4.4 Shielding

When the cracks are not loaded until the plastic deformation occurs, the dislocation emission response caused by the deformation is not observed on the crack tip. No dislocation presence means that the total local stress intensity factor k (Equation 2.11) does not reach the critical stress intensity factor for dislocation emission. Since there is no dislocation at the vicinity of the crack tip up to the critical value, k^D (Equation 2.9) is equal to zero and consequently, the applied stress intensity factor K is equal to k.

The first dislocation is generated when the stress on it from the crack tip field exceeds the image stress as shown in Figure 4.1 (a) and (a'). The net stress is sufficient to move the dislocation away from the crack tip until the force on it is balanced by the lattice frictional force. After being emitted from the crack tip, it interacts elastically with the cracks, and, as a consequence, the stress field around the cracks is modified. Once emitted, the dislocation exerts a back stress (Equation 2.5) on the source (the crack tip), and the stress on the sources is decreased by the back stress of the dislocation. Therefore, the local stress intensity factor is no longer equal to the applied stress intensity factor because $k^D \neq 0$. This decrease in the local stress intensity factor caused by the dislocation is called dislocation shielding of the crack tip from the applied stress.

As the applied stress intensity factor is increased in order for the source to operate again, one of two different responses is observed: farther movement of the first dislocation or the emission of a second dislocation from the crack tip, under the net force (including the back stress from the first dislocation). In the former case, the dislocation travels farther away from the crack tip (Figure 4.1 (b)) although it contradicts one of the characteristics of a mode I crack pointed out by Cottrell [52]: fresh dislocations must be generated at the crack tip in order to provide the crack opening displacement if a crack propagates by plastic deformation. In this case, the increasing of the applied stress intensity factor is not enough to cause the crack tip further emission. In other words, the total local stress intensity factor cannot reach the critical value for further emission. However, the crack force increases, which exerts a repulsive force on the dislocation, and thus it drives the first dislocation farther away from the crack tip. Consequently, the total local stress intensity factor on the crack tip increases gradually while the shielding effect of the first dislocation decreases, because the back stress of the dislocation is inversely proportional to its distance r from the crack tip, namely $1/r$. In this case, generally the crack tip shows the latter response as shown in Figure 4.1 (c), the second dislocation emission, when the applied stress intensity factor is increased again. In the latter case, emission of the second dislocation (Figure 4.1 (b')), the increase is enough to cause further emission. Again, the crack force increases and causes not only the second dislocation to emit and move away from the crack tip, but also the first dislocation to travel farther away. In this case the first dislocation moves slowly, and thus the traveling distance is smaller than that of the former case. As a result, the shielding effect of the first dislocation decreases again, but not as much as the former case. The total shielding, which is the sum of the first and the second dislocation increases slightly.

As the applied force is raised, more dislocations are generated from the crack tip, and the dislocation density is higher near the crack tip and decreases away from the crack tip. After a certain number of dislocations are emitted, the emission stops because of the shielding effect of the already nucleated dislocations. The ceasing of the dislocation emission is followed immediately by the brittle crack propagation.

In the simulation, the crack tip can generate no dislocation for a few steps of loading because the loading is not enough to cause the crack tip to emit dislocations. Figure 4.2 shows the total local stress intensity factor k versus the applied stress intensity factor K. The calculation of the total local stress intensity factor is carried out using Equations 2.11. The dashed line indicates no dislocation at the vicinity of the crack tip. The total local stress intensity factor k suddenly decreases when the applied stress intensity factor reaches $0.2\,eV(\overset{0}{A})^{-2.5}$ at which the first dislocation is generated, and it shields the cracks. As the loading is increased, the rate of decrease at the total local stress intensity factor increases slightly.

4.5 Pinning Distance

When a dislocation is generated from a crack tip, it advances away from the crack tip until the force on it is balanced with the lattice frictional force or it is stopped earlier by imperfections.

The first dislocation emitted is always the farthest from the crack tip (Figure 4.3 (a)) because at every loading step, it is affected by the net force that drives it far from the crack tip. In the simulation, the first dislocation, except the case of the 400,000 atoms size, is hindered by the fixed boundary condition of the model (Figure 4.3), which, in effect, acts like a rigid layer. This distance where the dislocation is stopped is effectively a *pinning distance*.

For the size of 400,000 atoms, there is no pinning effect and the first dislocation moves away from the crack tip to its equilibrium distance about $530A^o$. The crack propagates before the dislocation reaches the fixed boundary because the emitted dislocations suppress continued nucleation and favor a transition to cleavage. This result agrees with a Peierls type model [42] in which the dislocations within 10-100nm of the crack tip may prevent further emission of the dislocation and favor a transition to cleavage.

When dislocations do not travel away from a crack tip, dislocation shielding can eventually become strong enough to prevent further emissions because it is inversely proportion to the square root of the distance r, and it causes the crack to resume brittle propagation. Therefore, pinning distances, where the dislocations are stopped, play an important role in brittle propagation of cracks and the number of dislocations emitted. As pinning distances are enlarged, dislocation shielding becomes smaller and, if enlargement is enough, the shielding cannot prevent further emission. Therefore, it is necessary to increase applied stresses to observe the cleavage propagation.

The applied stress intensity factor (K) required to propagate the crack tip increases at first and then remains basically constant as the maximum distance that the first dislocation can move away from the crack tip increases, as shown in Figure 4.4. Probably, this behavior is due to dislocation shielding. The maximum distance of the emitted dislocations from the crack tip is the equilibrium distance for the case of the 400000-atom size. For the smaller computational blocks, the emitted dislocations are stopped by the fixed boundary, and hence the maximum distance of the emitted dislocations is equal to the pinning distances. On the other hand, the total local stress intensity factor at the crack tip k (Equation 2.11), and the local stress intensity factor along the slip plane K_{IIslip} (Equation 2.13) remain basically constant as the maximum distances of dislocations are farther from the crack tip as shown in Figure 4.4. For distances larger than $300 A^o$, the local stress intensity factor starts to increase slightly.

