7.6 A NEW APPROACH TO FRACTURE MECHANICS USING VOLTERRA DISLOCATIONS, WITH APPLICATIONS TO THERMO-MECHANICAL FRACTURE — A. Sheng, G. Po, N.M. Ghoniem (University of California, Los Angeles)

OJBECTIVE

This report presents a dislocation-based technique for fracture modeling that is capable of simulating complex crack systems, particularly those under thermo-mechanical loads. The main application for fusion energy is in the design of Plasma-Facing components, especially those made of tungsten, where fracture and plasticity control the mechanical behavior during plasma transients.

SUMMARY

Complex fracture phenomena involving multiple interacting cracks in three-dimensional geometries have proven difficult to model computationally. This may be a result of the way cracks are typically conceptualized - as a disruption to an otherwise perfect continuum. As a result, existing fracture-modeling methods are generally limited to simple geometries containing a small number of cracks. The mechanical response of the first wall/blanket and divertor systems to plasma transients will inevitably involve analysis of multiple interacting cracks in 3-D geometries. We present here a different strategy for fracture modeling in which cracks are represented by distributions of discrete Volterra dislocations. This new approach overcomes many of the computational difficulties of state-of-the art fracture mechanics based on the Finite Element method.

PROGRESS AND STATUS

Introduction

Fracture is an everyday occurrence with consequences that can range from inconvenient to catastrophic and incredibly costly. As the complexity and performance requirements of modern engineering applications grow, the ability to accurately model and predict failure becomes increasingly valuable and necessary. The similarity between the elastic fields of cracks and linear distributions of dislocations has been recognized for some time [1, 2]. A fracture modeling technique exploiting this resemblance is presented and shown to be a promising alternative to existing methods.

The method outlined herein is an extension of the Parametric Dislocation Dynamics (PDD) method developed by Ghoniem et al. [3] to investigate crystal plasticity. In PDD simulations, discrete crystal dislocations are represented by parametric space curves, and their collective interactions in 3-D is completely resolved [3, 4, 5]. This allows us to model cracks with complex shapes and their mutual interactions, since a crack may be considered a distribution of dislocations on the crack plane. Examples of crack problems in 3D finite geometry will be given to illustrate the utility of the proposed method. Additionally, an example of crack propagation is shown in 2D.

Volterra Dislocation-Based Fracture Mechanics

A loaded crack can be completely described by a distribution of dislocations with suitable Burger's vectors ***b***. The crack tip, which is fixed prior to propagation, determines the size and shape of the crack and is represented by a fixed dislocation loop conforming to the same contour. Enclosed by this loop is a series of additional loops that are free to expand and contract according to the applied load, their mutual interactions, as well as their interactions with the crack-tip loop.

The classical Griffith-Inglis crack in an elastic body may be subjected to three different load configurations, referred to as modes I, II, and III. Cracks under mode-I and mode-II loading consist of climb-edge and glide-edge dislocations respectively, while mode-III cracks consist of screw dislocation distributions. The configurational force that drives the motion of these dislocations is given by the Peach-Koehler formula. For a 2D crack under mixed mode-I and mode-II loading, dislocations are driven along the crack line by the Peach-Koehler force components shown in Figure 1.

When tractions are applied to an elastic body, forces cannot be transferred across crack surfaces. Dislocation velocities are proportional to the Peach-Koehler force so that when in mechanical equilibrium the stress on each dislocation is zero, satisfying this traction-free crack surface condition.

