which have been recently developed to predict brittle or ductile behavior in crystalline materials. The last section of this chapter consists of a critical study of previous research done in this area by MD simulation.

In chapter four, the new boundary is applied to the study of brittle materials at low temperatures, α-iron. There, it is studied the influence of other types of boundaries on crack propagation, the influence of the continuum solution (anisotropic or isotropic), and the crack tip structure and stress field.

Chapter five is devoted to the study of ductile materials, copper. Blunting of the crack tip is studied during its first stages by observing the lattice deformation and atomic motions occurring during the nucleation of dislocations.

In the last chapter conclusions are given along with some suggestions for future work.
Chapter Two

Computer Molecular Dynamics Techniques

2.1 Equations of Motion
2.2 Potential Functions
2.3 Numerical Integration of Equations of Motion.
   Accuracy of Numerical Integration
2.4 Stress Boundary Method
2.5 Determination of Equilibrium Position and
   Simulation of Thermal Effects
2.6 Determination of the Atomic Stress
2.1 Equations of Motion

In MD calculations (chapter 1 ref.(1-4)), a three-dimensional system of N particles is treated by setting up 3N classical equations of motion which are coupled through an assumed two-body interatomic potential. This set of N differential equations is then integrated numerically on a computer to give the spatial trajectories and velocities of all the particles as a function of time.

In the present simulation, a classical system of N point particles of mass m is assumed to obey Newtonian mechanics, in which case the equations of motion are given by

\[
\frac{d^2 \vec{r}_i}{dt^2} = \frac{1}{m} \vec{F}_i(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n) + \frac{\vec{F}^{ext}_i}{m}, i = 1, 2, \ldots, n \quad (2-1)
\]

where \( \vec{r}_i \) is the position coordinate of the ith particle, \( \vec{F}_i \) and \( \vec{F}^{ext}_i \) are the vector forces on the ith particle due to other particles and exterior forces respectively. For central, conservative, pairwise additive potentials, the pair force \( \vec{F}_{ij} \) between two particles i and j of the system is

\[
\vec{F}_{ij}(r_{ij}) = -\frac{\partial \phi(r_{ij})}{\partial r_{ij}} \quad (2-2)
\]

where \( \phi(r_{ij}) \) is the pairwise potential between particles i and j and \( r_{ij} \) the separation vector between these two particles.
2.2 Potential Functions

Empirical and semi-empirical potential functions can be constructed in which adjustable parameters are determined by matching certain calculated properties of the system to experimental results. Two fundamental assumptions are almost universally employed: central forces and pairwise additivity. Pairwise additivity means that the potential energy between two atoms is unaffected by the presence of other nearby atoms. The central force assumption means that the force between atoms is directed along the line joining the centers of mass and so is a function only of the atomic separation. The next discussion goes into commonly known empirical and theoretical potential functions which have been used in our computer simulation.

The interatomic force law used in the simulation of α-iron is derived from the interatomic potential constructed by Johnson (1,2), Fig. 2.1. This potential is based upon two central interactions which extend through the separations of first and second nearest neighbors. It is cut off smoothly to zero at a point midway between the second and third nearest neighbors. An empirical form is used with the constants selected to match the elastic constants $c_{11}$, $c_{12}$, $c_{44}$, and the Erginsoy et al. (3) radiation damage potential at close approach.

A form extensively used for metals is the Morse potential

$$\phi(r) = D \left[ \exp (-2\alpha(r-r_0)) - 2 \exp (-\alpha(r-r_0)) \right]$$  \hspace{1cm} (2-3)
2.1 Interatomic potential and force law for α-iron. Johnson potential.
where $\alpha$ and $D$ are constants with dimensions of reciprocal distance and energy, respectively, and $r_0$ is the equilibrium distance corresponding to the minimum of the potential (4).

The most important characteristic of this potential pertaining to our MD simulation of fracture is that the three parameters $D$, $\alpha$, and $r_0$ of the potential for several f.c.c. and b.c.c. metals have been determined using experimental values for the energy of vaporization or vacancy formation energy, the lattice constant, and the compresibility (5,6).

The elastic constants and equation of state which were computed using the Morse parameters, agreed with experiments for both face-centered and body-centered cubic metals (5). All stability conditions are also satisfied. This shows that the Morse potential can be applied to problems involving any type of mechanical deformation of cubic metals.

In our simulations of ductile materials, copper, we have applied a Morse interatomic potential with the parameters derived from the vacancy formation energy, lattice constant and bulk modulus(6), Fig. 2.2. The interatomic potential approaches very closely to zero after second nearest neighbor interaction, therefore, forces due to first and second nearest neighbors only were considered.

The estimates of the validity of the potentials in metals given in the preceding paragraphs apply to a perfect crystal and small deformations. An additional complication is introduced if defects are present, i.e. free surface, vacancy, or with large deformations, around the crack tip. The potential computed from
2.2 Interatomic potential and force law for copper. Morse potential.
the elastic constants, energy of vaporization, vacancy formation energy, lattice constant, and compressibility refer to a perfect lattice and reflect its electronic distribution. The presence of a defect, however, alters the electronic distribution, and it is difficult to estimate how this altered distribution would affect the atoms in the vicinity of the defect. In these cases only a satisfactory reproduction, by using MD and the interatomic potential, of the most significant experimental values in relation to the particular simulation study to be performed can confirm the validity of the potential. In particular in our simulation of fracture mechanics our potential function should reproduce satisfactorily deformation curves until the points where the maximum ideal stresses, \( \tau_c^{\text{id}} \) and \( \sigma_c^{\text{id}} \), are reached. These two stresses are of special significance in any study of fracture mechanics because they determine ultimately the fracture behavior. The lack of experimental data for these critical values, however, prevents us from confirming the validity of our potentials at large deformations.
2.3 Numerical Integration of Equations of Motion.

Accuracy of Numerical Integration.

The algorithm used in this thesis to move the particles forward in time by an amount \( \Delta t \) is given by

\[
\begin{align*}
\mathbf{r}(t+\Delta t) &= \mathbf{r}(t) + \mathbf{v}(t) \Delta t + \frac{1}{2} \left[ 4 \mathbf{a}(t) - \mathbf{a}(t-\Delta t) \right] \Delta t^2 \\
\mathbf{v}(t+\Delta t) &= \mathbf{v}(t) + \frac{1}{6} \left[ 2 \mathbf{a}(t+\Delta t) + 5 \mathbf{a}(t) - \mathbf{a}(t-\Delta t) \right] \Delta t
\end{align*}
\]

where \( \mathbf{r}(t) \), \( \mathbf{v}(t) \) and \( \mathbf{a}(t) \) are the position, velocity and acceleration of a particle at the time \( t \). This algorithm, used by P. Schofield in MD simulation of liquids (7), allows a relatively large time step to be used.

We have checked the accuracy of this algorithm by comparing its power series expansion in time with the expansion of the exact solution for the harmonic oscillator.

(a) Exact solution corresponding to harmonic oscillator

\[
\begin{align*}
\mathbf{x}(t) &= \mathbf{x}(0) + \frac{\mathbf{v}(0)}{\omega} \sin(\omega t) \\
\mathbf{v}(t) &= \mathbf{v}(0) \cos(\omega t)
\end{align*}
\]

Substituting \( t \) by \( t+\Delta t \) in the above equations and expanding \( \sin(\omega(t+\Delta t)) \) and \( \cos(\omega(t+\Delta t)) \) in powers of \( \Delta t \)
\[ x(t+\Delta t) = x(t) + v(t) \Delta t + \frac{\Delta t^2 a(t)}{2} - \frac{v(t) w^2 \Delta t^3}{3} + \frac{v_o \sin(\omega t) w^4 \Delta t^4}{4!} \]  \hfill (2-5)

\[ v(t+\Delta t) = v(t) + a(t) \Delta t + v_o \omega^4 \omega t \left( -\frac{w^2 \Delta t^2}{2!} \right) + v_o \omega^3 \omega t \left( \frac{w^3 \Delta t^3}{3!} \right) + v_o \omega^2 \omega t \left( \frac{w^4 \Delta t^4}{4!} \right) \]

(b) Algorithm (2-4), expanded in powers of \( \Delta t \)

\[ x(t+\Delta t) = x(t) + v(t) \Delta t + \frac{\Delta t^2 a(t)}{2} - \frac{v(t) w^2 \Delta t^3}{3} + \frac{v_o \sin(\omega t) w^4 \Delta t^4}{4!} \]  \hfill (2-6)

\[ v(t+\Delta t) = v(t) + a(t) \Delta t + v_o \omega^4 \omega t \left( -\frac{w^2 \Delta t^2}{2!} \right) + v_o \omega^3 \omega t \left( \frac{w^3 \Delta t^3}{3!} \right) \]

Equation (2-6) shows that the algorithm used by Schofield is correct to order \((\Delta t)^3\) and \((\Delta t)^2\) for the positions and velocities, respectively, when it is tested against the harmonic oscillator solution.

This algorithm has the advantage that it needs fewer terms to calculate \(r(t+\Delta t)\) and \(v(t+\Delta t)\) than the ordinary central difference method for the same order of accuracy and the drawback that the evaluation at time \(t+\Delta t\) is carried out using the values at \(t\) and \(t-\Delta t\), therefore, a different procedure is needed to initialize the numerical integration at time \(t=0\).

The time step size has to be chosen small enough that the integration procedure generates a stable and accurate solution to the equation of motion. If the time step size is too large, then
the equations of motion will fail to conserve total energy and will result in an unstable trajectory. On the other hand, it also has to be chosen as large as possible because the computational time per time step does not depend on the time step size, and the net cost of the simulation over a fixed duration will vary inversely as the time step size. The numerical integration should also span an oscillation period in a number of time steps, about 20, such that the net change during any single time step is not too large. The accuracy of the numerical integration can be measured by the precision to which the total energy is conserved. A series of simulations with different time step sizes at different temperatures was carried out on a perfect lattice composed of 200 particles to determine the maximum time step size that gave reasonable conservation in the total energy. Time step size as large as 0.1 of an oscillation period gave absolute deviations of about 0.05% per time step, and were considered acceptable. However, more conservative step sizes, about 0.02 of one oscillation period, were used.

The accuracy of the numerical integration can also be measured by the accuracy of the reversibility of the trajectory. The trajectory can be retraced simply by reversing velocities and other odd time derivatives at the time step of retracing or by using a negative value for $\Delta t$ at every time step. The accumulated error in the total energy during a computation period of one thousand time steps (500 time steps before reversing trajectories), was less than 2%.
2.4 Stress Boundary Method

The selection of a particular boundary condition depends upon what one wishes to calculate. If the goal were to simulate an infinite perfect system the behavior is approximated by describing the motion of N particles in a finite computational cell of volume V with periodic boundary conditions. The simulation is usually carried out at a constant density. New techniques have been developed which allow variation in shape and size of the periodically repeating molecular dynamic cell, such that the stress instead of the density is kept constant. In this formulation the shape and size of the system can change according to dynamical equations given by the lagrangian of the system. This new improvement of periodic boundary conditions is well suited to the study of structural transformation in solids under external stress and at finite temperature.

If one wants to use this procedure to study the behavior of defects, such as cracks, vacancies, interstitials, free surfaces, etc., two difficulties arise. First, the system must be large enough such that image defects in the periodic cells do not interact with the original defect, and second, the stresses are not uniform along a parallel boundary but they are determined by the distance to the core of the defect. In this case, periodic boundary conditions, either under constant density (fixed volume) or under fixed uniform stress do not introduce substantial advantages to the simulation. We will apply in the future this method to the simulation of a perfect sample under a tensile
2.3 Location of atomic regions.
stress.

In the simulation of fracture mechanics two general methods have been implemented during the past few years. One applies a constant and uniform stress along the boundary of a sample containing a microscopic crack, usually of a few interatomic spacings in length. This method, despite the computational simplicity, has the drawback that the simulation corresponds neither to the case of a macroscopic crack nor to the case of a crack surrounded by a reasonably large amount of material (9). The other method arranges the atoms at the boundary according to the solution given by a continuum linear theory and studies the behavior within the system, where linear theory is in general not valid, using MD simulation, Fig. 2.3.