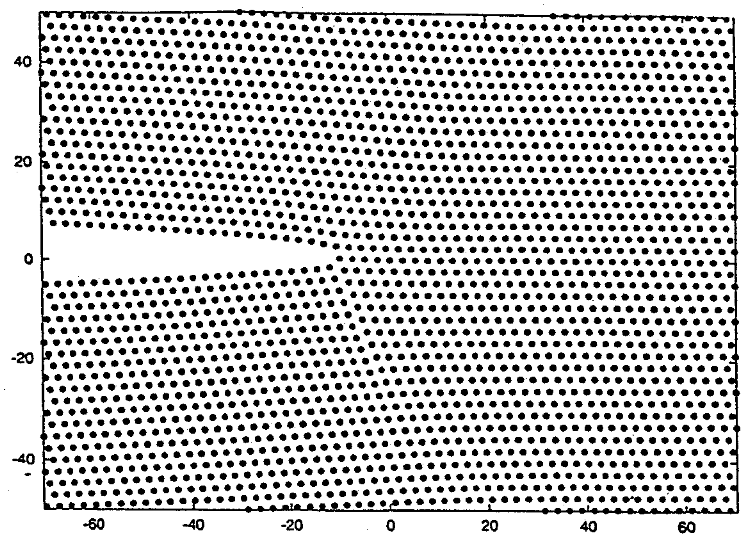
The applied stress intensity factor (K), the local stress intensity factor at the crack tip (k), and the local stress intensity factor along the slip plane (K_{IIslip}) versus the number of dislocations emitted at failure for all sizes are given in Figure 4.5. As the number of dislocations emitted increase, the applied stress intensity factor required to propagate the crack tip increases at first, and then becomes constant. On the other hand, both local stress intensity factors remain basically constant up to 12 dislocations, and then they begin to increase slightly.

The observed applied stress intensity factor at the crack tip and the total local stress intensity factor (in Figures 4.4 and 4.5) are larger than the Griffith value, because of the shielding that is induced by the distribution on the inclined plane. Equivalently, the larger local stress intensity factor is required since available work supplied by the applied stress intensity factor is partitioned between creation of a nonlinear core on the inclined plane and the cracks advance on the 0^o plane.

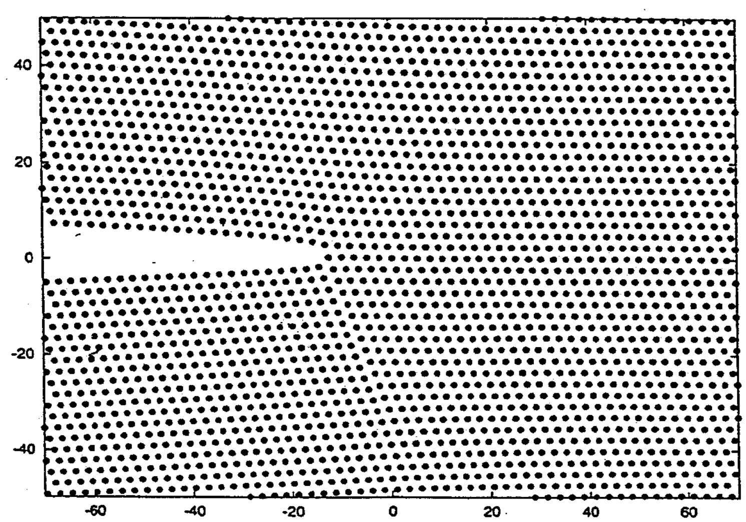
It is also clear that the total local stress intensity factor at the crack tip remains more than the local stress intensity factor along the slip plane as the number of dislocations continue to increase. Thus it can be concluded that dislocation nucleation is the preferred response to the applied stress. Consequently, the material showing such a behavior is classified as intrinsically ductile.

The effect of the maximum distance on the number of dislocations emitted is given in Figure 4.6. The number of dislocations generated increase rapidly at first and then more slowly when the maximum distance of the emitted dislocations increases. The reason of this behavior may be due to dislocation shielding and crack blunting.

It can be concluded that if there are some imperfections in a real material, which are near to a crack tip, they stop the movement of dislocations, and hence the shielding becomes strong enough to prevent further dislocation emission. Therefore, it causes the crack tip to resume brittle propagation.

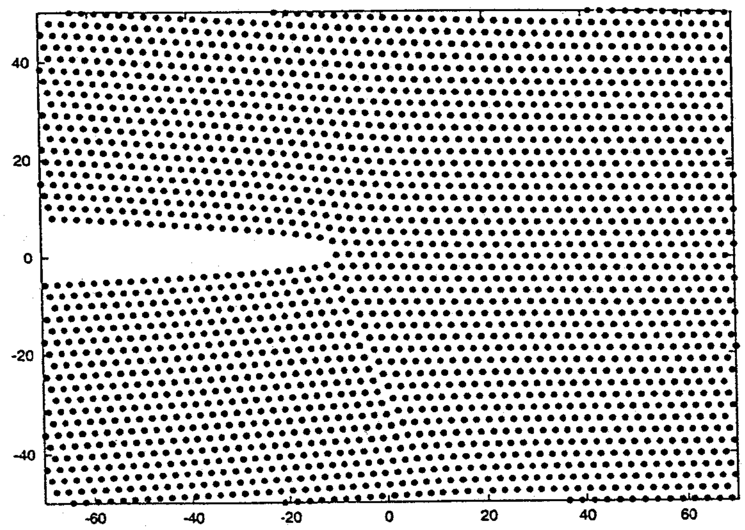


(a) The first dislocation is emitted at $K = 0.2\ eV(\mathring{A})^{-2.5}$ for the size of 18,000 atoms. The crack is blunted by the dislocation.

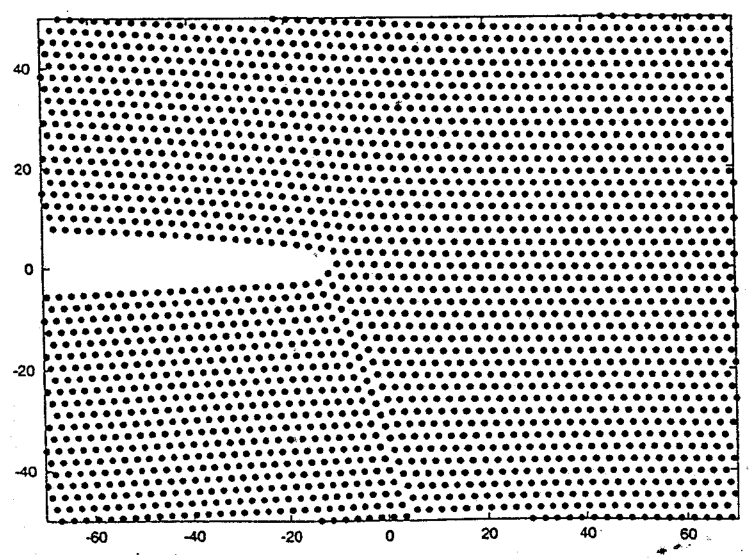


(a') The first dislocation is emitted at $K = 0.2\ eV(\mathring{A})^{-2.5}$ for the size of 33000 atoms. The dislocation blunts the crack tip.