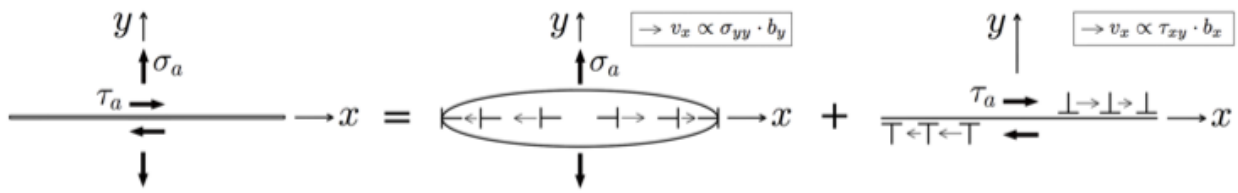

Figure 1. 2D mixed mode-I and mode-II crack

The fixed crack-tip dislocation experiences an unbalanced Peach-Koehler force as a result of the dislocation pileup. It can be shown that this unbalanced configurational force is equivalent to the J-integral described in classical fracture mechanics. The stress-intensity factor for each fracture mode can then be calculated using the relationship:

$$K_I = \sqrt{J_I E}\,, \quad K_{II} = \sqrt{J_{II} E}\,, \quad K_{III} = \sqrt{2 J_{III} \mu} \qquad (1)$$

The number of distributed dislocations and the magnitude of their Burger's vectors have a close relationship with the crack opening displacement (COD). Analytical expressions for the COD of numerous crack problems have been found using LEFM. In cases where the COD is available from these results, the Burgers vector magnitude is exactly the ratio of the COD to the number of dislocation dipoles or loops. For cases in which the COD is not known exactly, an estimate can be made based on the observation that the ratio of the COD to the crack length is proportional to the ratio of the applied load to the shear modulus. Note that as the number of dislocations in the distribution increases, the resolution of the approximate crack opening shape improves as shown in Figure 2 for a 2D mode-I crack in an infinite body.

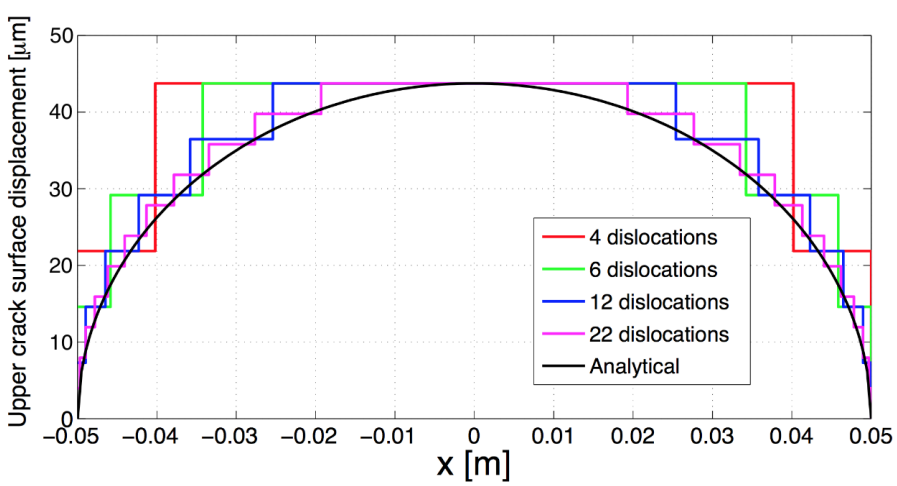

Figure 2. Mode I crack profile with increasing number of dislocations

Applying Dislocation Dynamics to Model Fracture

A fixed dislocation loop following the same contour as the crack tip is used to specify the crack size and shape. A dislocation loop is placed inside this fixed loop and allowed to equilibrate under the applied load. Once the free dislocation has reached its equilibrium position, a new loop is seeded inside the previous one, and the system is again allowed to equilibrate. This process is repeated until a newly seeded dislocation immediately begins to collapse (i.e. the applied load is no longer sufficient to drive the expansion of the seeded dislocation), as depicted with dislocation dipoles for a 2D mode-I crack in Figure 3.