This second category of boundary condition, which is generally applied when a simulation of real materials is performed, can be subdivided into two new types of boundary conditions. The first type has been used during the last decade in simulations of dislocations and cracks. We have used it previously in the simulation of a crack tip. It consists of fixing the position of the particles at the boundary according to a known continuum elastic solution appropriate to the type of defect and stress that is applied. The volume of the system is therefore fixed during the simulation. This method has been called fixed boundary condition (10). An improvement was introduced later that allows small changes of the volume of the system. This method applies a continuum linear Green's function that relaxes the forces between the continuum and the atomic region (11). The method,
Regions for the flexible boundary method in the case of a crack tip.
however, introduces new computational complexities in the simulation and it is not always possible to determine the Green's function of the defect that is being simulated.

The most important drawback of this type of boundary is that it imposes serious constraints on the system if the atomistic processes to be observed require variations in the shape and size of the atomic system. In particular our simulation of fracture mechanics, we expect large non-linear effects close to the crack tip in the form of large strains, corresponding to a high concentration of stress. Non-linear extension would be prevented if we fixed the boundary as in the method described above.

To solve this problem a new type of boundary condition has been developed in the present work which allows free relaxation of the atomic system. The new type of boundary fixes the stress at the boundary instead of the displacements. If these stresses can be assumed constants during the simulation and the linear elasticity solution valid at the boundary, we can expect a correct simulation. This will be the case if we use a system large enough such that the non-linear region does not extend to the boundary. The initial configuration of the crack tip is generated by using the solution for crack problems in anisotropic elasticity given by Sih and Liebowitz (12)
\[ \frac{c^2 - c''}{c''} = \frac{c^2 - c'}{c'} = \frac{c^2 - c''}{c''} \]

Here \( a' = a, a'' = a', \) and \( a'' = a' \) are the three optical components.

\[ \cos \phi \frac{c^2 - c''}{c''} \]

\[ \tan \left( \frac{\theta}{2} \right) \]

\[ 2a'' = \frac{2a}{r} \]

\[ \theta = \frac{2a + a''}{4a'} \]

when

\[ (2 - 7) \]

\[ \left\{ \begin{array}{l}
(1 - \cos \theta) + \cos \phi \cos \theta \\
(1 - \cos \theta) - \cos \phi \cos \theta
\end{array} \right\} \]

\[ \left\{ \begin{array}{l}
(1 - \cos \theta) + \cos \phi \cos \theta \\
(1 - \cos \theta) - \cos \phi \cos \theta
\end{array} \right\} \]

\[ \left\{ \begin{array}{l}
(1 - \cos \theta) + \cos \phi \cos \theta \\
(1 - \cos \theta) - \cos \phi \cos \theta
\end{array} \right\} \]
where \( u \) and \( v \) are the displacements along the \( x \) and \( y \) direction for the plain strain case, zero \( z \)-displacement, and \( r, \theta \) the atomic position in terms of a polar coordinate system located at the crack tip. After the initial configuration is generated we have to determine the forces exerted by the rest of the material on the atomic crack tip. The rest of the material is assumed infinite and completely surrounding the crack tip. Two alternative ways can be applied to determine these forces. The one used here consists in the determination of the forces exerted by the exterior atomic layers on the rest of the atomic system. The number of atomic layers depends on the range of the interatomic potential. Two atomic layers are necessary in the case of a Johnson's potential with second nearest neighbor interaction. To make this calculation we divide the atomic system in three regions as in the standard flexible boundary method and determine the forces of region 3 atoms on region 2, Fig. 2.4. The last step consists of substituting the exterior atomic layers, region 3, by the equivalent forces and leave these constant for the rest of the simulation.

The other alternative, although more direct, offers more practical difficulties. It consists in determining the forces acting on each particle at the boundary from the stresses given by the anisotropic elasticity solution(12). The difficulty arises at the moment of transforming these stresses in the equivalent forces acting on each particle, i.e., stresses should be distributed between several layers.
2.5 Determination of the Equilibrium Configuration and Simulation of Thermal Effects

Several different types of computer methods can be used to obtain the static equilibrium configuration of the defect. In the dynamic simulation of a crystal, each atom vibrates continuously about its static equilibrium position. The array of atomic positions can be obtained by computing the time average portion of each atom. In instances where only the time average portions are desired, for example, equilibrium position at 0 K, excluding quantum effects, the dynamical method can be amended so that the atomic motion is progressively damped as the atoms approach their static equilibrium positions.

There are several procedures for reaching the static equilibrium configuration. One applies a quasi-dynamical method where the velocity of each atom is set to zero each time the kinetic energy of the entire system reaches a maximum. This procedure is suggested by the circumstance that the velocity magnitude of a mass point in simple harmonic motion is maximum at the time it is passing through the static equilibrium position, zero net force position. Several variations of this basic idea have evolved. As a mass point in simple harmonic motion approaches the static equilibrium position, the dot product of its velocity and the restoring force is a monotonically decreasing positive quantity which vanishes at the equilibrium position and then becomes negative. On this basis, Evans and Beeler introduced the idea of setting the velocity of any atom to zero whenever the dot product
of the velocity and force becomes negative, in a static equilibrium calculation. This individual atom criterion for damping leads to a significantly faster convergence than the maximum total kinetic energy criterion. An individual atom criterion for damping is especially necessary when two or more markedly different atom masses are involved.

The procedure used in this work consists of introducing a frictional force in the equations of motion of each particle after the system has been allowed to run for several oscillations of the total kinetic energy

\[ m \frac{d^2 \vec{r}_i}{dt^2} = \vec{F}_i(\vec{r}_i, \vec{v}_i, \ldots, \vec{r}_n) - \alpha \frac{d\vec{r}_i}{dt} \quad (i = \xi) \]

The damping constant has to be chosen small enough that the system is not so overdamped that it is quenched, and as large as possible so the system will reach the minimum internal energy configuration in a reasonable period of time. Usually the damping constant is chosen to be around half the time average value of the critical damping constant estimated by Hooke's law. We did several tests with different damping constants and found that for values close to the critical damping, the average time for the system to reach the minimum energy configuration was about 300 time steps. The total procedure, therefore, consists of several periods of free relaxation without damping alternating with periods of frictional damping until the system temperature has decreased to a few degrees. The final configuration corresponds to a stable state of minimum potential energy and further damping.
to still lower temperatures does not lead to any significantly
different configuration of the relaxed atomic configuration.

In our simulation of fracture mechanics the initial config-
uration is a quasi-equilibrium position generated from the con-
tinuum elasticity theory. We have studied the effect of damping
on the simulation when it is introduced at different stages dur-
ing the relaxation. When atomic damping is introduced after sev-
eral oscillations of the total kinetic energy it is observed that
the kinetic energy acquired during the expansion of the system is
enough to break the weak crack tip bond which is already close to
the rupture point and propagate the crack, Fig. 2.5. The crack
tip bond length experiences a small increment during the first 20
time steps, Fig.2.5a. This corresponds to the relaxation time at
the crack tip because the continuum theory does not provide atom-
ic equilibrium, especially, at the crack tip. Only after the
sound wave generated by the expansion of the system, and
generated at the boundary, reaches the crack tip, 40 time steps
later, the crack tip bond starts to suffer large elongation,
Fig.2.5a. The kinetic energy absorbed during the expansion of the
system due to the work done by the exterior forces is enough to
break the crack tip bond and propagate the crack. It is interest-
ing to notice that the kinetic energy is not completely ran-
domized, the velocities components are greater along the
y-direction( direction of maximum elongation), and zero along the
z-direction. In the cases where a Maxwellian distribution of
velocities was introduced, after obtaining the equilibrium con-
figuration of the crack by introducing a large damping factor at
2.5 a) Variation of crack tip bond length during relaxation. $K_t = 0.9 K^0$. ● Damping. ○ No damping.
b) Variation of the temperature of the system during relaxation. $K_t = 0.9 K^0$. ● Damping. ○ No damping.
the beginning of the simulation, we did not get crack propa-
gation. This method will be adopted in the simulation of systems
close to the Griffith's critical value.

As an interesting confirmation of results in Fig.2.5 we have
determined analytically the time taken by the sound wave to
reach the crack tip from the boundary. A typical value for the
elastic constants of $\alpha$-iron, Young's and shear moduli, is $10^2$
dynes/cm² and the density of the system is about $10$ gr/cm³,
hence the velocity of the sound $w$ is

$$w \propto \sqrt{\frac{\text{elastic constant}}{\text{density}}} \approx \sqrt{\frac{10^6}{10}} \approx 3 \times 10^3 \text{ Å} \cdot \text{sec}^{-1} \quad (2-9)$$

the time to reach the crack tip assuming a distance of $5\text{ Å}$
interatomic spacings is about $t \approx (5 \cdot 3 \text{ Å}) / (3 \cdot 10^3 \text{ Å} \cdot \text{sec}^{-1}) \approx 5 \cdot 10^{-13} \text{ sec}$
which agrees satisfactorily with the 40 time steps reported in
Fig.2.5a (time step = $1.00 \cdot 10^{-14} \text{ sec}$).

If one is interested in studying thermal effects, the simu-
lation begins with the set of static relaxed position
coordinates, which correspond to a particular potential energy
and density and was obtained by the method indicated above, and
the velocities coordinates from a Maxwellian velocity
distribution which corresponds to a particular temperature. Then,
the initial state where all the thermal energy is in the form of
kinetic energy will rapidly exchange energy between potential and
kinetic energies and achieves time averaged distribution of ener-
gy which is approximately equipartitioned. The velocity components are sampled from a random number sequence which is characterized by a Maxwellian distribution so that the orientation of the initial velocity vectors is randomly distributed. Then the velocity components are adjusted so that the net momentum and torque of the system is identically zero and the kinetic energy of the system is approximately twice the desire equilibrium temperature.
2.6 Determination of the Atomic Stress

Born and Huang derived a general expression for the stress tensor at a given particle in a system of interacting particles in equilibrium. When the atomic interaction is described by a central force potential $V(r)$, the energy of the system of atoms is

$$E = \frac{1}{2} \sum_{i,j} V(r_{ij}) \tag{2-10}$$

where $r_{ij}$ is the separation of atom $i$ and $j$. In this case the component of the stress tensor at atom $i$ is (14)

$$
\sigma^{\alpha\beta}(i) = \frac{1}{2 \Omega} \sum_{j \neq i} \frac{\partial V(r_{ij})}{\partial r_{ij}} \left( \frac{r_{ij}^{\alpha}}{r_{ij}} \right) \left( \frac{r_{ij}^{\beta}}{r_{ij}} \right) \tag{2-11}
$$

where $r_{ij}^{\alpha}$ and $r_{ij}^{\beta}$ are the $\alpha$ and $\beta$ components of the vector $r_{ij}$, respectively, and the atomic volume.

We have applied this expression to the determination of the stress field in our atomic system. After all the components of the stress tensor have been calculated at each atomic position the principal stresses were determined by using the Mohr's circle. Fig. 2.6 shows the stress field surrounding the crack tip in a simulation of $\alpha$-iron. The stress field will be analyzed again in sec. 4.10. Arrows and bars indicate tension and compression respectively.
Principal stresses in α-iron obtained by using the atomic stress tensor. Arrows indicate tension and bars indicate compression. Results were obtained using the initial configuration given by the linear anisotropic solution at $K_i = 0.8K_c$, (Sec. 4.4).
Chapter Three

Continuum and Atomistic Studies of Fracture Mechanics

3.1 Griffith Theory of Brittle Materials
3.2 Britteness and Ductility of Crystalline Materials
3.3 MD Simulation of Fracture Mechanics—Previous Works
The following sections summarize the general concepts and theories of macroscopic fracture mechanics which will be studied at an atomic level in the present work. A general description and critical study of the most recent MD simulations of fracture mechanics is given in Section 3.3.

3.1 Griffith Theory of Brittle Materials

The observed strength of ordinary window glass is less than one-hundredth of its theoretical strength. This discrepancy between the strength ordinarily observed and the theoretical strength led Griffith (1,2) to postulate that the low observed strengths were due to the presence of small cracks or flaws in low strength glass. In considering this problem, we shall first follow the approach of Griffith and then discuss the analysis of Orowan which involves atomic parameters that are pertinent to our MD simulations.

Because the extremities of cracks have the ability to act as stress raisers, Griffith assumed that the theoretical stress was obtained at the crack tip, even though the average stress was still far below the theoretical strength. According to this concept, fracture occurs when the stress at the ends of the crack exceeds the theoretical stress. When this occurs, the crack is able to expand catastrophically.