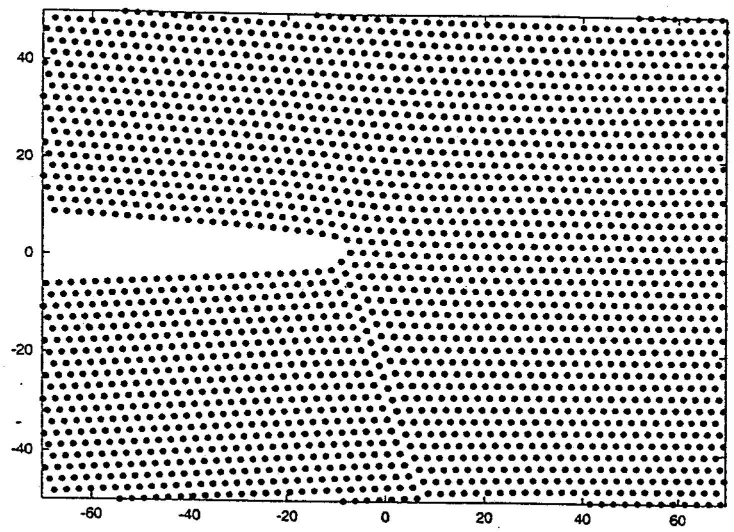
Figure 4.1 Some steps of two different simulation blocks: 18000 and 33000 atoms.



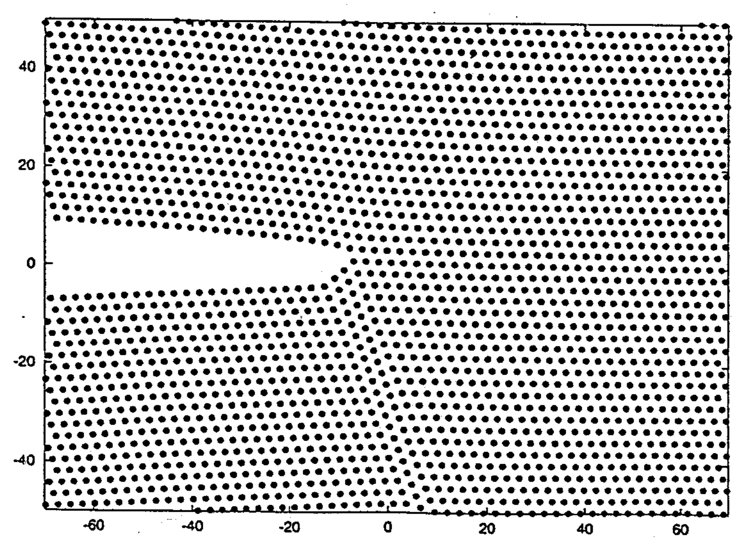
(b) Farther movement of the first dislocation at $K = 0.225\ eV(\mathring{A})^{-2.5}$ (18000 Atoms).



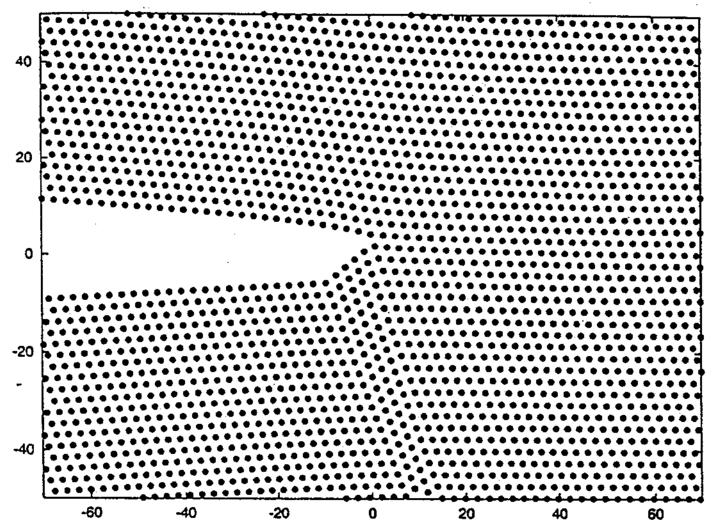
(b') The second dislocation is emitted at $K = 0.225\ eV(\mathring{A})^{-2.5}$ (33000 Atoms). The geometry of the crack is shaped as a blunted crack with a sharp corner.



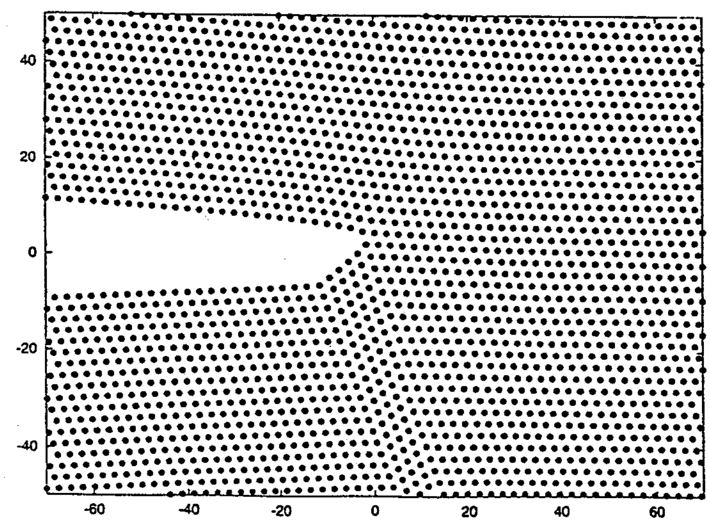
(c) The second dislocation is emitted at $K = 0.25\ eV(\mathring{A})^{-2.5}$ (18000 Atoms). The crack becomes a blunted crack with a sharp corner.



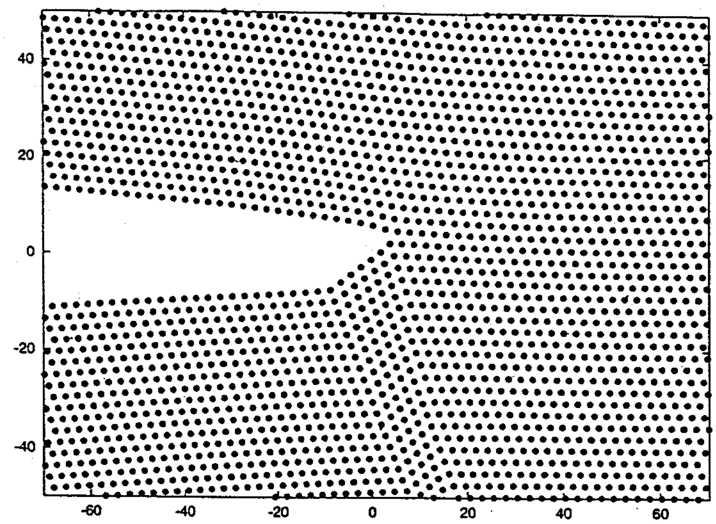
(c') The dislocation emission continues at $K = 0.275\ eV(\mathring{A})^{-2.5}$ (33000 Atoms).