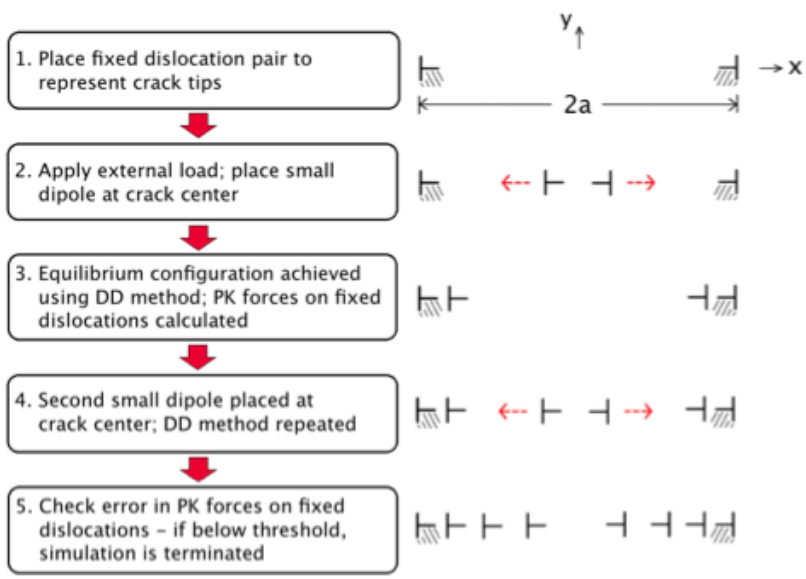

Figure 3. DD crack modeling procedure

For a crack in an infinite body, this procedure is sufficient for determining the stress intensity factor *K*. An additional procedure is required for a crack in a finite body, where the influence of the boundaries on the elastic field of the crack must be accounted for. In addition to the traction-free crack surfaces, the free boundaries of the finite domain must also be free of traction. To satisfy this condition, an additional step that will henceforth be referred to as the boundary correction procedure must be performed.

Based on a technique developed by van der Giessen and Needleman to calculate the elastic fields of dislocations in finite bodies [6], the boundary correction procedure utilizes the superposition principal to decompose the finite-body crack problem into two separate elastic problems. The first consists of a dislocation distribution in an infinite body – the same problem as described above. Calculating the dislocation stresses on virtual surfaces in the infinite body that match the free surfaces of the finite body, one finds that the stresses are non-zero and thus the traction-free boundary condition is not satisfied. The second problem consists of the finite body without the crack, with tractions applied to the surfaces that are the opposite of those calculated on the virtual boundary in the infinite body problem. The boundary correction procedure is illustrated for a 2D mode-I crack in Figure 4.

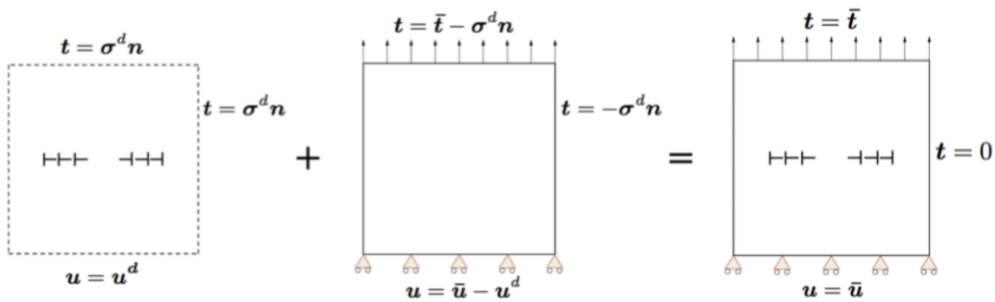

Figure 4. Boundary correction procedure for finite-body cracks

Examples

Mode-I Penny Crack in Infinite Body

For this example, a penny crack in an infinite body was modeled. The crack radius is *a* = 500 nm and a uniform stress of 100 MPa is applied in the mode-I loading direction as shown in Figure 5a. The dislocation loops used to model the crack are represented by parametric space curves in the PDD method. Results of the PDD fracture method are presented in Figure 5b for a number of dislocation loops ranging from two to eight loops. The shear modulus used is G = 80 GPa and the Poisson's ratio taken to be v = 0.3 to represent a generic material.