Griffith's idea was to set up a model for a crack system in terms of a reversible thermodynamical process. The system,
defined in Fig.3.1, is an elastic body B containing an internal crack S of length 2C, and subjected to loads applied at the outer boundary L.

The first step in the treatment was to find an expression for the total energy of the system. To do this the individual energy terms that change as a result of crack formation are considered. First, it can be expected in general that the outer boundary of the crack system will undergo some displacement, such that the applied load does an amount of work $W_L$. (For a truly reversible system an increase in this work can be identified with a corresponding decrease in the potential energy of the loading system). Second, the strain energy $V$ stored in the elastic medium must be sensitive to variations in the system geometry. Third, the mere act of creating new crack surfaces requires the expenditure of free surface energy $V_s$. For a static crack system the total energy is the sum of these three terms:

$$V = (-W_L + V_s) + V_s \quad (3-1)$$

Since forces transmitted to the crack region are determined by the loading system and elastic medium, it is convenient to refer to the bracket term in Eq.(3-1) as the mechanical energy of the system. If we were to be concerned with a dynamic crack system, we would have to add a kinetic energy term to Eq.3-1.

Thermodynamic equilibrium is then attained by balancing the
Figure 3.1 Static plane crack system. L applied loading, S crack surface.

Figure 3.2 Energetics of Griffith crack in uniform tension.
mechanical and surface energy terms over a virtual crack extension. The mechanical energy must decrease as the crack extends. On the other hand, the surface energy term must increase with crack extension, since the cohesive forces of molecular attraction across \( \Sigma_c \) must be overcome during the creation of the new fracture surfaces. Thus, the bracket term in Eq. 3.1 favors crack extension, while the second opposes it. This is the Griffith energy balance concept, a formal statement of which is given by the extended equilibrium requirement

\[
dV/dc = 0 \quad (3-2)
\]

Griffith attempted to confirm his theory by applying it to a real situation. He needed a model for a crack in order to calculate the energy terms in Eq. 3.1. For this he took advantage of the Inglis analysis (3), considering the case of a narrow elliptical crack in a remote, uniform tensile stress field. Then, for experimental verification he had to find a well behaved model material, isotropic and closely obeying Hooke's law at all stress level prior to fracture. Glass was selected as the most easily accessible material satisfying these demands.

In evaluating the mechanical energy of this model, Griffith used a result from linear elasticity theory, namely that for any body under constant applied stress during crack formation,

\[
W_c = 2 \ V_f \text{(constant stress)} \quad (3-3)
\]
From the Inglis solution of the stress and strain field, the strain energy density is easily computed for each volume element about the crack. Integrating over dimensions large compared with the length of the crack then gives, for unit width of the crack (measured along the crack front), (3,4)

\[ V_\varepsilon = \frac{k c^2 \sigma_a^2}{E} \text{ (plane stress)} \quad (3-4a) \]

for a thin plate, or

\[ V_\varepsilon = \left(1 - \nu^2\right) c^2 \sigma_a^2 / E \text{ (plane strain)} \quad (3-4b) \]

for a thick plate. Here \( \sigma_a \) is the applied tension normal to the crack plane, \( E \) is Young's modulus, \( \nu \) is Poisson's ratio, and \( 2c \) is the length of the crack. For the surface energy of the crack system, Griffith wrote for unit width of crack

\[ V_s = 4c \gamma \quad (3-5) \]

with \( \gamma \) the surface energy per unit area. The total system energy Eq. (3-1) thus becomes for the case of plane strain

\[ V = -\pi c^2 \sigma_a^2 \left(1 - \nu^2\right) / E + 4c \gamma \quad (3-6) \]

The Griffith equilibrium condition, Eq. (3-2), may now be
applied to eq. (3-6); this gives as a critical condition for fracture

$$K_{IC}^G = \left( \sigma a \sqrt{\pi c} \right)_{IC}^G = \left[ \frac{2 E \gamma_f}{(1-\nu^2)} \right]^{\frac{1}{2}} \quad (3-7)$$

for constant stress, plane strain conditions, Fig. 3.2. $K_{IC}^G$ is called the critical stress intensity factor and it is a property of the material for a given fracture mode.

In the above case, the analysis has been applied to a crack in a brittle elastic solid where its movement does not involve plastic deformation. It is significant that the same approach can also be applied to problems where the movement of the crack involves plastic deformation with the assumption that the plastic region around the crack tip is negligibly small in comparison with the outer zone (Irving approach). In this case we may substitute $\gamma$ by $\gamma_f$, where $\gamma_f$ is the plastic work done in forming a surface of unit area. Under these circumstances the energy to break atomic bonds must include the energy due to all the mechanisms of plastic relaxation produced during crack extension.

Orowan (4), on the other hand, used the stress at the crack tip in his approach. In both theories, however, a flat plate containing a crack of elliptical cross section was considered. The stress and strain around a elliptical hole of this type, with the indicated orientation of the tensile stress, have been computed by Inglis (3). According to these calculations the stress
, at the end of the crack is

\[ \bar{\sigma}_E = 2 \sigma_a \left( \frac{c}{\rho} \right)^{\frac{1}{2}} \]  \hspace{1cm} (3.8)

where \( 2c \) is the length of the major axis of the elliptical hole, \( \sigma \) is the applied stress, and \( \rho \) is the radius of curvature at the ends of the ellipse. We know that (4)

\[ \sigma_t^{\text{corr}} = \left( \frac{E}{a} \right)^{\frac{1}{2}} \]  \hspace{1cm} (3.9)

where \( a \) is the interatomic distance.

If the fracture is to spread, \( \sigma_E \) must equal \( \sigma_t^{\text{corr}} \), and

\[ 2 \sigma_a \left( \frac{c}{\rho} \right)^{\frac{1}{2}} = \left( \frac{E}{a} \right)^{\frac{1}{2}} \]  \hspace{1cm} (3.10)

This relationship can now be solved, yielding for the plane strain case

\[ K_{IC}^{\text{Orowan}} = \left( \sigma_a^{\text{corr}} \right)_{IC}^{\text{Orowan}} = \left[ \left( \frac{\pi f}{8a} \right) \frac{2 \sqrt{E}}{(1-\nu^2)} \right]^{\frac{1}{2}} \]  \hspace{1cm} (3.11)

where \( \sigma_a \) is the average applied stress at which the crack will spread. This relationship is Orowan's version of the Griffith criterion for brittle fracture. It differs only slightly (in a small numerical factor) from Griffith's original relation. Notice that as the crack length increases, the stress to keep it moving decreases. This signifies that once the crack starts moving it is able to accelerate to high velocities.
3.2 Brittleness and Ductility of Crystalline Materials

There is an extensive literature covering all the continuum aspects of crack tip plasticity. In this section a model of dislocation nucleation at the crack tip and the influence of such defects in predicting brittle or ductile behavior as described by Kelly, Tyson and Cottrell (KTC) (5) and by Rice and Thomson (RT) (6) are discussed.

A criterion for brittle fracture in crystals can be established in terms of the spontaneous emission of dislocations from a sharp crack. The stress field near the crack tip in a linearly elastic medium is of the form \( \sigma_{ij} = K(2\pi r)^{1/2} \phi_j(\theta) \) where \( K \) is the stress intensity factor and \( (r, \theta) \) are polar coordinates with the origin at the crack tip. At the crack tip itself where \( r \to 0 \) a non-linear treatment is required as the interatomic bonds are stretched beyond the region of harmonic behavior. As the stress intensity factor increases, lattice fracture will occur at the crack tip in the non-linear region. Failure can occur by bond rupture in either tension or shear, which will determine whether the behavior is inherently brittle or ductile.

Two treatments have been presented in the literature to predict the failure mode from known material properties. Kelly, Tyson and Cottrell proposed the criterion that an ideal (defect free) solid may sustain a fully brittle crack only if the theoretical strength in tension is exceeded before the theoretical
strength in shear within the local field of the crack tip. The criterion makes no comment of the nature of any deformation that might occur. One only needs to consider the theoretical strength calculations in relation to the stress distribution at the crack tip, coming back to the equations of linear elasticity for an evaluation of this field. The final expression proposed by KTC was that brittle fracture will be observed if

\[
\left( \frac{\tau_{\text{Shear}}}{\tau_{\text{Conhesive}}} \right)_{\text{ideal}} > \left( \frac{\tau_{\text{Shear}}}{\tau_{\text{Conhesive}}} \right)_{\text{max}}
\]

where the subscript "ideal" and "max" refer to the ideal properties of a perfect lattice and to the maximum values attained at a crack tip respectively.

Rice and Thomson (6), on the other hand, have argued that a necessary criterion for brittle fracture is stability against emission of dislocations from the crack tip. They have treated this nucleation process within the approximation of linear elasticity and the Peierls model of a dislocation core. The specific question addressed by these workers is whether the shear deformation is sufficient, not merely to nucleate a dislocation at the crack tip, but also to propagate it within the stress field into the surrounding crystal. They considered first the balance between the following crack dislocation interaction forces: (a) force on dislocation arising from the stress field of the crack (b) surface tension force caused by creating surface ledges at the (blunted) crack, (c) image force of dislocation in the free
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surface of the crack. The first term repels the dislocation from the crack tip, while the remaining two attract it. One then compares the core of the dislocation versus the distance in which the dislocation starts to be repelled from the crack tip.

Rice and Thomson thus conclude that covalent and ionic solids, along with h.c.p. metals, are stable against dislocation emission, while f.c.c. metals are unstable; and b.c.c. comprise and intermediate case. The KTC criterion probably leads to an underestimate of the brittle tendencies of the solids because of not considering the subsequent propagation of newly generated shear deformation (dislocation).

Both treatments require approximations in their quantitative development. The stress analysis of linear elasticity is used to evaluate \( \frac{\tau_{\text{shear}}}{\tau_{\text{con}} \text{crit}} \) around the crack tip in the KTC criterion and the forces on dislocations near the crack tip in the RT model. Better models of the non-linear and atomistic behavior of materials are also required to evaluate \( \frac{\tau_{\text{shear}}}{\tau_{\text{con}} \text{crit}} \) and dislocation core structure with greater accuracy.
3.3 Computer Molecular Dynamics of Fracture Mechanics

Previous Works

During the last years a number of studies of fracture in crystalline solids using atomistic models have appeared. One can classify them in two categories. The first type is concerned with a specific material or group of materials, and its purpose is to be as realistic as possible with respect to both crystal geometry (dimensionality of the system, boundary conditions, etc.) and interatomic force laws. These models must yield information regarding atomic processes in the given class of materials. Examples are provided by the work of Kanninen and Gehlen (7,8,9) and Sinclair (10).

Gehlen and Kanninen worked on $\alpha$-iron in a three-dimensional system on which the atoms interact through a central pair potential constructed by Johnson (sec.2.4). This potential is based upon two body interactions which extend out to first and second nearest neighbors. An empirical form is used with the constants selected to match the experimentally determined elastic constants of the material. The atoms are initially put into a configuration approximating the defect being simulated. The boundary atoms are held fixed in the positions given by the linear elasticity continuum solution (fixed boundary condition). The final position of atomic equilibrium is evaluated by letting the atoms
inside the system move freely according to the interatomic forces.

Based on this model Gehlen and Kanninen tried to check the validity of Griffith's criterion. All the macroscopic variables, elastic constants and surface energy were specified by the potential function and the critical stress intensity factor was determined by calculating the condition of maximum elongation for the crack tip bond. The estimated values for the critical stress intensity factor were found to be greater than those necessary to produce an exact correspondence with Griffith's equation. A possible reason for this discrepancy, as noted by the authors, is that the boundaries were fixed. This inflexibility could impose a serious constraint, in the form of residual forces between the atomic and the continuum regions, especially if the atomic boundaries are close to the crack tip. To avoid these difficulties the authors used a new procedure called flexible boundary to attenuate the effects of incompatibility between the two regions. Using this improved boundary the stress intensity factor was still found to be about three times the theoretical Griffith's value. To explain this, a kink parallel to the crack front was introduced in the simulation. This crack with the kink had a critical stress of motion very close to Griffith's estimate.

Our studies in the next chapter show that it is possible to obtain an accurate correspondence with Griffith's value when
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one uses a boundary condition flexible enough such that non-linear effects are not as constrained as in previous boundaries methods.