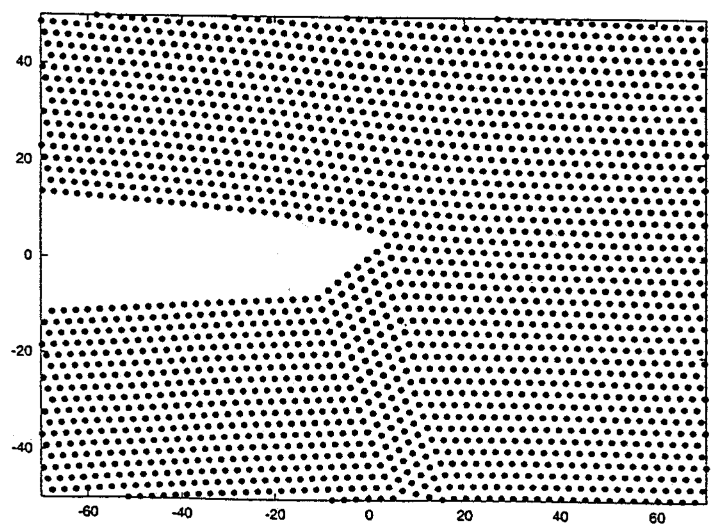
(d) The dislocation emission continues at $K = 0.35\ eV(\overset{0}{A})^{-2.5}$ (18000 Atoms).



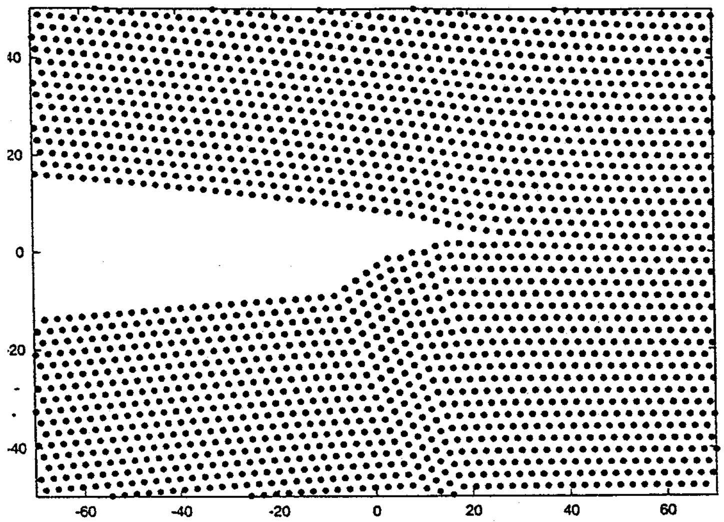
(d') The dislocation emission continues at $K = 0.35\ eV(\overset{0}{A})^{-2.5}$ (33000 Atoms).



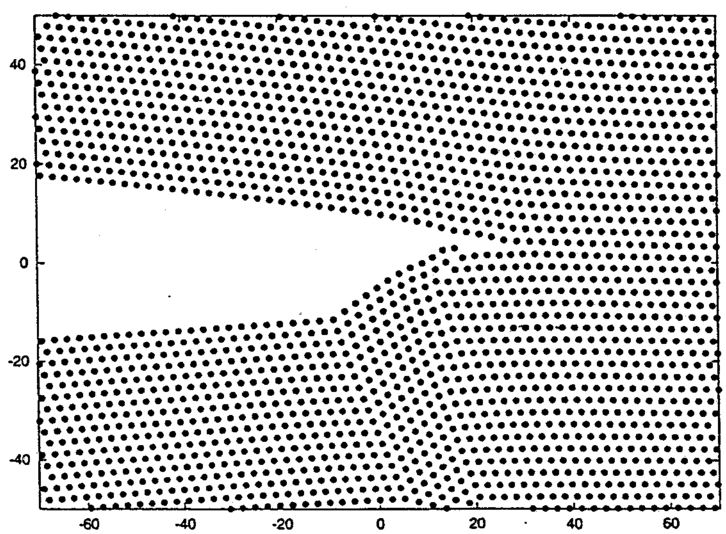
(e) The dislocation emission continues at $K = 0.425\ eV(\overset{0}{A})^{-2.5}$ (18000 Atoms).



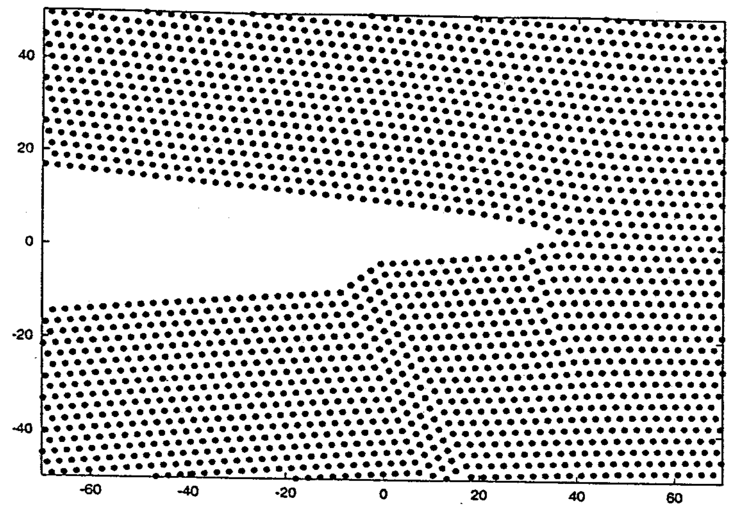
(e') The dislocation emission continues at $K = 0.425\ eV(\overset{0}{A})^{-2.5}$ (33000 Atoms).