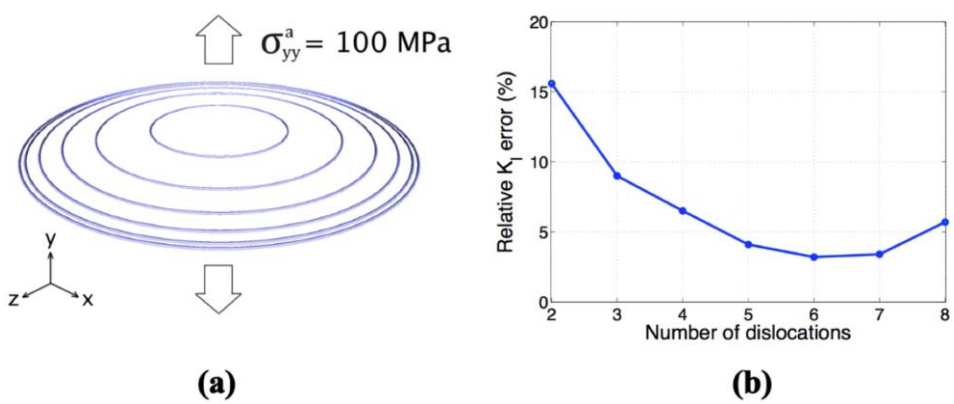

Figure 5. (a) Iso-displacement contours for a penny crack (b) Relative error in K_I given by PDD simulation, as compared to analytical solution [7].

Mode-I Penny Crack in Cylinder

A penny crack with a radius of *a* = 500 nm is placed in the center of a cylinder of radius *b*. The bottom face of the cylinder is held fixed, and a traction of 100 MPa is applied uniformly to the top face as shown in Figure 6.

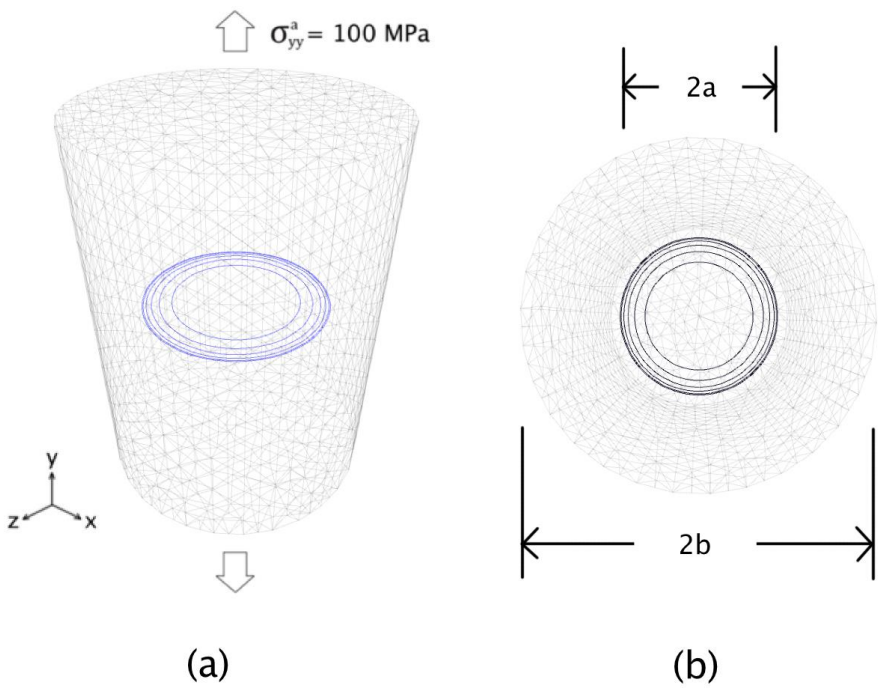

Figure 6. (a) Iso-displacement contours for a penny crack in a cylinder (b) Top-view of penny crack in cylinder

Results from the PDD crack simulation are given in Figure 7 for a range of cylinder radii.

