A Unified Discrete Defect Dynamics Framework for Plasticity and Fracture

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Computational modeling of complex fracture phenomena, where multiple cracks propagate and interact in three-dimensional geometry is a very challenging task that has not been satisfactorily demonstrated. Despite huge technological incentives, most of the exisiting methods are limited to simple geometries and a small number of interacting cracks. The main reason appears to be the conceptual way that cracks are currently modeled as a disruption to an otherwise perfect continuum.

We have developed a fundamentally different approach to modeling discontinuities and defects in materials, namely the method of Parametric Dislocation Dynamics (PDD), where discrete crystal dislocations are represented by parametric space curves, and their collective interactions in 3-D is completely resolved [Amodeo and Ghoniem (1990); Ghoniem et al. (2000); Po and Ghoniem (2013)]. It has been known for a while that cracks can be represented by a suitable distribution of discontinuities (Volterra or Somigliana type dislocations), where the Burgers vector can be either fixed (Volterra), or locally variable (Somigliana). Thus, such objects can provide enormous flexibility in modeling complex-shape cracks and their mutual interactions, if only a computational method can be developed. We present here a new approach to modeling complex facture phenomena by extending the robust framework of our PDD method. We show that suitable choices of the Volterra Burgers vector enables dislocation arrays to represent 2-D cracks in modes I, II, and III [Ghoniem and Huang (2006); Takahashi and Ghoniem (2013)]. Moreover, it is shown that the Peach-Koehler force, which is the basis for motion and equilibrium in PDD simulations, is equivalent to the J-integral in fracture mechanics problems. Crack propagation is shown to be a natural extension to dislocation motion in PDD simulations. Several examples of crack problems in 3-D finite geometry will also be given to illustrate the utility of the proposed approach.

Dislocation-based Fracture Mechanics

A crack may be considered a distribution of dislocations along the crack plane with fixed dislocations representing crack tips. Cracks under mode-I and mode-II loading consist of distributed climb-edge and glide-edge dislocations respectively, while mode-III cracks consist of screw dislocation distributions. When tractions are applied to an elastic body, the resulting forces cannot be transferred across crack surfaces. To satisfy this condition, the distributed dislocations must be in mechanical equilibrium with the exception of the fixed dislocations at the crack tips.

The configurational force that drives dislocation motion is given by the well-known Peach-Koehler formula. For a 2D crack under mixed mode I and mode II loading, dislocation motion along the crack line is driven by the force component shown in Fig. 1. The dislocation velocities are proportional to the Peach-Koehler force so that when the dislocations reach their equilibrium positions the stress on each dislocation is zero. Thus at each equilibrium position, the traction-free crack surfaces condition is satisfied. The unbalanced Peach-Koehler force on the fixed crack-tip dislocations is equivalent to the J-integral around the crack tip. The stress-intensity factor K can then be calculated for each fracture mode using the relationship:

$$K_I = \sqrt{J_I E}\,, \quad K_{II} = \sqrt{J_{II} E} \tag{1}$$

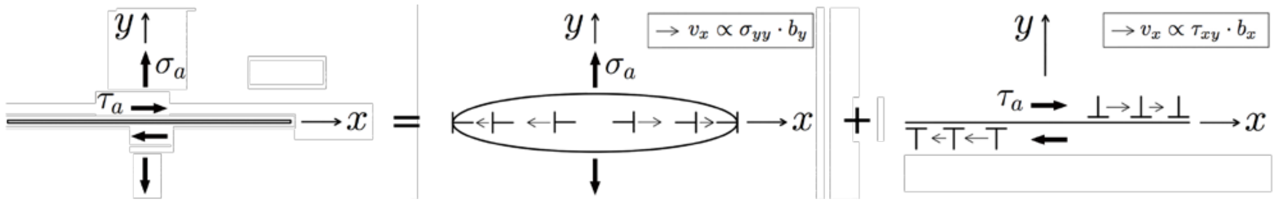

Figure 1. 2D mixed mode-I and mode-II crack

The number of dislocations used in the distribution and the magnitude of the Burgers vector has a close relationship with the crack opening displacement (COD). LEFM has provided the COD analytically for a large number of crack problems, and shown that the ratio of the COD to the crack length is proportional to the ratio of the applied load to the shear modulus of the material. For problems in which the COD is given analytically, the Burgers vector is exactly the ratio of the COD to the number of dipoles or loops in the distribution. It follows that the crack representation is improved with an increasing number of dislocations used to model the crack. This is shown in Fig. 2 for a 2D mode I crack in an infinite body. For more complex cracks where the COD is not given exactly, the Burgers vector magnitude is estimated using the same relationship.