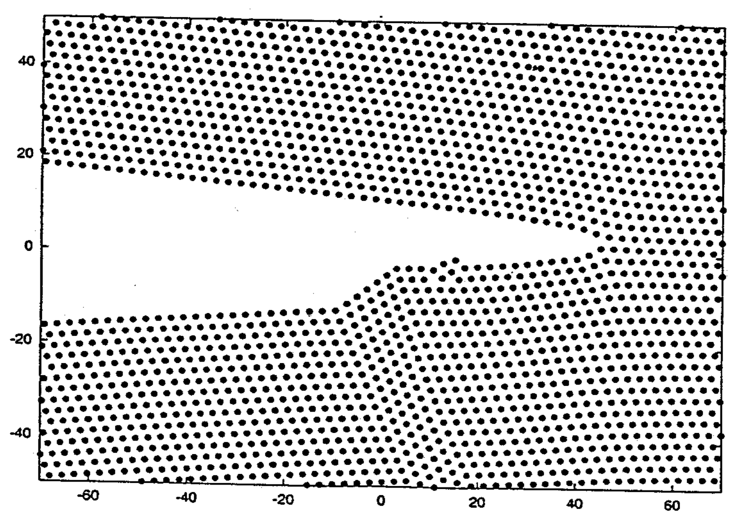
(f) The crack just starts the propagation at $K = 0.525\ eV(\overset{0}{A})^{-2.5}$ (18000 atoms)



(f') Before the crack propagates at $K = 0.575\ eV(\overset{0}{A})^{-2.5}$ (33000 atoms).



(g) The crack propagates. The dislocations emitted nearer to the crack tip come back. After propagating forward a short distances, the crack tip emits dislocations (18000 atoms).



(g') The crack propagates. The dislocations nearer to the crack come back. The dislocations are emitted on the parallel slip plane after the crack propagates forward (33000 atoms).

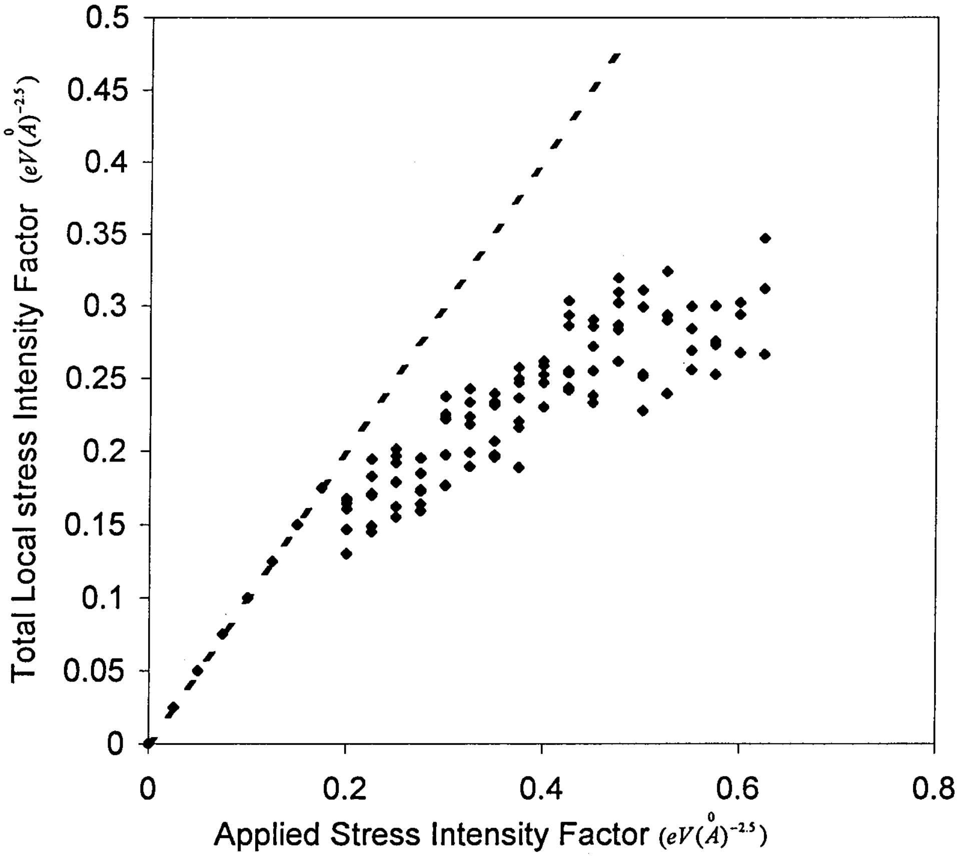
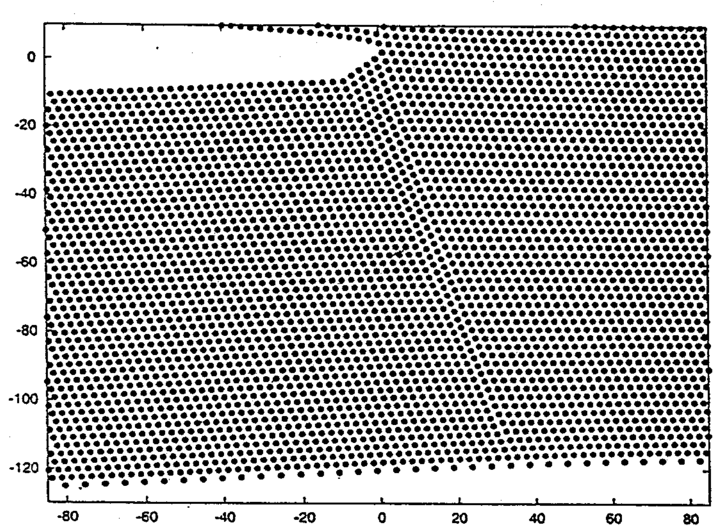
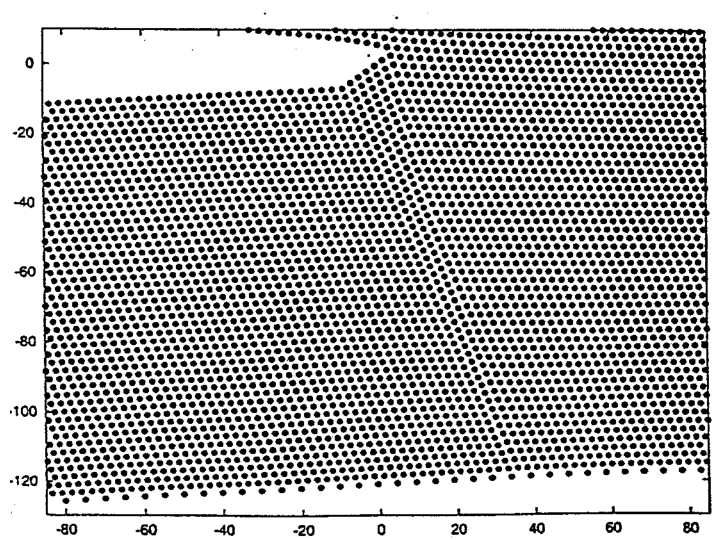


Figure 4.2 The total local stress intensity factor at the crack tip versus the applied stress intensity factor. The total local stress intensity factor is calculated from Equations 2.11 and 2.16. The dashed line indicates no dislocation. When the first dislocation is emitted at $K = 0.2\ eV(\overset{0}{A})^{-2.5}$, the total local stress intensity factor for the crack tip decreases suddenly because of dislocation shielding. As the applied stress increases, more dislocations are emitted from the crack tip.