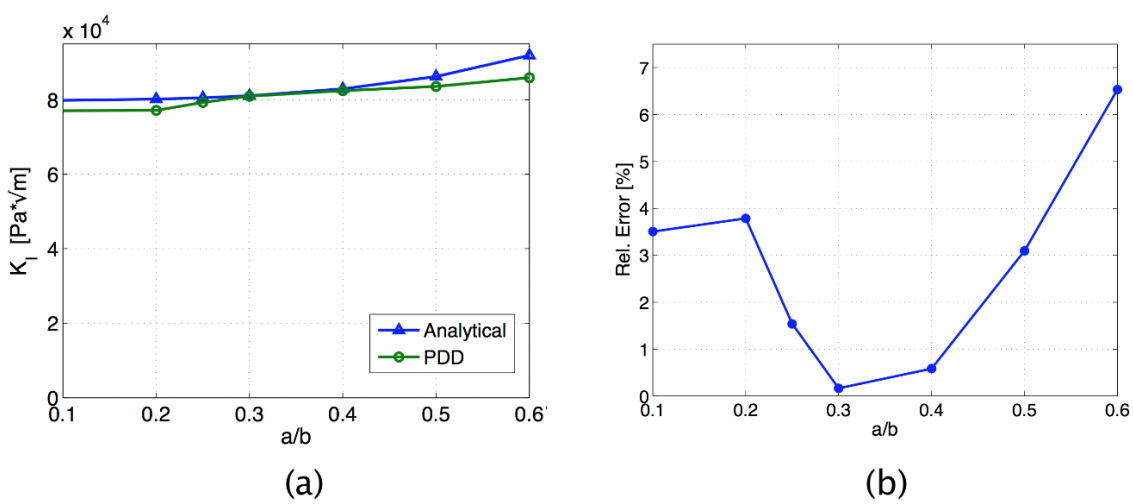

Figure 7. (a) Penny crack SIF vs. a/b (b) Relative SIF error. The analytical solution is obtained from reference [7]

<u>Mode-I Penny Crack in Rectangular Pillar</u>

A penny crack with a radius of 500 nm is placed in the center of a rectangular pillar with a width of 1500 nm, a thickness of 1050 nm, and a height of 2000 nm. A traction of 100 MPa is applied to the top face in the mode-I loading direction as shown in Figure 8a. Note that because the crack shape does not conform to that of the boundary, the crack dislocation loops take on the elliptical contour shown in Figure

8b due to the non-axisymmetric boundary effect. Note that the dislocations are more tightly compacted at $\theta = 90°$ compared to at $\theta = 0°$ due to the increased severity of the boundary effect.