The second type of atomistic models is highly idealized from the viewpoint of crystal geometry (two dimensional systems, free uniform stress boundary, etc.) and interatomic force laws. They cannot, therefore, represent directly any particular real material. Nevertheless, they do serve to provide insight into general characteristics of static and dynamic propagation of cracks with a minimum of computational difficulties compared with the previous method. Examples of idealized atomistic models include the works of Thomson, Hsieh and Rana (11, 12, 13) in which a new phenomenon called "lattice trapping", the crack analogy of the Peierls resistance to a dislocation motion, is studied. They used two models which were subjected to a "lattice static" analysis. In the first model, a one-dimensional system, the crack was depicted as two semi-infinite chains consisting of points of atoms linked horizontally by stretchable elements. The chains were subjected to opening forces applied vertically to the free ends. In the two dimensional model an infinite square lattice of atoms linked by stretchable and bendable elements was considered. The crack was opened either by a vertical wedging force or by vertical tensile forces distributed uniformly at infinity. The "lattice-static" analysis began with an assumption concerning the form of the atomic interaction, and proceeded to calculate an equilibrium configuration consistent with appropriate boundary
conditions. This involved considerable mathematical complexity, and one had to restrict the analysis to the simplest force law for the linking elements. Accordingly it was assumed that the elements were Hookean up to a critical breaking point. The lattice trapping behavior has been tested by Sinclair(14) with other atomistic models and using different types of potentials. These results seemed to indicate that the phenomenon of lattice trapping is almost completely attenuated when more realistic interatomic force laws are used in the simulation.

Highly idealized models have been used in the studies of Ashurst and Hoover(15), Weiner and Pear(16), and Paskin(17). Ashurst and Hoover used a two-dimensional triangular lattice in which the particles interact by truncated Hook's law forces and the exterior stresses acted directly over the boundaries. Their static results for the energy, entropy, stress concentration and crack structure are consistent with expectation from macroscopic elasticity theory. The dynamic theory of crack propagation is, according to the authors, less well developed and supersonic crack velocities could be produced by the proximity of the exterior boundaries. Under these conditions crack propagation can outrun lattice relaxation.
CHAPTER 4. Simulation of Brittle Materials. Results for \( \alpha \)-Iron

4.1 Atomic Model
4.2 Surface Energy and Elastic Constants
4.3 Tensile Test Simulation
4.4 Stress Boundary Method
4.5 Effects of Anisotropy on Crack Propagation
4.6 Determination of the Critical Stress Intensity Factor
4.7 Comparison of Stress and Fixed Boundary Methods
4.8 Effects of Finite Simulation System Size
4.9 Test for Ductility in \( \alpha \)-Iron
4.10 Stress and Displacement Field in the Crack Tip Region
In this chapter a study of fracture mechanics, by studying the atomic arrangements at the tip of a cleavage crack in α-iron, is described. A new boundary condition is applied to the crack tip. This new method has solved the problems of previous boundary conditions, for example: great deviations from Griffith theory in the case of brittle materials, lack of flexibility at the boundaries and constraints against the emissions of dislocations (chapter 5).

Using this new method an atomistic study has been performed of the crack tip structure and properties, stress and strain field surrounding the crack tip, anisotropic effects, and a comparative study with other boundary conditions which have been applied previously to MD simulation of fracture mechanics.
4.1 Atomic Model

The atomic system to be used in the present simulation is a three dimensional b.c.c. lattice of iron atoms, α-phase, interacting through the Johnson's potential described in section 2.2. The b.c.c. system is characterized by four close-packed directions, the {111} directions, Fig.4.1, and by the lack of a truly close-packed plane such as the (111) plane of the f.c.c. lattice or the basal plane of the hexagonal lattice. The slip direction in the b.c.c. crystal is the close-packed direction, {111}; the slip plane, however, is not well defined. Experimental tests on iron single crystals show that any plane that contains a close packed {111} direction can act as a slip plane. In further agreement with the lack of a close packed plane is the high ideal shear stress; in this case the ratio of ideal shear and cohesive stress ( \( \sigma_{sh} = 0.66 \cdot 10^5 \text{dynes/cm}^2 \), \( \sigma_{\infty} = 3.00 \cdot 10^5 \text{dynes/cm}^2 \) ) takes a value close to the critical point 0.5 (chapter 3, KTC criterion), separating brittle from ductile behavior. Experimental tests assign b.c.c. materials to an intermediate position between ductile, f.c.c. materials, and highly brittle covalent materials, diamond, Si, etc. Recognition of the slip system of the material is necessary in order to orient the crack configuration in a position where dislocation emission and propagation of the crack can be easily produced and clearly observed.

The first step in constructing the atomic model is to gener-
4.1 Body-centered cubic cell. Dashed lines indicate close-packed ⟨111⟩ directions. Atoms are labeled for reference in Fig. 4.2.
ate a b.c.c. lattice of iron atoms, Fig.4.2. Periodic boundary conditions are applied perpendicular to the plane of the figure (z-direction). This condition imposes a constant thickness to the sample during the simulation. The situation, therefore, corresponds to the plane strain case.

The interatomic force law used in this work is derived from the interatomic potential constructed by Johnson (1,2), as given in section 2.2. This potential is based upon two-body interactions which extend through the separations of first and second nearest neighbors. It is cut off smoothly to zero at a point midway between the second and third nearest neighbors. An empirical form is used with the constants selected to match the elastic constants $c_{11}$, $c_{12}$, $c_{44}$, and the Erginsoy et al (3) radiation damage potential at close approach.

After a perfect lattice has been generated we fix arbitrarily the position of the crack tip, point x in Fig.4.2. The positions of the atoms in the initial configuration are determined by linear elasticity theory as will be described in section 4.4. The way the stress is applied to the sample is specified by the particular boundary method used. Two types of boundary methods will be applied, section 2.4, the fixed boundary and the stress boundary. Different sizes of the simulation system will be used, in all cases there are only two layers of atoms along the z-direction.
4.2 Coordinate system for defining two adjacent (001) planes, denoted by closed and open circles. Also shown is the crack tip location at X.
4.2 Surface Energy and Isotropic Elastic Constants

The surface energy and the elastic constants of the material are necessary to determine the Griffith's critical stress and the initial configuration when using the continuum elasticity solution. The surface energy is taken as the work required to completely separate the crystal along some given plane starting from the undeformed perfect configuration. Its value depends only on the atomic structure of the material and the interatomic potential. In particular, using values appropriate for separation on a (100) plane in \( \alpha \)-iron and for Johnson's potential (4), it is found that \( \gamma = 0.081 \text{eV/Å}^2 \) (1300 erg/cm\(^2\)). It might be noted that Johnson's potential has not been constructed to specifically account for the surface energy. Consequently, there is no reason to expect this value to be realistic. For comparison, an estimate can be obtained using the value of 2320 ergs/cm\(^2\) at the melting point as given by Hondras (5), together with a temperature dependance of 0.49 ergs/cm\(^2\)/°C given by Tszin-tan et al (6). These give a value of 3160 ergs/cm2 at absolute zero. Although this estimate is well above the value obtained from the interatomic potential, we will use the latter value in the determination of Griffith's critical value in order to be consistent with the atomic potential used in the simulation.

Estimates of the isotropic elastic constants can be obtained from the three independent elastic stiffness constants\( (c_{11}, c_{12}, c_{44}) \) using, for example, the procedure outlined by Hirth and Lothe (7). Here the Voight averages, give the expressions for
the shear modulus $\mu$ and Poisson's ratio $\nu$

$$\mu = \frac{1}{5} \left( C_{11} - C_{12} + 3 C_{44} \right)$$  \hspace{1cm} (4.1)$$

and

$$\nu = \frac{\frac{1}{2} \left( C_{11} + 4 C_{14} - 2 C_{44} \right)}{2 C_{11} + 3 C_{12} + C_{44}}$$  \hspace{1cm} (4.2)$$

Inserting experimental values for $\alpha$-iron (11): $c_{11} = 1.2$ and $c_{12} = c_{44} = 0.6$ (eV/A$^3$), Eqs. (4.1) and (4.2) give $\mu = 0.48$ (11,100 Ksi) and $\nu = 0.25$ whereupon $E = 1.20$ (27,800 Ksi).

With the knowledge of the elastic constants, in particular Young modulus and Poisson's ratio, and the surface energy derived from Johnson's potential we can determine the critical stress intensity factor given by Griffith's theory. From chapter 3, the expression for the plane strain case is

$$\left( J_\alpha \sqrt{\pi c} \right)^6 K_{Ic}^6 = \sqrt{\frac{2 E \gamma}{1 - \nu^2}}$$  \hspace{1cm} (4.3)$$
4.3 Tensile Test Simulation

In order to examine the validity of the Johnson potential at higher stresses we have performed a MD simulation to calculate the stress-strain curve in a tensile test of a perfect sample of α-iron. The simulation was carried out with a system composed of 81 particles, two atomic layers along the z-direction, without lateral constraints, Fig.4.3a. Uniform tensile forces directed along the y-direction were applied on layers a-a', b-b', c-c' and d-d', Fig.4.3a. Progressively higher tensile stresses were applied along the [100] direction, y-axis, in order to determine several points on the stress-strain curve. After a new stress was applied the equilibrium configuration was determined by applying the relaxation method indicated in section 2.5. Each relaxation period took about 100 time steps, and a time step double the normal value used in other dynamic simulations was applied. The temperature of the system increased by the work done by the exterior forces, but it was kept low, about 50°K, by the artificial damping imposed on the equations of motion of the particles. It is to be expected that if the additional stresses were small enough the new equilibrium configuration achieved would be independent of the precise manner of increasing the stress. This was found to be the case at a high stress level (past point B in Fig.4.3b) where we obtained the same result whether the stress was applied all at once or applied incrementally starting at point B. The strain was measured on the unit cell situated at the center of the system to avoid sur-
4.3 (a) Simulation system of b.c.c. iron for tensile test, N=81 particles. Two layers are shown. Tensile forces are applied directly on the boundary atoms along rows a-a', b-b', c-c' and d-d'. Configuration shown is the equilibrium structure at $\sigma = 0.5 \times 10^6$ dynes/cm$^2$ (point A in Fig. 4.3b). Notice the b.c.c. structure is still preserved. Atomic bonds for the particle at the center of the system are indicated by dashed lines.
face effects. Deviations close to 30 per cent were found when this strain was compared with the strain at the boundaries. No size effects have been studied in this test, therefore further studies to determine accurately the influence of the boundary and the distribution of stress in a big sample will be performed. Direct comparison with experimental data on iron whiskers tested in uniform tension along the [010] direction (8) showed a good agreement with our MD results at low stresses (Fig.4.3b, dashed line). Deviations from linearity in iron whiskers began to be prominent at e=0.02 elastic strain, and the elasticity modulus /e decreased 15 per cent at ξ=0.03 and almost 40 per cent at =0.05, the maximum measured strain. In our MD tests we found at low stress levels, less than 0.5 10 dynes/cm , that the system was stable and preserved the body-centered cubic structure, Fig.4.3b. At higher stresses, starting of flat part of the curve 4.3b, a significant change in the shape of the atomic cell was found, resulting in a large elongation along the y-direction that corresponds to the rupture of atomic bonds between second nearest neighbors in this direction, and a large lateral contraction, Fig.4.3c. The system was found to have changed to a body-centered tetragonal structure. Similar behavior was found in other computational studies with long range Morse potentials. For example, Milstein (9) in a review of theoretical mechanical behavior of single crystals under load, indicates that similar behavior has been found with other b.c.c. structures and different types of potentials. M.Parrinello (10) has developed a Lagrangian formalism to simulate systems under a wide variety of
(b) Stress-strain curve produced by tensile test in simulation system of Fig.4.3(a). Circles denote actual strains produced at the various stress levels. Dashed line indicates the experimental results in iron whiskers (8).
(c) Relaxed atomic configuration obtained at $\sigma=1.0 \times 10^6$ dynes/cm$^2$ (point B in Fig. 4.3(b)) showing a body-centered tetragonal structure. All the second nearest neighbor bonds along the y-direction are broken.
(d) Displacement field corresponding to Fig.4.3(c). Open circles indicate final position of equilibrium. A body-centered tetragonal structure has been created by large elongation along the y-direction and simultaneous contraction along the x-direction.
stresses. The advantage of this new formalism is that it allows to apply periodic boundary conditions without fixing the volume of the system. Oscillatory potentials which reproduce the phonon spectrum at the transition point between the two phases would also be interesting for testing. The interest in these simulations is that they can provide a better understanding of deformations in whiskers, twinning, martensitic transformations, and the mechanical properties of small structures such as metallic integrated circuits.