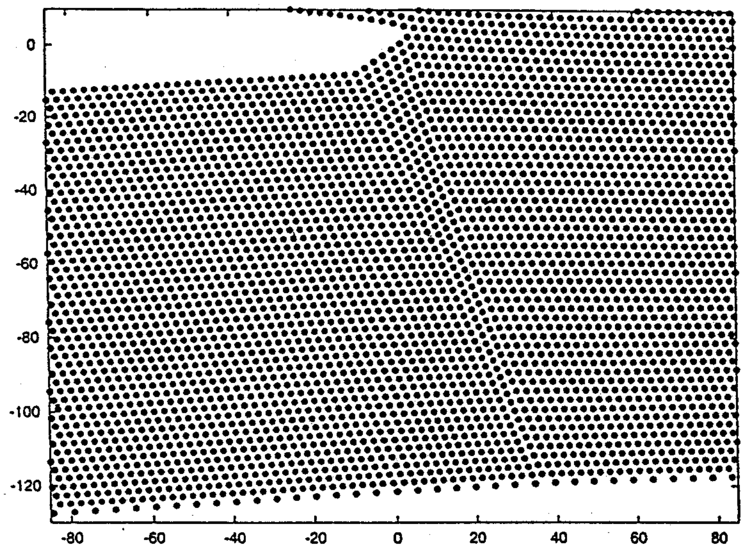


(a) The first dislocation is stopped by the fixed boundary at $K = 0.375\ eV(\overset{0}{A})^{-2.5}$.

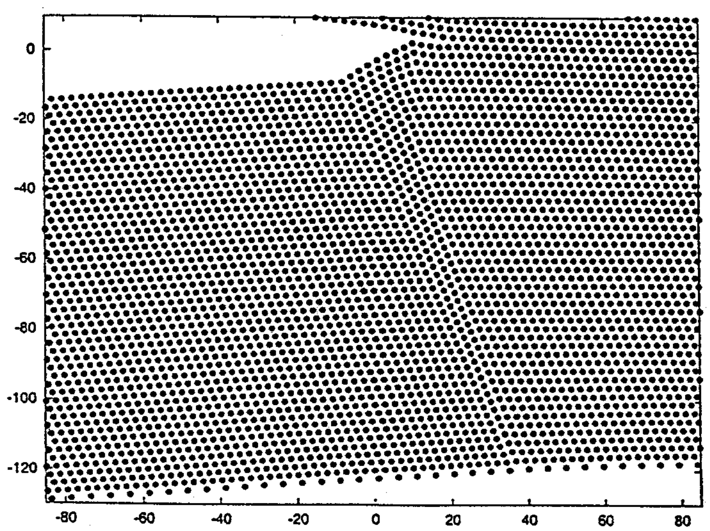


(b) The crack emits one more dislocation at $K = 0.4\ eV(\overset{0}{A})^{-2.5}$

Figure 4.3 Some steps in the size of 33000 atoms after the first dislocation is stopped by the fixed boundary.



(c) The dislocation emission continues at $K = 0.425\ eV(\overset{0}{A})^{-2.5}$.



(d) The dislocation emission continues at $K = 0.45\ eV(\overset{0}{A})^{-2.5}$.

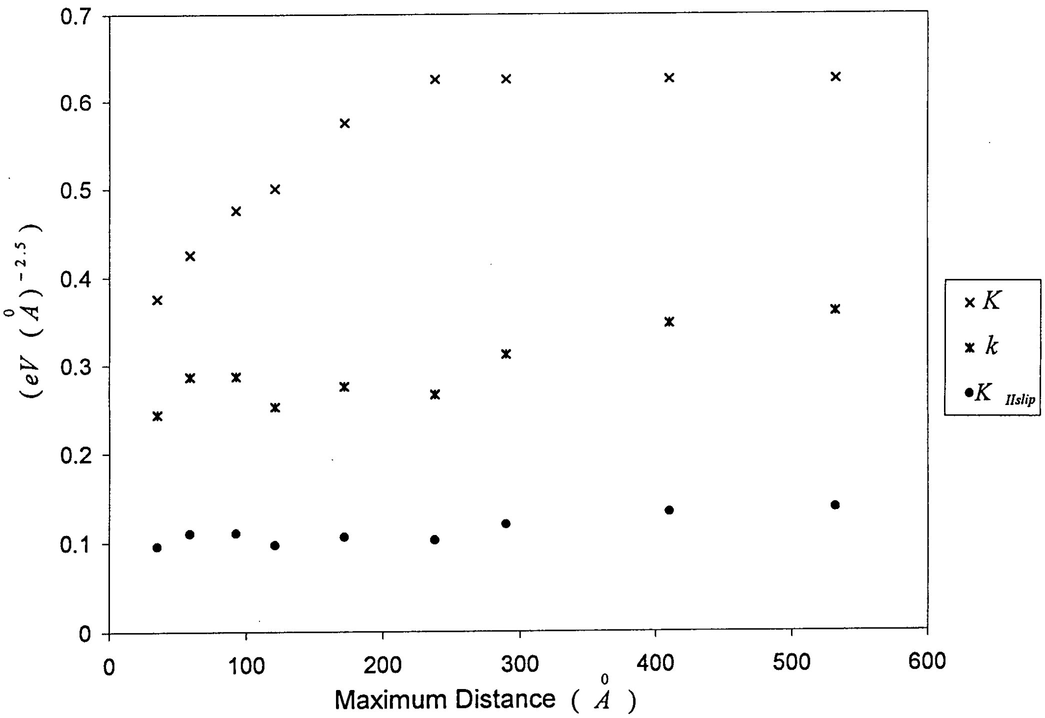


Figure 4.4 The applied stress intensity factor (K), the local stress intensity factor at the crack tip (k), and the local stress intensity factor along the slip plane (K_{IIslip}) versus the maximum distance at failure for all sizes. The maximum distance is the equilibrium distance for the size of 400,000 atoms (the last point), while it is pinning distances for the other sizes since the dislocations are stopped by the fixed boundary condition of the model.