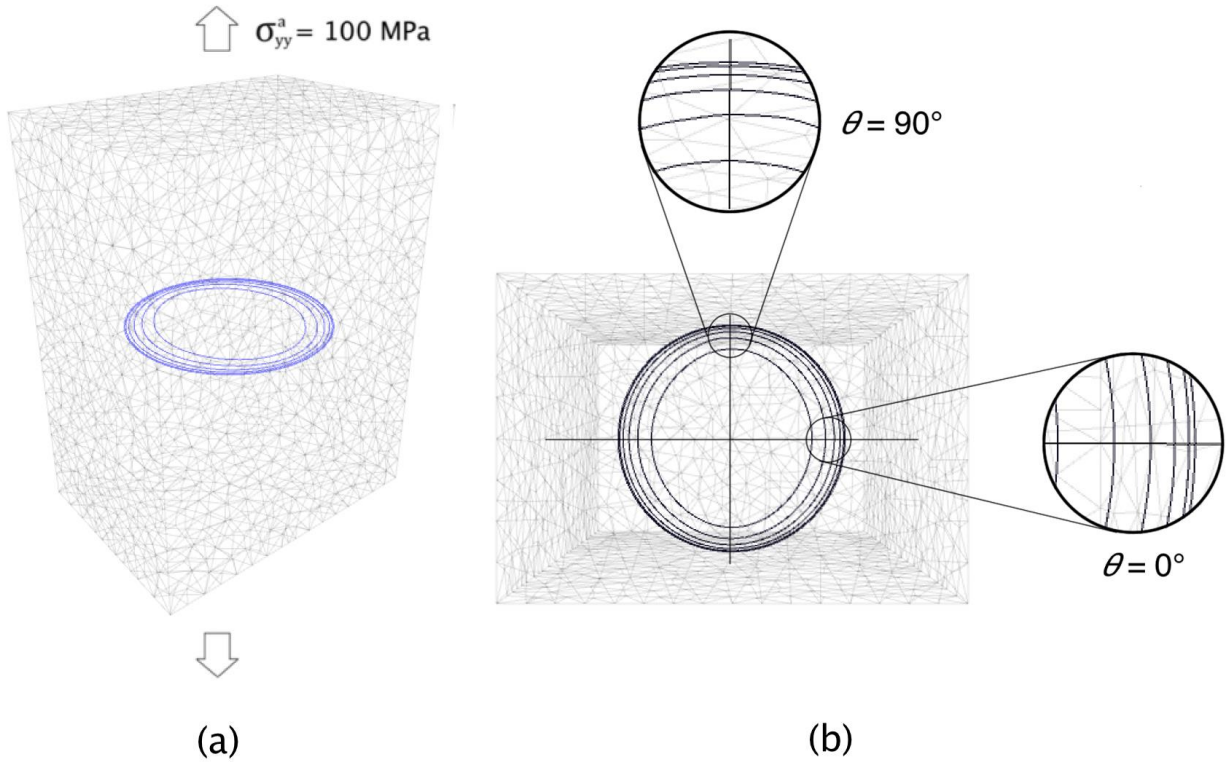

Figure 8. (a) Iso-displacement contours for a penny crack in a rectangular pillar (b) Top view of penny crack in a rectangular pillar

This boundary effect is further illustrated in the K_I results from the PDD simulation shown in Figure 9, which are plotted against the angular position θ.

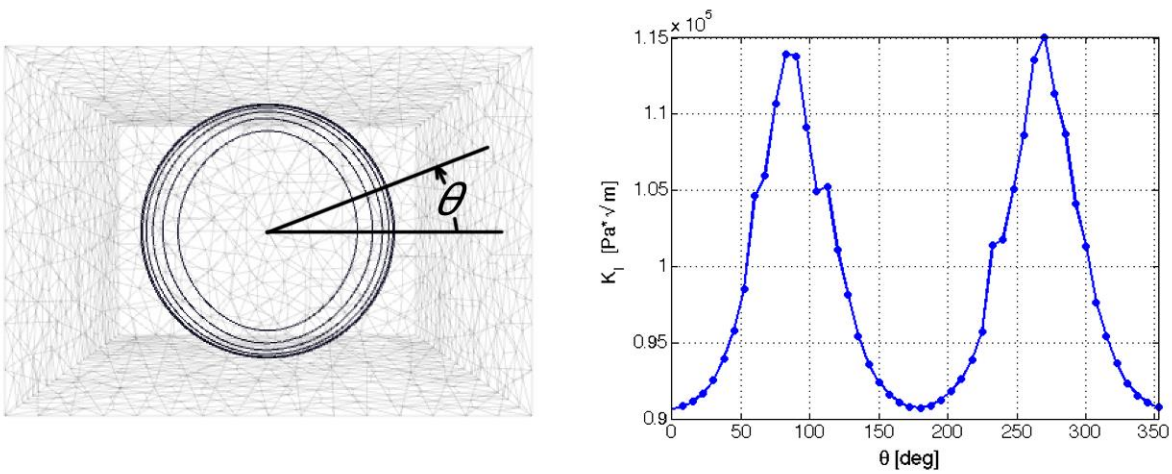

Figure 9. Stress Intensity Factor K_I vs. angular position θ for penny crack in rectangular pillar