At this time there are not experimental tests that confirm the non-linear part of the stress-strain curve and the values of the ideal cohesive and shear stress in $\alpha$-iron. Our purpose for future simulations is to study in greater detail these transitions with the Lagrangian formalism for the boundary and different types of potentials.
4.4 Stress Boundary Condition

A general description of the boundary condition used in the present work is given in section 2.4. In this section we explain how the new method is applied to the simulation of ε-iron.

The initial configuration of the crack tip in ε-iron is generated by using the solution for crack problems in anisotropic elasticity given by Sih and Liebowitz (11). The displacement field in the close proximity of the crack tip for a body subjected to a uniform tensile load (section 2.4.):

\[ u = k_1 \sqrt{r} F_1 (\theta, c_{11}, c_{12}, c_{44}) \]  \hspace{1cm} (4-4)
\[ v = k_1 \sqrt{r} F_2 (\theta, c_{11}, c_{12}, c_{44}) \]

where \( u \) and \( v \) are the displacements along the \( x \) and \( y \) direction for the plane strain case, zero \( z \)-displacement, and \( r, \theta \) the atomic position in terms of a polar coordinate system located at the crack tip fig.4.4 (higher order terms in \( r \) have been neglected). After the initial configuration is generated we have to determine the forces exerted by the rest of the material on the boundary atoms. The rest of material is assumed infinite and completely surrounding the crack tip. Two alternative methods can be used to determine these forces. The one used here consists of first determining the forces exerted by the external material (still discrete) on the atomic simulation system. The number of atomic layers in the external material depends on the range of interatomic potential. Only two atomic layers are needed in the
4.4 Crack tip stresses showing components in rectangular coordinates.
case of Johnson's potential with second nearest neighbour interaction. Then the external material as represented by the two atomic layers is removed and substituted by its equivalent forces. The boundary forces remain constant during the period of simulation.

The other method, although more direct, entails practical difficulties. It consists of determining the forces acting on each particle at the boundary from the stresses given by the anisotropic elasticity solution (11). The difficulty arises at the moment of transforming these stresses to the equivalent forces acting on each particle, i.e. stresses should be distributed between several layers.

To obtain the relaxed configuration an artificial damping is introduced in the equations of motion, see section 2.5.
4.5 Effects of Anisotropy on Crack Propagation

The one important class of metals in which cleavage is most frequently observed is the b.c.c. metals, although the alkali metals, sodium, potassium, etc., are b.c.c., and do not cleavage. The cleavage plane in the body-centered lattice is usually \{100\}, although there are a few examples in which cleavage along the \{110\} plane has been observed (12).

In previous simulations by Gehlen et al. (13,14), cleavage along \{110\} plane in \(\alpha\)-iron was observed despite the fact that experimental tests clearly show propagation in the \{100\} plane. The simulation results believed to be due to the use of an isotropic linear elasticity solution for the arrangement of the initial configuration. The effects of the anisotropy of the crystal were neglected in the early simulations (13,14), because the differences in the atomic positions of the relaxed configurations were very small. However, in later simulations (15), propagation along \{100\} was found when an anisotropic solution was used to specify the initial configuration. Thus the results of references 13,14 and those of reference 15 suggest that the cleavage direction observed by simulation depends on whether anisotropic effects are considered in the linear elasticity solution.

We have examined the effects of anisotropic solution in the cleavage direction in \(\alpha\)-iron. Fig.4.5 shows the results of two instantaneous configurations obtained at right the same stage of crack propagation in a model system of about 200 particles with \(K_r\).
4.5 Atomic configuration obtained in MD simulation of a crack in α-iron. (a) Initial configuration. (b) Instantaneous configuration during crack propagation obtained using the isotropic linear elasticity solution to specify the initial configuration. (c) An instantaneous configuration during crack propagation obtained using the anisotropic linear elasticity solution to specify the initial configuration.
=1K_{rc}^6. The result given by the initial configuration specified by the isotropic linear elasticity solution shows cleavage in the (110) plane, Fig.4.5b, whereas the result based on the anisotropic solution shows cleavage in the (010) plane, Fig.4.5c, which is in agreement with experimental observations. These two configurations closely resemble those obtained by Gehlen et al. (13-15). It should be noted that their simulation systems were somewhat smaller in the x and y directions than ours, but their total number of particles was more than ours since these systems had more than two layers along the z-direction. Secondly, Gehlen et al. used the flexible boundary method (section 3.3) in contrast to the present method of stress boundary. Both Fig.4.5b and Fig.4.5c are instantaneous configurations because the crack was unstable and if the simulations were not terminated the crack would continue to propagate. A larger system would be needed to provide sufficient material in front of the crack tip to enable the simulation to continue. Further simulations with larger model systems show that the cleavage direction is in addition sensitive to system size. Fig.4.6 shows the results of N=673 using again stress boundary condition and the same stress intensity factor K_{r} =K_{rc}^6. The initial configuration was determined by the anisotropic linear elasticity solution as in Fig.4.5c. One observed in this case an apparent cleavage along the (110) plane, Fig.4.6a, but with continued simulation the cleavage plane appeared to be established along the (010) plane, Fig.4.6b. Since the configuration at the crack tip is the same between Fig.4.5c and Fig.4.6a, the fact that in the latter case cleavage occurred along (110)
4.6 Same as Fig.4.5 except N=673 and initial configuration was determined by the anisotropic linear elasticity solution. (a) Initial cleavage propagation along (110) plane. (b) Subsequent cleavage along (010) plane as simulation continued.
must be due to the effect of a larger system.

It is significant that Fig.4.6b shows that subsequent cleavage takes place along (010) even though initial cleavage plane was (110). This suggests that the initial configuration is unimportant in subsequent crack propagation and that probably the more important factor is a change in the local stress field as a consequence of the response of the entire system which results in higher tensile stresses favoring propagation along (110). It follows that if we were to carry out the simulation in the N=673 system with an isotropic solution for initial configuration we will still obtain cleavage along (010). If this were the case, then the use of isotropic or anisotropic solution would not give any significantly results provided a sufficiently large system is used and the crack is allowed to propagate beyond the breaking of the first few bonds.

In addition to the possible effects of the initial configuration, the asymmetry of the crack tip relative to the plane y=0 is also an important reason for the tendency of the crack to start the cleavage along the (110) plane. In sec.4.8 we show MD results obtained with a different system orientation. In that case the symmetry of the crack did not favor propagation along the (110) plane, and crack propagation was indeed observed to take place along the (010) plane, independent of the size and the continuum solution employed for the initial configuration.
4.6 Determination of the Critical Stress Intensity Factor.

An important result in the simulation of fracture is the determination of the value of the critical stress intensity factor. For mode-I fracture a sharp crack surrounded by an infinite amount of material is (sec.3.1)

\[ K_{IC}^C = \left( \frac{\sqrt{a}}{\pi c} \right)_{IC}^6 = \sqrt{\frac{2 \alpha r}{J_{IC}}} \quad (4-5) \]

The expression for this critical stress intensity factor \( K_{IC}^C \) was derived following Griffith theory in sec.3.1. Using the experimental elastic constant and the surface energy \( \gamma \) calculated from the Johnson potential one can evaluate \( K_{IC}^C \) using Eq.(3-7). Each simulation begins with a fixed value of \( K_\gamma \) which can be expressed as a constant times \( K_{IC}^C \). The critical value determined by MD simulation, \( K_{IC}^{MD} \), is estimated by carrying out simulations at successively higher values of \( K_\gamma \) until crack propagation commences. In previous simulations (13-14) using a model system of several hundred atoms and the flexible boundary method described in sec.2.4, the critical value was found to be appreciably higher than the Griffith's prediction, about three times \( K_{IC}^C \). Several reasons were given for this discrepancy: inadequacies in the Johnson potential, in particular the fact that this potential does not account for non-axial force, the quasi-3-dimensional nature of the model, absence of imperfections such as vacancies and impurities, etc. In a different simulation (14) a kink was introduced into the crack system parallel to the crack front, and the critical stress intensity factor in this case was found to be
close to $K_{ic}^o$. We have studied the crack tip configuration using a model system of $N=200$, the isotropic linear elasticity solution for initial configuration, and the flexible boundary method. Fig.4.7 shows the results at three values of $K_{i}$, $1K_{ic}^o$, $2K_{ic}^o$, and $3K_{ic}^o$. The configuration in Fig.4.7c is not in equilibrium since the crack is propagating. Fig.4.7d was obtained at $3K_{ic}^o$ with the fixed boundary method, the constraint imposed by the fixed border of the system prevents the crack front from moving very far. At $K_{i} = 2K_{ic}^o$, Fig.4.7b shows a relaxed configuration with no signs of bond rupture. Notice that at $K_{i} = 3K_{ic}^o$ a cleavage along the (110) plane could be observed, Fig.4.7c, which is the same behavior as Fig.4.5c obtained using the the stress boundary condition at $K_{i} = K_{ic}^o$.

We have made a series of simulation using the stress boundary method in an attempt to determine the critical value of $K_{ic}^{MD}$. These simulations involved three different size systems, two orientations of the z-axis, and both isotropic and anisotropic linear elasticity solutions for the initial configuration. In all cases the simulation began at zero temperature, as the simulation progressed the system started to heat up as a result of work done on the system. Since this is an artifact due to the sudden way in which forces are applied to the system, which is not initially close to the final position of equilibrium, it is appropriate to remove this energy. This was done in all cases, except as noted otherwise, by means of the frictional damping technique discussed in section 2.5.

Table 4.1 shows the results of the most significant
4.7 Atomic configuration of a crack system in α-iron at various stress intensity factors $K_i$, determined using the flexible boundary method. (a) $K_i = K_{ic}$, (b) $K_i = 2K_{ic}$, (c) $K_i = 3K_{ic}$. Case (d) was obtained at $K_i = 3K_{ic}$ but using the fixed boundary method.
<table>
<thead>
<tr>
<th>Simulation</th>
<th>Number of Particles</th>
<th>Orientation z-axis</th>
<th>Elasticity Solution Used</th>
<th>Stress Intensity Factor</th>
<th>Crack Stability and Cleavage Plane</th>
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<tbody>
<tr>
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<td>Stable</td>
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<td>1.2</td>
<td>Propagation,(010)</td>
</tr>
<tr>
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</tr>
<tr>
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<tr>
<td>5*</td>
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<td>Propagation,(010)</td>
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<tr>
<td>6</td>
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<td>1.2</td>
<td>Propagation,(010)</td>
</tr>
<tr>
<td>7</td>
<td>673</td>
<td>[101]</td>
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<td>1.2</td>
<td>Propagation,(010)</td>
</tr>
<tr>
<td>8</td>
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<td>[101]</td>
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<td>Recession</td>
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<tr>
<td>9</td>
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<td>Propagation,(010)</td>
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<tr>
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</tr>
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</tr>
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<td>[001]</td>
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<td>0.8</td>
<td>Propagation,(010)</td>
</tr>
</tbody>
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Table 4.1 Crack propagation characteristics in α-iron as obtained by MD simulations using model systems of various sizes and stress boundary method, (*) runs were made without frictional damping.
simulations along with comments on the crack stability and the direction of propagation. Table 4.2 presents the estimates of the range of $K_{IC}^{m0}$ values for stress boundary simulations. In addition, it shows the results of similar runs using the fixed and flexible boundary method. No results were obtained for the flexible boundary simulations for $N > 140$ since such runs are prohibitively time consuming as the system size gets large.