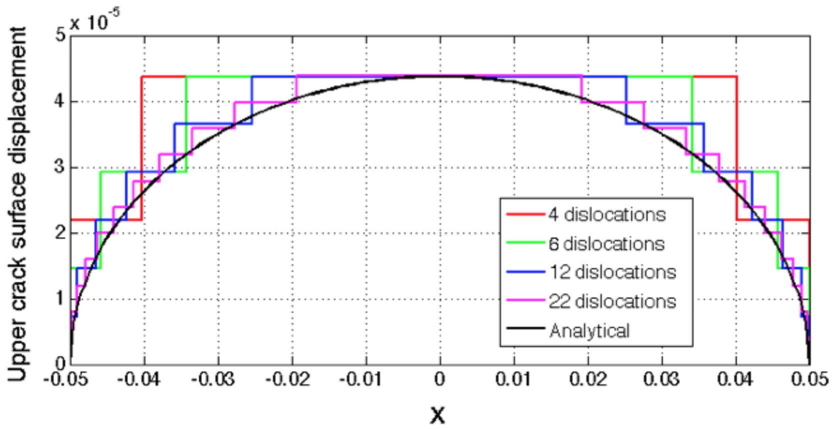

Figure 2. Mode I crack profile with increasing number of dislocations

Applying the dislocation dynamics fracture modeling method to a slanted crack oriented at an angle β gives the results shown in Fig. 3. The numerical results are in close agreement with the analytical stress intensity factors given by:

$$K_I = \sqrt{\pi a}(\sigma_{yy} \sin^2 \beta + \sigma_{xx} \cos^2 \beta) \quad (2)$$

$$K_{II} = \sqrt{\pi a}(\sigma_{yy} - \sigma_{xx}) \sin \beta \cos \beta \quad (3)$$

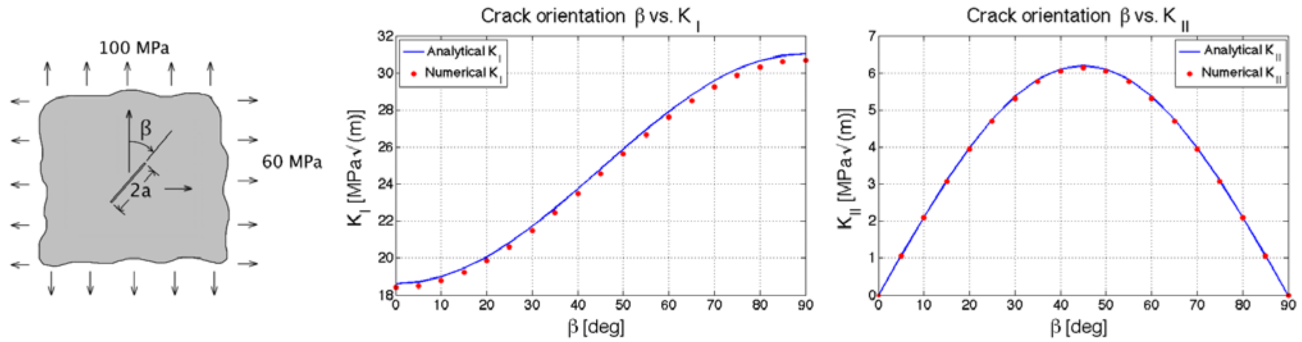

Figure 3. Mode I and mode II stress intensity factors for an inclined crack

The distributed dislocation loops used to model three-dimensional cracks are represented by parametric space curves as shown in Fig. 4a. Results of the PDD simulation for a mode I penny-shaped crack in an infinite body are shown in Fig. 4b for Burgers vector magnitudes ranging from 0.06 nm to 0.14 nm. The diameter of the crack is $2a = 1$ μm and the uniform tensile stress applied is 100 MPa.

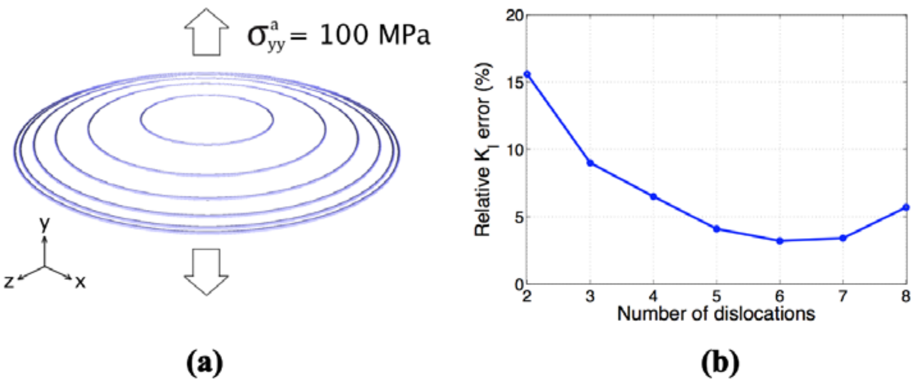

Figure 4. (a) Penny-shaped crack (b) Relative error in K_I given by PDD simulation

Conclusion

A new method for fracture modeling is proposed based on the Parametric Dislocation Dynamics (PDD) method developed for simulating crystal plasticity. A crack is represented by a distribution of dislocation loops in which the outer dislocation loop at the crack tip is fixed. The driving force behind dislocation motion, the Peach-Koehler (PK) force, is proportional to the dislocation velocity. Thus the traction-free crack surfaces condition is satisfied at each dislocation in mechanical equilibrium. The developed method has a number of computational advantages: (1) any complex shape crack can be represented in 2-D and 3-D geometries; (2) the PK (J-intergral) provide a natural mechanism that governs crack propagation and crack-crack interactions; (3) crack problems in finite domains can be solved without the need for re-meshing or special crack elements.

The unbalanced Peach-Koehler force on the fixed crack-tip dislocations is equal to the J-integral around the crack tip, allowing for direct calculation of the stress intensity factor. Two examples of the dislocation dynamics method for modeling cracks are shown – a 2D slanted crack in an infinite plate and a 3D penny-shaped crack in an infinite body. For both examples, the simulation results for the stress intensity factors are shown to be in good agreement with analytical solutions.

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