Mode-I 2D Crack Propagation in Finite Plate

A simple 2D crack propagation example is presented in which a 50.8 × 50.8 mm square plate containing a 20 mm long center crack represented by a distribution of three dipoles is subjected to a “fixed grips” loading condition. A prescribed vertical displacement of 0.25 mm is applied to the upper and lower surfaces of the plate at successive time steps, m, as shown below in Figure 10.

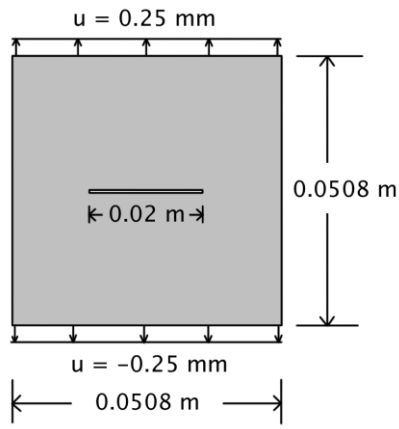

Figure 10. 2D plate containing a center crack under fixed-grips loading

To represent a generic material, the fracture toughness used is 130 MPa√m. Under the prescribed loading conditions, the stress intensity factors at the crack tips are found to exceed the fracture toughness. This initiates the crack propagation process. For each time step *m*, the crack tip is shifted a distance proportional to the Peach-Koehler force acting on the crack-tip dislocation and a new equilibrium configuration is solved for using the average stress along the crack line.

Under the fixed-grips loading condition, crack growth results in a relaxation of the material which decreases the stress intensity factor despite the increased crack length. This procedure is repeated until the calculated stress-intensity factor drops below the fracture toughness of the material (final K_I = 126 MPa√m). Figure 11 shows the crack as it increases in length over a period of time. Figure 12 shows the y-component stress field of the crack at the time steps corresponding to those shown in Figure 11.