Table 4.1 shows the effects of anisotropy studied in sec.4.5. In simulation 2 and 3 same cleavage plane was obtained by using whether the isotropic or the anisotropic solution. When the isotropic solution was applied, simulation 3, initial propagation along the (110) plane was observed, however, the cleavage plane changed to the (010) plane after the crack propagated a few interatomic displacements, Fig.4.6b. Simulation 5 shows the effects of lack of damping in the equations of motion, sec.2.5. In this case crack propagation was obtained with a stress intensity factor smaller than in simulation 2. Size dependence of the stress intensity factor is observed when working with small systems. For large systems, simulations 1 and 2, $K_{IC}^{m0}$ was in a range between $1K_{IC}^{m0}$ and $1.2K_{IC}^{m0}$ and for small systems, simulations 12 and 13, the range goes from $0.7K_{IC}^{m0}$ to $1K_{IC}^{m0}$. For systems greater than 200 particles dependence on the size decreases. For example, simulations 9 and 10 performed with systems composed of 238 particles showed the same range for the stress intensity factor as that for a system composed of 673 particles. Effects of the size of the system on the critical stress intensity factor and stress surrounding the crack tip are studied in greater detail in
<table>
<thead>
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<th>N*</th>
<th>Stress</th>
<th>Fixed</th>
<th>Flexible</th>
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<td>2.5-3.0</td>
<td>2.5-3.0</td>
</tr>
<tr>
<td>141</td>
<td>0.9-1.0</td>
<td>2.5-3.0</td>
<td>2.5-3.0</td>
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<tr>
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<td>1.0-1.2</td>
<td>2.5-3.0</td>
<td>---</td>
</tr>
<tr>
<td>673</td>
<td>1.0-1.2</td>
<td>2.5-3.0</td>
<td>---</td>
</tr>
</tbody>
</table>

Table 4.2 Ranges of values of $K_{IC}^{MD}$, the critical stress intensity factor determined by MD simulation using different size systems (N) and various boundary methods, divided by $K_{IC}^{G}$ (the Griffith theory prediction). (*) Number of particles refers to region-1 and region-2 only in the case of fixed and flexible boundaries.
sec.4.8.

Table 4.2 shows the estimated ranges of values of $K_I$ obtained by using the stress boundary method and by using the fixed and flexible boundary methods. With the latter methods at each $N$ one run was made at $K_I=2.5K_{Ic}$ which gave a stable crack and another at $K_I=3K_{Ic}$ giving crack propagation. No further attempt was made to reduce this range, mainly because of the computational expenses involved. One sees from table 4.2 that there is a slight system size dependence in the stress boundary results for the small systems; this dependence is no longer present for $N > 200$. The fact that the small system gives a lower critical stress intensity factor is due to the proximity of the linear forces to the crack tip, which should be applied in a linear region far from the crack (in our case at the boundary of systems composed of more than 200 particles). It is reasonable that similar variations also exist in the fixed and flexible boundary results; all we can conclude is that they should lie within the rather large range shown.

The present MD simulation results show that there is a range of stress intensity factors where the crack is stable, in opposition to Griffith's continuum theory that predicts a unique critical stress. This behavior may be related to the lattice trapping effect suggested by Thomson, ref.(11) chapter 3, which is produced by the discrete nature of the system. As it was mentioned there, when long range interatomic potentials that go smoothly to zero are applied, this effect can be completely attenuated (ref.(14), chapter 3).
4.7 Comparison of Stress and Fixed Boundary Methods

A definitive comparison of different boundary methods is difficult because of ambiguity in normalizing the different simulations. With the tensile load applied through the initial displacements of atoms, we might compare simulation results obtained using the same value of stress intensity factor $K_i$. We have already seen in sec.4.6 that the critical stress intensity value given by the stress and the fixed boundary methods are quite different. It follow that simulation results at the same value of $K_i$ will be quite different. Another normalization procedure is to compare simulations with the same value of the crack tip bond length. This is a reasonable procedure since the region of greatest interest is at the crack tip and one would expect the crack tip configuration to be least sensitive to the direct influence of the approximation introduced at the simulation system boundary.

In this section we consider a comparison of the displacement, strain and stress distributions obtained in two simulations (N=673), one using the stress and the other the fixed boundary, which are normalized to the same crack tip bond length, $d$. The value chosen is $d=3.0 \text{ Å}$ which is just below the distance of maximum force (cf.Fig.2.1). Fig.4.8 shows the direction leading from the crack tip along which the various distributions will be evaluated. Figs.4.9 and 4.10 show the stress and fixed boundary results respectively.

In the case of stress boundary method the initial positions
4.8 MD simulation system (N=673) showing the crack tip position and the atoms along the y-direction at which displacement, stress, and strain distributions will be evaluated. The atoms are indicated as \( \otimes \) and they are numbered with atom 1 being the nearest to the crack tip and atom 10 being the atom in the boundary region which consists of the two outermost rows. In the stress boundary method, forces are applied on the atoms in the boundary region while these atoms are allowed to move. In the fixed boundary method, the atoms in the boundary are held fixed.
Displacement, strain and stress distributions along the y-direction (cf. Fig.4.8) in a crack system obtained by MD simulation with $N=673$ and stress boundary method at $K_i=K_{ic}$. Results derived from an initial configuration based on anisotropic linear elasticity are denoted by crosses or dashed curve, while results based on the relaxed configuration are denoted by open circles and solid curve. The only exception is in (b) where the crosses denote stresses calculated using the procedure in sec.2.6 and the linear elasticity displacement shown in (a).
4.10 Same as Fig. 4.9 except the fixed boundary method is used instead of the stress boundary method. $K_I = 1.4K_{IC}$. 
of atoms in the simulation systems in Fig.4.9(a) were evaluated from the anisotropic linear elasticity solution, Eq.(2.7). The final positions were obtained from the relaxed configuration achieved after 200 time steps at $\Delta t=2\times10^{-14}$ sec. with frictional damping. Notice there occurred a considerable relaxation at each atom position which seems to reach a more or less constant value near the system boundary which is located at atom 10. This additional displacement is a direct result of non-linear forces close to the crack tip. It is interesting that the system has undergone an expansion which is uniform except very close to the crack tip. It should be noted that the far field displacement will have the same value no matter how large is the simulation system. In other words, $d$ is a consequence of the relaxation that has occurred in the non-linear region around the crack tip. By making the system even larger than the present size will not change the differences in atomic displacements between the MD results and the initial linear elasticity solution. This effect is also indicated by the strain distribution, as it can be seen the far-field strain in the simulation system has converged to the linear elasticity value. The stress distribution shown in Fig.4.9(b) indicates a stress relief at the crack tip when non-linear effects are allowed. The linear elasticity solution is singular at the crack tip. The initial stress distribution was evaluated using the initial atomic positions in Fig.4.9(a) and the atomic stress expression in sec.2.6. This procedure will yield a finite stress even at the crack tip. The MD results show a decrease in stress near the crack tip such that the
distribution has a maximum two interatomic distances away. This behavior has also been observed in a MD simulation in a two dimensional square lattice and fixed boundary (16). In the stress boundary method the force on the boundary atoms, in this case atom 10, was kept constant. Even though the boundary stresses were allowed to move during relaxation, (see Fig.4.9(a)), the resulting stresses at 7,8 and 9 gave a distribution that goes smoothly to the fixed value at atom 10. This demonstrates the property of the boundary method of maintaining a constant stress at the boundary while allowing the system to expand in response to the non-linear interaction in the interior.

The fixed boundary results given in Fig.4.10(a) show a smaller displacement of the atoms as a result of the immobility of the boundary. The position of atom 10 was fixed during the simulation because it was a boundary atom. The interior atoms, therefore can only relax under the constraint of the system size being held fixed. This is the principal reason for the smaller displacement obtained relative to the stress boundary method. Correspondingly the strain is smaller in the interior, whereas at the boundary both methods gave essentially the same value.

The stress distribution obtained with the fixed boundary method, shown in Fig.4.10(b), does not joint smoothly onto the boundary values at atom 10. Thus at the boundary (atom 10) we calculate a stress value using the procedure described in sec.2.6 and find it to be the same as the initial stress. The stress at atom 9 depends on the bond length between atoms 9 and 10, and since the strain in this bond decreases by virtue of the relax-
ation (system expansion) the stress also decreases. This effect is an unsatisfactory consequence of the fixed boundary method. At the opposite end one sees that even the initial stress distribution shows a maximum away from the crack tip. This behavior will be discussed in sec.4.10.

The comparison of the simulation results is given in Fig.4.11. The two boundary methods are seen to give very similar results. Since the two simulations were carried out at different stress intensity factors, \( K_I = 1K_{ic}^6 \) and \( 1.4K_{ic}^6 \) for the stress and fixed boundary methods respectively, one can conclude that using different methods at the same value of \( K_I \) would give quite different displacement, strain and stress distributions. It is reasonable that Fig.4.11(a) shows the stress boundary method to yield a somewhat more flexible system in the sense of greater displacements in the non-linear region around the crack, a behavior that is consistent with the lower stress values shown in Fig.11.(f).

The displacements and stress distributions along the x-direction, half way between the crack and the superior boundary, are given in table 4.3. One can determine the magnitude of the non-linear region from the deviations of the relaxed stress field relative to the linear elasticity solution, as will be discussed in more detail in sec.4.10. It is interesting to note in Table 4.3 that the relative change in stress is about three times smaller than the relative change in displacement. The fact that the stress distribution is more slowly varying in response to the non-linear effects suggests that it is better to assume a constant
4.11 Comparison of results in Fig.4.9 and Fig.4.10
<table>
<thead>
<tr>
<th>Atom</th>
<th>$V_\varepsilon$ (elastic) $\AA$</th>
<th>$V_r$ (relaxed) $\AA$</th>
<th>$\frac{V_r - V_\varepsilon}{V_\varepsilon}$</th>
<th>$\sigma_\varepsilon$ (elastic) x10^2 dynes/cm²</th>
<th>$\sigma_r$ (relaxed) dynes/cm²</th>
<th>$\frac{\sigma_\varepsilon - \sigma_r}{\sigma_\varepsilon}$</th>
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<tr>
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</tr>
<tr>
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</tr>
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Table 4.3  Displacements and stresses along line a-a' (see Fig.4.9) with atoms numbered from left to right. Stress boundary method. $K_f = K_{ic}$. 

-96-
stress at the boundary than a constant displacement.
4.8 Effects of Finite Simulation System Size

Since all MD simulations involve model systems of finite size, it is clearly important to have some appreciation of the effects associated with finite system size. In computer simulation studies this is commonly known as number dependence, with the implicit understanding that there is one-to-one correspondence between the number of particles in the simulation system and the system size. In this thesis we have consistently used $N$, the total number of particles simulated, to denote the system size.

There exists no general method of determining in any quantitative manner the size effects except for the empirical procedure of studying the variation in a particular quantity with $N$ as the simulation is repeated with several system sizes. If $N$ is such that the quantity no longer varies significantly with further increases in $N$, one can conclude that the simulation results are reliable so far as error due to number dependence is concerned. Since different properties can have different rates of convergence, clearly one has to be cautious in interpreting the results of $N$ dependence study.

We have examined $N$ dependence in the tensile stress along the y-direction and the crack tip bond length in the MD results obtained using the stress boundary method at subcritical values of stress intensity factor. Fig.4.13 shows the variation of with $N$ at positions close to the crack tip,1 and 2 (cf. Fig.4.8),
4.13 Variation of $\sigma_{yy}$ at two atom positions with simulation system size as represented by $N$, the number of particles in the system. Results are for stress boundary method at $K_1 = 0.8K_{1c}$ with initial configuration given the anisotropic linear elasticity solution. The $N$ values are 81, 144, 238, 442 and 673. (a) Stress $\sigma_{yy}$ at atom 1. (b) stress $\sigma_{yy}$ at atom 2 (see Fig. 4.8).
at $K_i=0.8K_{ic}^G$. The observed behavior can be understood on the basis that increasing the system size, when size effects cannot be ignored, reduces further non-linear relaxation. As one can see from Fig.4.9 the non-linear relaxation causes the tensile stress to decrease at particle 1 and to increase at particle 2. This behavior is shown in Fig.4.13. Notice that on the basis of these results one could infer that convergence has been effectively achieved for $N>238$.