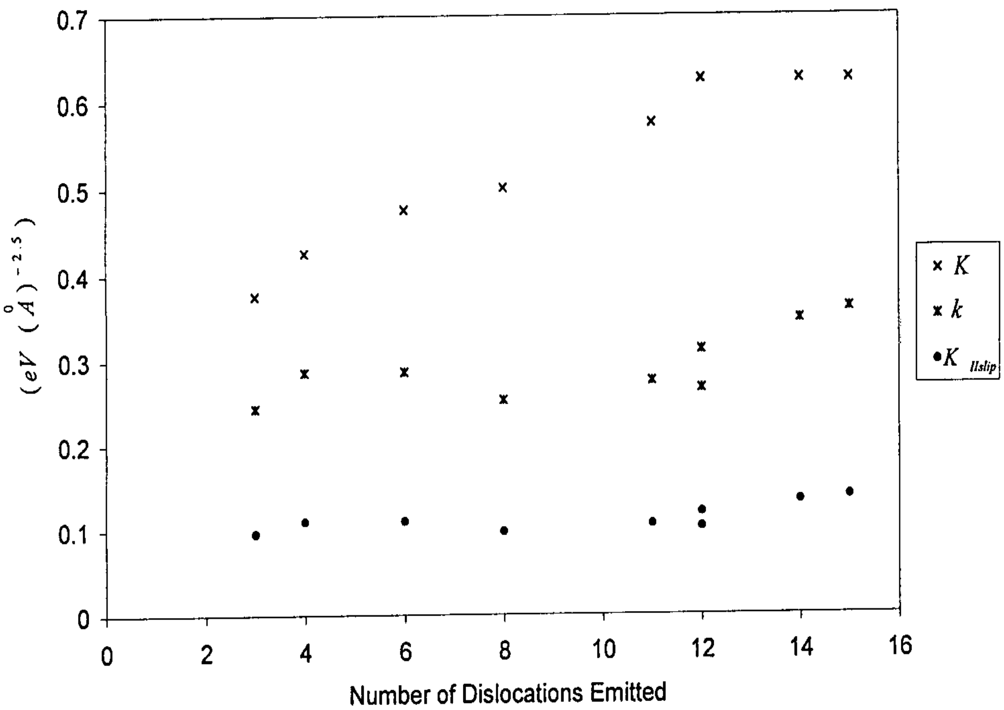


Figure 4.5 The applied stress intensity factor (K), the total local stress intensity factor at the crack tip (k), and the local stress intensity factor along the slip plane (K_{IIslip}) versus the number of emitted dislocations at failure for all sizes. As the number of dislocations increases, the applied stress intensity factor required to propagate the crack tip increases at first and then become constant, and the local stress intensity factors remain basically constant up to 12 dislocations. Thereafter, the local stress intensity factors start to increase slightly.

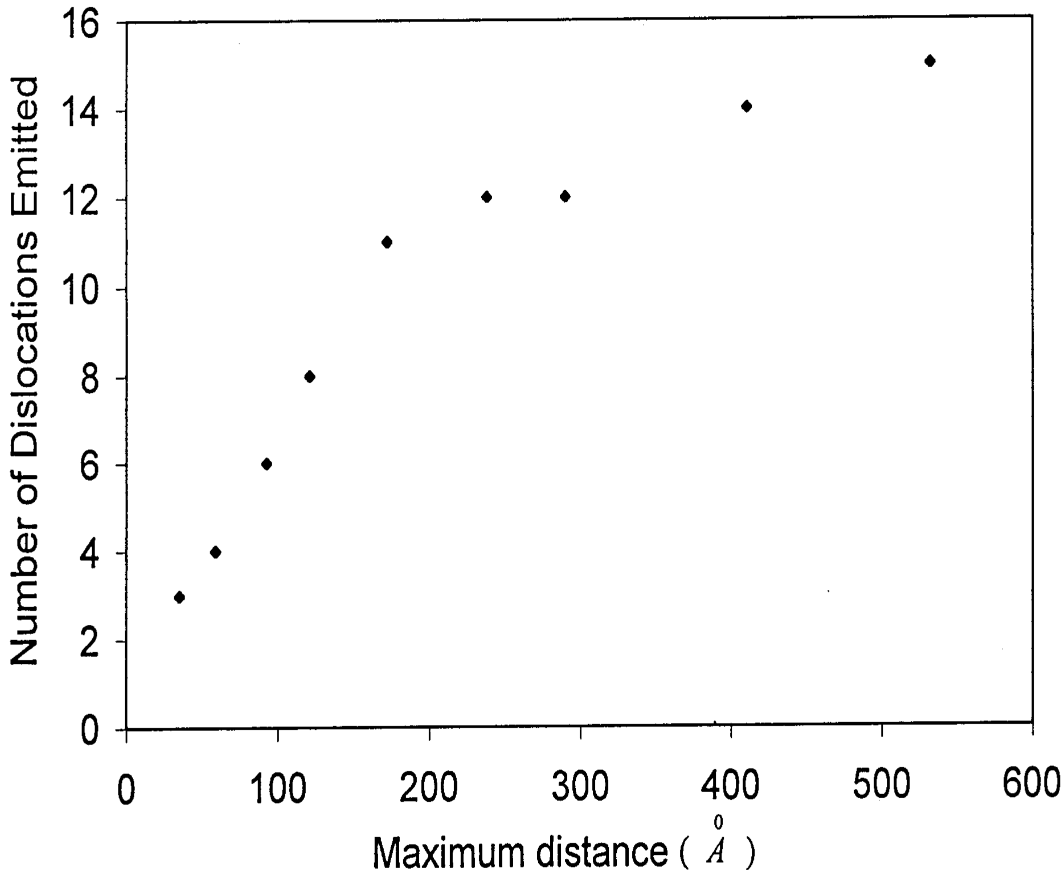


Figure 4.6 The effect of the maximum distances on the number of dislocations emitted. The number of dislocations increase rapidly at first and then slowly as the maximum distance of the dislocations emitted increases. This behavior may be due to dislocation shielding

Chapter 5

Discussion

The results show that cracks introduced in aluminum emit dislocations. In this orientation, the emission occurs along [112] slip direction inclined at an angle of 70.5^0 with respect to the crack tip. The emitted dislocations intersect the crack front, and the Burgers vector 1/6[112] has a component normal to the crack plane. Therefore, the cracks are blunted. This agrees with the fact that Rice and Thomson's requirement of blunting of a mode I crack are satisfied.

The cracks emit Shockley partial dislocations that lies on the parallel and adjacent slip $(11\bar{1})$ planes. The resulting parallel stacking faults are equivalent to twin. The dislocations generated are in the form of an inverse pileup because dislocation density is very high near the crack tip and it decreases gradually from the crack tip.