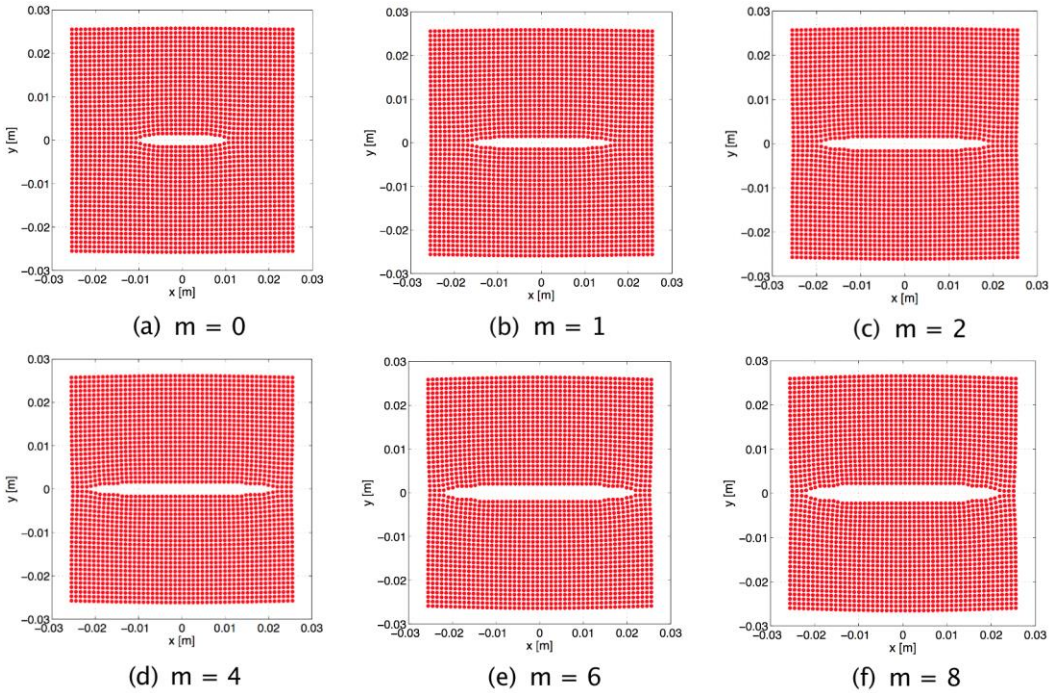

Figure 11. The displacement field associated with a propagating crack in finite geometry. (a) Initial crack length followed by (b-e) Crack size at different time steps, each with a displacement of 0.25 mm at the upper boundary. (f) Final crack length

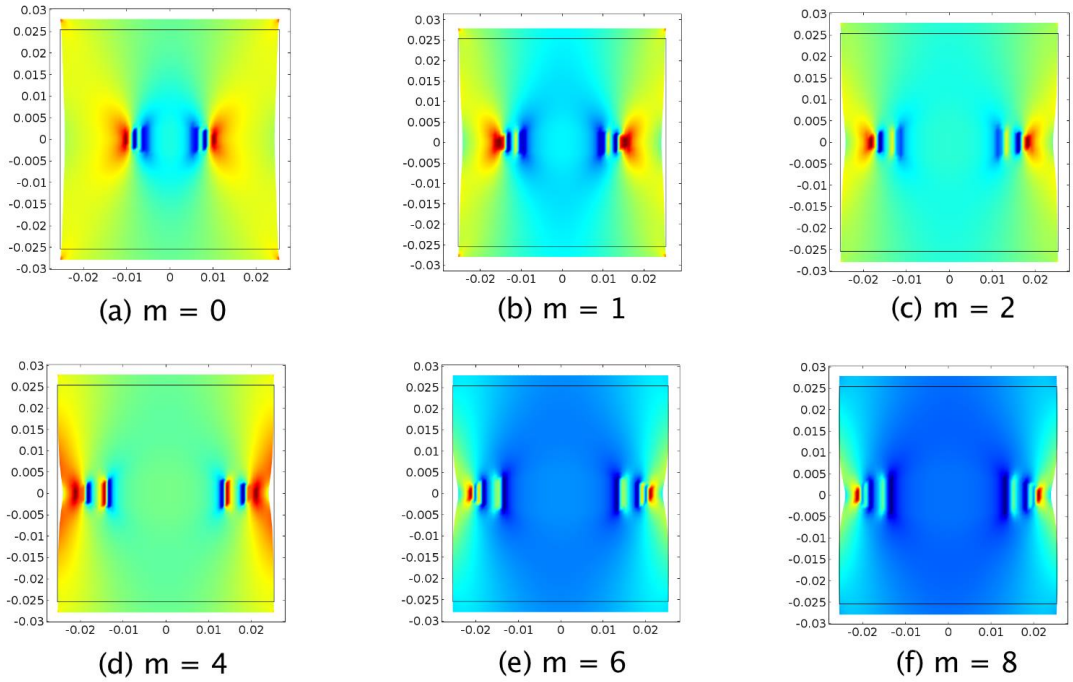

Figure 12. σ_y stress component for (a) Initial crack length followed by (b-e) Crack at different time steps (f) final crack length

Conclusions and Future Research

We have demonstrated the computational viability of the Volterra dislocation-based fracture mechanics method for solution of several fracture problems that have been traditionally challenging. These are: (1) 3-D cracks in infinite and finite geometry; (2) 2-D Mixed-mode cracks in finite geometry; and (3) a propagating crack in finite geometry. Future extensions and applications will be in the following areas: (1) single cracks in 3-D geometry in FW/B and PFC materials during plasma transients; (2) multiple interacting cracks in thermally shocked and mechanically loaded components.

References

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