It can be expected that number dependence will vary at different $K_i$ values. Intuitively one can anticipate that when $K_i$ is reduced, convergence will be obtained at smaller $N$. Fig.4.14 shows the change in crack tip bond length with $N$ at two $K_i$ values. The $K_i=0.8K_{ic}^G$ data also lead to the conclusion that systems with $N > 238$ are sufficiently large so far as number dependence is concerned. The interpretation of the decrease in crack tip bond length with increasing $N$ is that in small simulation systems one is applying forces derived from the linear elasticity theory at a distance close to the non-linear region. This has the effect, in the stress boundary method, of producing an excessive expansion of the system boundary and consequently the relaxed crack tip bond length is too large, favoring crack propagation. As the simulation system size increases, the boundary forces are applied at distances further away from the crack tip region. The effect of the expansion is reduced and consequently the crack tip bond length decreases. At the lower $K_i$ the data show essentially no variations with $N$. This implies that the non-linear region is sufficiently small that no unphysical effect
4.14 Variation of crack tip bond length with $N$ at two values of stress intensity factor, $K_1 = 0.8K_{ic}$ (open circles) and $K_1 = 0.5K_{ic}$ (closed circles). Stress boundary method.
is produced at these system sizes by applying the linear elasticity forces.

In the case of fixed boundary method, the number-dependent effects require a different interpretation. Because the boundary is not allowed to move, increasing $N$ will increase the extent of the non-linear region surrounding the crack tip. One then expects the crack tip bond length to increase with increasing $N$ until convergence is obtained. Previous MD simulation results (17) using both fixed and flexible boundary methods are in agreement with this interpretation, and they indicate the convergence is relatively much slower.
4.9 Test for Ductility of $\alpha$-Iron

In order to confirm our preceding results in sec. 4.5 which showed that $\alpha$-iron is brittle in the sense that crack propagation is not accompanied by dislocation emission, it is important to demonstrate that such dislocations are not emitted even with a model simulation system having an orientation that favors the emission of the dislocations. The Burgers vector of the dislocation should be along \{111\} direction since this is the close-packed direction in a b.c.c. structure. With our previous choice of system orientation (see Fig. 4.2) this vector would point out of the x-y plane. Now we want to choose an orientation such that the \{111\} direction lies in the x-y plane. We therefore choose x and y axis to be along [101] and [010] so that (101) is the x-y plane. The advantage of this model is the higher symmetry with respect to the cleavage plane (010), which gives greater stability against translation and rotation of the simulation system and also facilitates the visualization of any dislocation emitted.

The MD results corresponding to the case 6 in Table 4.1 are shown in Fig. 4.15. As before, we observed crack propagation at $K_t^c = K_t^{6c}$ and the cleavage plane is (010). The fact that the cleavage plane always turns out to be (010) in the present simulations (simulations 6, 7, and 8) suggests that symmetry effects are more important in determining cleavage plane than the type of linear solution applied. None of the simulations showed any dislocation emission which reinforces our foregoing conclusion that $\alpha$-iron is
4.15 MD simulation of a crack system oriented with x and y axis along [101] and [010] respectively (case no. 6 in Table 4.1), (a) configuration just prior to the onset of crack propagation, (b) configuration during crack propagation, (c) displacement field of configuration shown in (a).
brittle. However, the present simulation did reveal an interesting deformation which indicates that twinning has occurred in the non-linear crack tip region.

Fig.4.16 shows the same MD configuration as Fig.4.15(a) but with some of the nearest neighbor bonds outlined to show the difference in "cell" rotation. The region of twinning is indicated by the cross-hatched cells. The twinning direction is [111], the direction along which atoms move in order to form a new region with the same lattice structure but different orientation. The twinning plane, plane that separates the two crystals, is the plane (112) in agreement with experimental results. In experimental studies by high resolution electron microscopy, thin twins generated by cracks have been observed in b.c.c. materials (molybdenum). These experiments, nevertheless, were conducted under a different state of stress (18).
4.16 Configuration of crack system, Fig.4.15(a), with dashed lines drawn along some of the nearest neighbor bonds to show the region of twinning in the upper half of the simulation system. Line a-a' indicates the direction [111], the direction of twinning.
4.10 Stress and Displacement Field in the Crack Tip Region

In section 2.6 we have explained the procedure to calculate the stress at any atomic position given the position of its neighbors. This was called the atomic stress in contrast to the continuum stress given by the linear elasticity theory. One can evaluate the atomic stress using the initial configuration given by the linear elasticity theory, and the result will not be the same as the continuum stress if the stress is too high. The difference is due to the non-linearity of the interatomic force and was discussed in sec. 2.6.

The stress distribution of the relaxed crack configuration was first discussed in section 4.7 in connection with the effects of different boundary methods. Here we will consider additional simulation results on stress and displacement fields along different directions and at different stress intensity factors. Fig. 4.17 shows the stress field of the relaxed configuration obtained using the atomic stress method. The stress intensity factor applied was $0.8K_c$. Comparing this result with Fig. 2.8, the atomic stress field for the atomic configuration one can see the most pronounced effects of non-linear relaxation occur in the change of the tensile stress along the $45^\circ$ direction. Immediately in front of the crack the stress decreased and after three interatomic distances it increased rather suddenly. Near the boundary of the simulation system the stress remained essentially unchanged.

Quantitative changes in the displacement and stress
Principal stresses in α-iron at $K_f = 0.8K_f^c$. Arrows indicate tension and bars indicate compression. Results were obtained using the relaxed configuration after application of the stress boundary method.
distributions along 90°, 45°, and 0° directions are shown in Figs. 4.18, 4.19 and 4.20. Three stress intensity factors, 0.5, 0.8 and 1.2 $K_{Ic}$ were examined in each case. At 90° the results at $K_I = 1.0K_{Ic}$ were shown in Fig.4.9 and discussed in sec.4.7. The present results at $K_I = 0.8K_{Ic}$ show the same features. At $K_I = 0.5K_{Ic}$ the effects of non-linear relaxation are quite small, as we might expect. The results at $K_I = 1.2K_{Ic}$ show dynamic effects since at this stress intensity factor the crack is propagating.

Along the 45° direction the results at $K_I = 0.5K_{Ic}$ show essentially no effects of the relaxation in the displacement distribution, but there was an increase in the stress in the region close to the crack tip. At $K_I = 0.8K_{Ic}$ one sees clearly the changes noted in Fig.4.17, that is, the relaxed stress distribution near the crack tip was considerably reduced relative to its value for the initial configuration, and after three interatomic distances it increased sharply. At the transition the displacement field went from a contraction to an expansion. Again there are transient effects at $K_I = 1.2K_{Ic}$. They might be relevant in a study of dynamical effects of crack propagation.

Along the 0° degree direction all the effects are small by comparison with the results for the other two directions. The displacements fields along the crack surface are shown in this case, and we can see a significant crack expansion at $K_I = 1.2K_{Ic}$.

-111-
4.18 Displacement and stress distributions along 90° direction (y-axis) in simulation of α-iron at three stress intensity factors, (a) $K_I = 0.5K_{IC}$, (b) $K_I = 0.8K_{IC}$, (c) $K_I = 1.2K_{IC}$. Same condition as in Fig. 4.9. Open circles denote results obtained using the initial configuration and close circles correspond to the relaxed configuration.
Fig. 4.18 b
Fig. 4.18 c
4.19  Same as Fig.4.18 except the direction is along 45°.
4.20 Same as Fig. 4.18 except the direction is along 0°. Three additional atom positions shown refer to the surface of the crack.
Fig. 4.20 b
Fig. 4.20c
Chapter Five
Simulation of Ductile Materials-
Results for Copper

5.1 Simulation of F.C.C. Materials - Atomic Model.
5.2 Nucleation of Dislocations at the Crack Tip.
5.3 Crack Tip Structure in Ductile Materials.
A fundamental understanding of the process of fracture propagation in ductile metals requires consideration of a very complex elastic-plastic problem. One major source of difficulty in the analysis of the problem is that large changes in boundary configuration accompany dislocation emission from the crack and any nearby growing cavities. Another difficulty, particularly in the case of semibrittle materials, is that the yielding can be too anisotropic and non-uniform for a continuum plasticity theory to be applicable. Zones of diffuse yielding, spreading over many grains, are frequently observed, and for such cases the application of continuum plasticity theory with the help of a finite element computational method is probably the best approach. However, finite element methods have difficulty in handling cases where the yield spreads in thin bands. Several treatments have been made of the spread of yield in thin bands. The best known is that of Bilby, Cottrell and Swinden (BCS), which is based on yield zones coplanar with the crack, and is carried through analytically. All of these models have neglected the effects of crack blunting. They may therefore, successfully predict properties depending mainly on the long range stress field of the crack, such as the yielded zone size and the total plastic crack opening. However, if dislocation nucleation at the crack tip is subject to some barrier, or if it is desired to study the crack propagation process, then it must be necessary to find those details of the stress and strain fields which depend critically on the blunted crack profile.

In relation to the problems just mentioned we have stud-
ied the behavior of a ductile material, copper, paying special attention to the specific features provided by MD simulation: atomic configuration of the crack tip during the nucleation of dislocations and shape and structure of the crack tip after the crack is blunted by dislocation emission. In these studies in addition to the atomistic processes observed by MD simulation, we have tried to relate the results of our simulations to experimental data and macroscopic theories (4,5,6).
5.1 Simulation of F.C.C. Materials-Atomic Model.

The system to be studied is composed of copper atoms interacting through a Morse potential, section 2.2. As in the case of b.c.c. materials an understanding of the effect of lattice structure on the mechanical properties of f.c.c. materials is essential to selecting an appropriate atomic orientation for the crack tip.

In the f.c.c. structure the close-packed directions are the <110> directions. These are the directions that run diagonally across the faces of the unit cell, Fig.5.1. There are four planes in the face-centered cubic lattice, called octahedral planes, with indices (111),(111),(111), and (111). Each octahedral plane contains three close-packed directions, therefore, the total number of octahedral slip systems is 4x3=12. The only important slip systems in the face-centered cubic structure are those on the octahedral plane. There are several reasons for this. First, slip can occur much more easily between close-packed planes than between planes of lower atomic density; that is, the critical resolved shear stress for slip between octahedral planes is lower than for other planes. Second, there are twelve different ways that octahedral slip can occur, and the twelve slip systems are well distributed in the space. It is therefore almost impossible to strain a face-centered cubic crystal and not have at least one {111} plane in a favorable position for slip.

With these features in mind we have selected the atomic ar-
5.1 Face-centered cubic cell. Dashed lines correspond to directions of minimum shear stress, \(<\overline{112}\>). Point 0 lies at the center of the triangle formed by sites 2, 7, and 9 which are on a close-packed plane \((111)\).
rangement for the crack tip that most facilitates the observation of dislocations, given that emission is highly probable under any orientation. Fig.5.2 shows the lattice structure of a f.c.c. material looking at the unit cell from the direction [101]. Two atomic layers have been drawn. Periodic boundary conditions are applied along the z-direction. The crack has been incorporated into the system by placing the crack front along the z-direction, Fig.5.3a, and the crack tip at an intermediate point between particles 5 and 8, Fig 5.3b.

In the next section we study this atomic model with two different types of boundary conditions. In the first case, a somewhat unrealistic case, an uniform tensile stress was applied to the system. Given that the stress at the boundary does not represent exactly the stress field when the crack is surrounded by large amount of material, section 2.4, we applied in a second simulation the stress boundary method.
5.2 Two adjacent (101) planes in a f.c.c. structure as viewed along [101]. Lattice sites are numbered according to Fig.5.1, close and open circles denote sites on different planes. Coordinate system shown is the one used in this chapter.
5.3 Initial crack tip configuration in simulation of copper, (a) Lateral view showing orientation of the crack front. (b) Crack tip location in the coordinate system indicated in Fig.5.2. X indicates location of the crack tip.
5.2 Nucleation of Dislocations at the Crack Tip.

Despite the lack of direct experimental evidence about core structure of dislocations and atomic motions during nucleation and propagation of dislocations, it is known (2) that in f.c.c. materials the Burgers vector of a 1/2 [011] dislocation can be decomposed in two parts, corresponding to two partial dislocations, according to the reaction, Fig.5.4,

\[ \frac{1}{2} (011) = \frac{1}{6} (11\bar{2}) + \frac{1}{6} (12\bar{1}) \]  \hspace{1cm} (5-1)

with the two Burgers vectors of the partial dislocations lying along the direction of minimum shear stress (directions \( \langle 11\bar{2} \rangle \) and planes \( \{111\} \), \( \tau_{\text{com}} = 0.012 \cdot 10^6 \) dynes/cm² (3)), Fig.5.1. The atomic positions corresponding to the initial configuration of the crack tip and unit cell of the face-centered cubic structure have been numbered consistently in all the figures of this section to facilitate their comparison under different orientations. The generation and motion of a dislocation in face-centered cubic structures does not occur in the simple manner described in other lattice structures. As it can be deduced with the aid of a ping-pong ball model of the atomic arrangements, Fig.5.4, a zig-zag motion of atoms demands less lattice strain.