The dislocations are emitted on one side of the crack because of the crystallographic orientation. There is only one slip planes because the (111) plane is not a mirror plane. The emitted dislocations cause the crack to become a blunted crack with a sharp corner. Emission of further dislocations maintains the geometry of crack tip since the crack tip stays at the same layer. The stress concentration at the corner may be as strong as the stress concentration of a sharp crack. Therefore, the sharp corner reduces the effect of the blunting.

The emission stops because of the strong shielding effect after a certain number of dislocations are generated from the crack tip. This is followed by the brittle propagation without the cracks branching in the blocks. Therefore, dislocation emission is initially favored, but there is a cleavage transition for a critical number of emitted dislocations. After cracks propagate, some dislocations, especially the last emitted ones, which are closer to the crack tip, come towards to the crack tip. This result agrees with the experimental result obtained by Zhang *et al.* [55].

We obtained that the applied stress intensity factor required to propagate the crack tip increases at first, and then becomes constant as the maximum distance that the dislocations can move away from the crack tip increases. On the other hand, the total local stress intensity factor at the crack tip and the local stress intensity factor along the slip plane basically remain constant as the maximum distance of emitted dislocations increases.

As the number of dislocations emitted increase, the applied stress intensity factor required to propagate the crack tip increases at first and then becomes constant. On the other hand, both local stress intensity factors remain basically constant up to 12 dislocations, and then they begin to increase slightly.

The observed applied stress intensity factor at the crack tip is larger than the Griffith value, because of the shielding that is induced by the distribution on the inclined plane. Also, the larger local stress intensity factor is required since available work supplied by the applied stress intensity factor is partitioned between creation of a nonlinear core on the inclined plane and the cracks advance on the 0^{o} plane.

The local stress intensity factor along the slip plane remains less than the total local stress intensity factor at the crack tip as the number of dislocations emitted increases. Therefore, dislocation nucleation is the preferred response to the applied stress. Consequently, the material showing such a behavior is classified as intrinsically ductile.

The number of dislocations generated increase rapidly at first and then more slowly when the maximum distance of the emitted dislocations increases. The reason of this behavior may be due to dislocation shielding and crack blunting.

Imperfections such as grain boundaries, impurity atoms and point defects in crystals may stop the movement of dislocation. If these imperfections prevent dislocations from moving far way from the crack tip, the shielding can become strong enough to prevent further dislocation emission. Therefore, it causes the crack tip to resume brittle propagation. Consequently, fracture toughness of a material that has imperfections may decrease because of the pinning of dislocations.

Chapter 6

Conclusions

It was obtained that aluminum is a ductile material at 0 ^{o}K in which cracks generate dislocations, which shield the cracks. Therefore, it can be concluded that aluminum is an intrinsically ductile material at high temperature since ductility increases with temperature. It is clear that dislocation emission is initially favored, but there is a cleavage transition for a critical number of emitted dislocations. The Rice and Thomson Model predicts the behavior of aluminum, as does Kelly *et al.*'s simple theory. Also the result obtained is in agreement with Rice's recent model [24].

One of the advantages of the atomistic simulations is that phenomena difficult to observe experimentally may be predicted: Twinning, which has never been observed experimentally in aluminum because of the high stacking fault, was observed in the present study. Therefore, the simulation predicts that aluminum may produce twinning at low temperature (0 ^{o}K). At high temperatures, twinning in aluminum is not a preferred mode of the deformation because the twinning stress is much higher than the stress required for slip.

The dislocations are generated only one side of the cracks, and thus they cause the cracks to shape as a blunted crack with a sharp corner. Emission of the dislocations maintains the geometry of the crack tip because the crack tip stays at the same layer. The influences of the change in crack tip shape on the applied stress intensity factor was not considered explicitly, but probably does not play a significant role because the blunted crack maintains a sharp tip. The dislocation shielding reduces the local stress intensity factor at the crack tip. Consequently, the fracture toughness increases.

As the maximum distance that the dislocations emitted can travel away from the crack tip increases, the applied stress intensity factor required to propagate the crack tip increases at first, and then becomes constant. On the other hand, the total local stress intensity factor at the crack tip and the local stress intensity factor along the slip plane basically remain constant as the maximum distance of emitted dislocations increases. The behavior is consequence of dislocation emission.

The applied stress intensity factor required to propagate the crack tip increases at first and then becomes constant as the number of dislocations emitted increase. On the other hand, both local stress intensity factors remain basically constant because of dislocation shielding.

The observed total local stress intensity factor is larger than the Griffith value since available work supplied by the applied stress intensity factor is partitioned between creation of a nonlinear core on the inclined plane and the cracks advance on the 0^{o} plane.

Imperfections such as grain boundaries, impurity atoms and point defects in crystals may stop the movement of dislocation. If these imperfections may cause dislocations emitted to be pinned near to a crack tip, the shielding can become strong enough to prevent further dislocation emission. Therefore, it causes the crack tip to resume brittle propagation. Consequently, fracture toughness of a material that has imperfections may decrease because of the pinning effects.

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Notation

g surface energy

m shear modulus

b Burgers vector

g_{us} unstable stacking energy

k_I local mode I stress intensity factor

k_{II} local mode II stress intensity factor

k_{III} local mode III stress intensity factor

k_{Ic} fracture toughness

f_c elastic force per unit length on a crack

u Poisson's ratio

q inclination of the slip plane

f component of the angle mode by Burgers vector

R_e resistance to dislocation emission

R_c resistance to cleavage

s applied tensile stress

t shear stress

F force on an emitted dislocation

r position of a dislocation

K applied load

s^D back stress

k total local stress intensity factor at a crack tip

K_{IIslip} local stress intensity factor along a slip plane

Vita

Murat Durandurdu was born on April 9, 1969 in Kirsehir, Turkey. After completing his high school education, he was accepted at Department of Physics at Karadeniz Technical University in Trabzon. During his undergraduate education, he was awarded with two honors and six high honors, and he hold an undergraduate scholarship of Turkish Physics Foundation, which offers some fifteen scholarships to successful undergraduates from allover Turkey.

After graduation with the highest grade and high honors, he was accepted as a graduate student at the same university. During his graduate education, he was awarded with a scholarship by Turkish Government to pursue his graduate study in the USA. He came to the USA in 1995 and started his graduate study at Department of Physics at the State University New Jersey, Rutgers. After getting his MSc degree, he was accepted at Department of Physics at Virginia Polytechnic Institute and State University. However he has transferred to the Materials Science and Engineering Department. After defending his thesis in June 1999, He will pursue his PhD study at Department of Physics at Ohio University.