Next, we show the results of our simulations on face-centered cubic structures of ductile materials, where the characteristics of partial dislocations described above are observed by MD simulation.
5.4 Two atomic layers with sites numbered according to Fig. 5.1 showing the directions of minimum shear stress and the relationship between a dislocation with Burgers vector $b = 1/2[01\overline{1}]$ and its two partial dislocations with Burgers vectors $b_1 = 1/6[\overline{1}12]$ and $b_2 = 1/6[12\overline{1}]$.
We have performed the simulation of ductile fracture with the atomic model described in the previous section, Fig.5.3b. The crack was formed by a layer of vacancies. The atomic system was pulled apart by a uniform tensile stress applied at the horizontal borders of the system. No stress was applied to the left and right vertical borders. Later on we found similar results with another system where the crack was assumed to be surrounded by an infinite amount of material. In this case, we applied the stress boundary method.

Fig.5.5a shows the configuration of the crack tip for $k=5.00 \times 10^7$ dynes·cm$^{-2}$. This configuration has been obtained after applying the relaxation method described in section 2.5. At this stage of the simulation the system is thermally agitated by introducing a Maxwellian distribution of velocities to the particles, $T=300^\circ$K. In agreement with the directions indicated previously the generation of the first partial dislocation occurs in the direction $(\bar{1}1\bar{2})$,7=0, Fig.5.5b. In this case particle 7 and all its images (for instance, particle 9) jump simultaneously in this direction (periodic boundary condition along the z-direction). The compression against the next row (particle 2 and its images) causes the nucleation of the first partial dislocation. When the dislocation moves ahead, subsequent atomic rows are forced to make the same type of motion. Fig.5.5b shows the nucleation and subsequent propagation of the first partial dislocation. In this case atomic displacements in the direction $(\bar{1}1\bar{2})$ has already taken place in the next rows of particles (indicated by arrows), and the partial dislocation has reached point A. The
generation of the second partial dislocation can be observed in Fig. 5.5c. This motion is entirely contained in the plane \(x-y\), and the direction is \((12\bar{1})\), in agreement with reaction (5-1). This second jump restores the original lattice structure after the dislocation has passed through. The second partial dislocation is located at position B in Fig. 5.5c, and remains separated from the first partial dislocation at position A. After the two dislocations have passed, shear deformation by an amount equal to a complete nearest neighbor separation has taken place in the material left behind. The two partial dislocations define what is called an "extended dislocation". We have determined the total Burgers vector of the extended dislocation. As can be seen in Fig. 5.5c, the total Burgers vector after the emission of the two partial dislocations is equal to the vector \(7-2\) which does not lie inside the plane \(x-y\). The Burgers vector indicates the strength and direction of the shear after the passing of the dislocation. The dislocations travel to the boundary of the simulation system where they give rise to a ledge structure, Fig. 5.5d. In the case of a very large system the dislocations would continue to travel until they are stopped by lattice friction (Peierls barrier).

We have shown thus far the results corresponding to a microscopic crack formed by a layer of vacancies obtained by applying a uniform stress at the boundary. We have also carried out a simulation of a smaller system (200 particles) using the stress boundary method. The results showed essentially the same behavior as observed in Fig. 5.5, but subsequent generation of
5.5 Atomic configurations of a crack in copper obtained by MD simulation, showing the emission of partial dislocations. Only the upper half of the system is shown since the system is assumed to be symmetric about the x-axis. (a) Initial configuration after static relaxation, t=0, (b) t=500\Delta t, (c) t=550\Delta t, (d) t=600\Delta t, where \Delta t=10^{-9} \text{ sec.}
dislocations and a more complete analysis of the structure of the crack tip has been performed.

In all our studies of copper a dynamic simulation was necessary in order to obtain the right type of behavior for the material. At 0°K the only possible displacement is by symmetry inside the plane x-y, (101) plane, which is the plane imposed by the exterior forces. For a realistic simulation motion outside the plane (101) must be allowed. In order to permit such displacements, a Maxwellian distribution of velocities, corresponding to certain temperature T, was assigned to the particles of the system after the system has reached a position of static equilibrium, (section 2.5). The introduction of a temperature in the system allowed displacements out of of the plane x-y, which were necessary to nucleate the first partial dislocation, (jump from position 7 to position 0). To observe the emission of this dislocation certain waiting time was necessary. The reason is that this process only occurred when all the atoms lying along the z-direction jumped simultaneously. In the case of a system with periodic boundary conditions and only two atomic layers along the z-direction this time was reduced. Only a few hundred time steps and low temperatures, about 100°K, were necessary in order to observe this process. The second partial dislocation was emitted right after the emission of the first one and required less energy to be nucleated for lying the direction of the jump inside the plane favored by the exterior stress (plane x-y). To make a realistic dynamic simulation of what happens in real materials at high temperatures, which would include the cre-
ation of dislocation loops by thermal effects, it would be neces-
sary to increase the number of layers of the system along the
z-direction and wait for a time long enough such that this proc-
ess can be observed. These two factors impose a severe limitation
in the simulation because they greatly increase the computing
cost. We have studied our quasi three-dimensional model because
it reflects the behavior of real materials at low temperatures
(symmetry along the z-direction).
5.3 Crack Tip Structure in Ductile Materials

In this section we shall show the results on copper obtained by using the stress boundary method. As we have indicated before, the simulations were performed at progressively higher stresses until either emission of dislocations or crack propagation was observed. After the static configuration was obtained by the relaxation method described in section 2.5, the system was agitated thermally to allow atomic displacements out of the x-y plane. The method thus permitted the observation of crack blunting by the emission of partial dislocations.

Figs. 5.6 shows the atomic configurations and displacement fields surrounding a crack tip at various stages of the simulation. Fig. 5.6a shows the initial static configuration at $0^\circ$K, $K_1 = 4.30 \times 10^7$ dynes/cm$^{3/2}$. The crack remains sharp because the particles are unable to move out of the x-y plane. When thermal motions are introduced ($T=300^\circ$K) the crack tip is blunted by the emission of partial dislocations in the way described in section 5.2, along the slip planes $\{111\}$ and slip directions $<11\bar{2}>$. Figs. 5.6b and c show the atomic structure and displacement field after 1000 time steps (time step=1.00 $10^{-14}$ sec.). Certain waiting time, larger than in the case with uniform stress, was necessary in order to observe the emission of the first partial dislocation. Emission has taken place by shearing of the planes c-c' and e-e', and each dislocation gives rise to a ledge structure at the boundary. Also shear deformation along other planes has been observed, row g-g'. As the simulation continues, the
5.6 Atomic configuration of a crack in copper, obtained by MD simulation using the stress boundary method, showing crack tip blunting. (a) Initial configuration after relaxation $t=0$, (b) configuration at $t=1000\Delta t$ and corresponding displacement field, (c) $t=1050\Delta t$ and corresponding displacement field, where $\Delta t=1.0\times10^{-14}$ sec.
crack is blunted by emission of dislocations on other \{111\} planes. Fig. 5.6d and e show the crack tip structure and displacements after 1050 time steps. Slip has occurred also on row b-b, Fig. 5.6d. All the slip planes intersect the apex of the crack tip and leave a net crack opening equal to the sum of the Burgers vectors of all the dislocations emitted from the crack. The final crack configuration takes a V-shaped tip, flat on the tip facets, and leaving a slip-free triangular region in front of the crack tip. At this stage, we have interrupted the simulation because the boundary has been deformed by the ledges left by the dislocations and the elasticity solution must be a poor approximation for the stresses at the boundary.

In order to study the effect of the size of the system on the crack tip structure, we have performed similar simulations with a system composed of 400 particles. Fig. 5.7 shows the blunting of the crack tip and the dislocation emitted. The further simulation was continued for 200 time steps. Due to the distortion of the boundary it was difficult to make further assumptions about the shape and behavior of the crack tip at this stage of the simulation.

Further study of the distribution of dislocations around the crack tip would involve larger models including regions where dislocations are stopped by the Peierls barrier. These studies impose limitations to our MD simulations due to the atomic dimensions of the crack tip. The structure and shape of the crack tip, and form in which dislocations are emitted resemble the structure found in several analytical and experimental
5.7 Atomic configuration of a crack tip in copper obtained by MD simulation. Same conditions as Fig. 5.6 except \( N = 359 \). (a) Configuration before blunting \( t = 1000 \Delta t \), (b) Configuration at \( t = 1050 \Delta t \), the crack tip has been blunted by emission of a dislocation. \( \Delta t = 10^{-11} \) sec.
studies of fracture in ductile materials. For example, Sinclair (4), using computer methods to solve the crack blunting problem with realistic dislocation assumptions, shows the same crack tip shape, Fig.5.5. Newmann (5), has demonstrated in cyclically loaded single crystals of copper how a crack aligned in the same orientation can blunt, during the tensile cycles, into a notch with a V-shaped tip, macroscopically flat on the tip facets. Further studies with high resolution electron microscopy, as the work done by Ohr (6), could provide a definitive experimental verification of the atomic features observed by MD simulation.
Chapter Six. Conclusions
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The fundamental atomic processes responsible for fracture behavior in semibrittle materials $\alpha$-iron and ductile materials Cu have been studied by MD simulation.

The simulations have been performed under realistic conditions: three dimensional systems, appropriate potential functions for each material, and a boundary method that allows a correct treatment of the highly stressed non-linear region surrounding the crack tip.

A new boundary method has been developed for the atomic simulation of fracture mechanics. With the use of this method the problems of previous simulations have been resolved, namely, large deviations from Griffith theory in the case of brittle materials and constraint against the emission of dislocations in the case of ductile behavior. The method has allowed a realistic simulation of real materials: confirmation of Griffith theory by MD simulation, the observation of the correct cleavage plane during crack propagation in $\alpha$-iron, and the nucleation of dislocations in copper along the directions of minimum shear stress.

The atomic structure around the crack tip was also studied. In the case of $\alpha$-iron a small amount of plastic deformation by twinning was observed. The analysis of the non-linear stress field has been performed by applying a new method that determines the stress tensor at each atomic position. These studies are the first simulations of ductile fracture in discrete models of real materials.
Given that only the potential function and lattice structure determine the mechanical properties of the material, it is important to select appropriate potential functions which reproduce the most important experimental data in fracture mechanics. While the potential functions applied in our simulations reproduce satisfactorily experimental values of several physical constants at small deformations, i.e. elastic constants, equation of state, vaporization energy, it is necessary to confirm the validity of the potential at large deformations. In future work studies of perfect crystals under different states of stress, (section 4.3 ref.10), should be performed by applying a Lagrangian formalism. This method allows changes in the volume of the system while still maintaining periodic boundary conditions and will permit the simulation of large deformations without surface effects.

In simulation of fracture there are properties that are especially significant: ideal cohesive stress, ideal shear stress, surface energy and stacking-fault energy. Given the lack of experimental results for the ideal stresses and uncertainties in the values of such surfaces energies, it is impossible to make further statements about the accuracy of the potential functions that we have applied in simulation of fracture. We expect that in the future more accurate experimental values of these constants and better potential functions derived from them can be incorporated in the present method of simulation.

The size of the system is limited by finite computer memory to a few hundred particles and only allows one to observe the
crack tip behavior during the first stages of crack propagation or crack blunting. During these first moments, however, the atomic structure plays an important role. We have observed atomic processes in our simulations, i.e. nucleation of twinning in α-iron, that will require experimental confirmation in the future by high resolution techniques, such as the work performed by Ohr applying electron microscopy (sec.5.3).

Further studies, including dynamic effects, would not involve too much effort after an appropriate simulation method has been established. For example, dynamic effects could be of importance during crack propagation. We have observed that the kinetic energy after a crack has started to propagate is concentrated around the crack tip and seems to favor the breaking of other atomic bonds. In this case normal modes of vibration localized around the crack tip could play an important role. Also the dynamic effects due to a finite temperature have not been included in this model. If all these effects were studied using the atomic model and boundary condition we have proposed, a great deal of new information about atomic effects in fracture of real materials could be obtained from MD simulations.
References

Chapter One


Chapter Two


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Chapter Three

Chapter Four

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Chapter Five


