NUMERICAL SIMULATION OF STATIC AND DYNAMIC SHADOW PATTERNS USING AN ATOMISTIC DESCRIPTION OF CRACK INITIATION AND PROPAGATION

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ABSTRACT

In this paper we model crack propagation from an atomic point of view. We seek to understand the phenomenology of crack propagation in a decreasing stress field. Our objective is to shed light on the interpretations and implications of optical measurements (Kalthoff, Beinert, and Winkler, 1977a) of stress intensities. Our computational method is to use the simplest interatomic potential which captures the important features of real interactions to charaterize the structure of cracks from a discrete point of view. In our atomistic approach the fracture criterion is not independently specified but rather follows, along with all other macroscopic constitutive quantities, from the interparticle forces.

We developed a recipe to estimate the average strength of the stress singularity from a direct simulation of the shadow pattern using the strain distribution around the crack tip. We applied this recipe to the steady state propagation of a crack in a finite strip and obtained good agreement with Nilsson's (1972, 1973) corresponding continuum solution.

KEYWORDS

Shadow patterns; dynamic; atomistic; crack propagation; triangular lattice fracture.

INTRODUCTION

An optical technique for estimating the dynamic stress intensity factors for propagating and arresting cracks has been developed by Kalthoff and coworkers (1977b, 1977c). The technique is based on the analysis of shadow patterns (Manogg, 1964) which result from changing specimen thickness near the crack tip. These patterns directly reveal the surface curvature, from which the strain distribution and the stress intensity can be inferred.

The desire to understand Kalthoff's dynamical results has stimulated this research. This paper describes the numerical simulation of shadow patterns; their interpretation and usefulness in predicting crack propagation and arrest.

MOTIVATION

The stress and strain fields of continuum fracture mechanics include unrealistic divergences at crack tips. These divergences can be avoided by using a detailed atomistic description. Such a description automatically characterizes the crack propagation process.

In real metals there are impurities, grain boundaries, dislocations, and sometimes microcracks. The mostly unknown dependence of the interatomic forces on these defects precludes quantitative agreement with experiments so that computer simulations can be expected to provide understanding of experimental trends rather than replication of experimental results. Some progress in describing the defects with a statistical mechanics approach has been made by Stout (1982). Atomistic fracture simulations have been carried out by Markworth and Hirth (1981), Ashurst and Hoover (1976), and Chang (1970).

TECHNIQUE

Our model consists of a lattice of interacting mass points representing the atoms. The motion is governed by interatomic forces. The model makes several other simplifications. Our basic philosophy is to choose the simplest possible description which enhances the understanding of the underlying phenomenology. There is no quantum mechanics in our model. Only nearest neighbour interactions are included and the potential form is very simple.

Figure 1 is a plot of our interatomic force as a function of bond length. Near the equilibrium position, the force decreases linearly with bond strain until the strain reaches a critical value at which the bond becomes unstable. Beyond the instability point, the force increases linearly until the strain is twice the critical value. For strains larger than twice the critical value, the force is identically zero. Typically in our calculations, the critical strain was 0.15; by comparison, for a 6-12 Lennard-Jones interaction, the critical strain is 0.109. Although the discontinuous derivatives of the piecewise-linear forces are unrealistic, these forces retain important features of real interactions: A repulsive part, which prevents atoms from

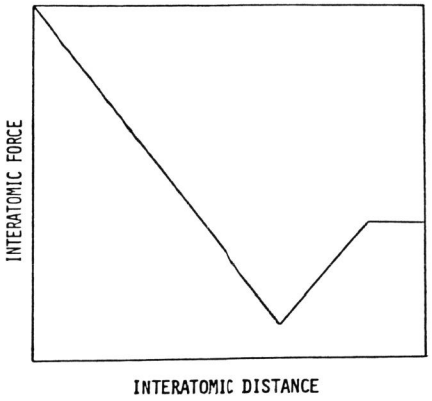

Fig. 1. The piecewise-linear force law used in molecular dynamics simulations of fracture.

coalescing, and an attractive part, which stabilizes the liquid and solid phases of matter.

The material modelled is the two dimensional triangular lattice whose thermodynamics and lattice dynamics are well known (Hoover, Ladd, and Hoover, 1981). The surface dynamics of this crystal has been discussed by Hoover and coworkers (1982). To model a crack in the crystal we "cut" a number of consecutive bonds in a row. This is done by ignoring the forces due to these bonds. Further details of the numerical model are available in (Moran, 1983).

RESULTS

We used nonuniform boundary displacements on the top surface of the strip shown in Fig. 2 to simulate crack propagation in a linearly decreasing strain field. We found that the location of the crack tip at arrest always corresponds to a strain lower than the strain necessary to initiate propagation. As the crack propagates in a decreasing strain field near threshold strain, the kinetic energy released at the tip is sufficient to carry the next bond along the crack path to the point of instability. Propagation continues in the decreasing strain field until the strain of the bond ahead of the crack is about 15% below threshold. The kinetic energy released is then no longer sufficient to carry the bond ahead of the crack to the instability point and the crack arrests.

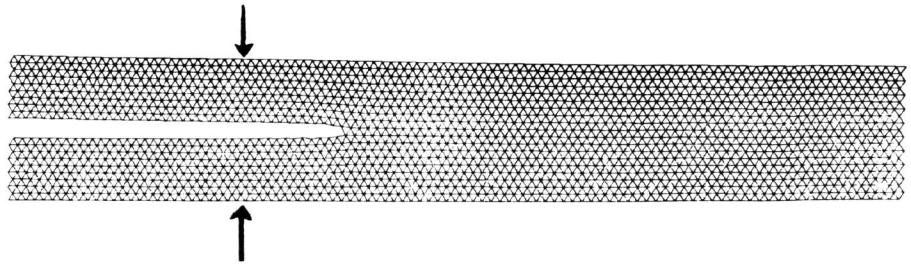

Fig. 2. "Tapered" specimen with arrested crack. The tapered slope of the upper boundary is almost too small to see, 1.6%. The arrows indicate the location of the crack tip corresponding to the critical stress instensity.

We simulated shadow patterns in our two dimensional calculation by using the plane stress equations to calculate hypothetical displacements perpendicular to the plane of the fracturing crystals. We sampled a large number of incident light beams and computed the image of these on a screen. To achieve a smooth shadow pattern using the discrete displacements at the nodal points of each triangle we developed a smoothing and interpolation technique for the triangular mesh.

We first calculated the vertical displacement of each node from a weighted average of the surrounding triangles. Next we calculated the tilt angle for each triangle from the vertical displacements of its three nodes. The position of each node's image on the virtual image plane was then calculated for

the three nodes in each triangle. In this way, individual nodes, which are common to as many as six triangles, have as many as six different images. The next step in the smoothing process was to average the coordinates of the individual point images that originate from a single node on the specimen. To each node we associated an average tilt from the surrounding triangles. The shadow pattern was next generated by using a bilinear tilt distribution in the triangular elements. Each triangle is no longer a plane mirror but a curved one. Using this interpolation scheme, the vertical displacement on the surface of the specimen is continuous and has continuous derivatives everywhere. The amount of light reflected by each triangle depends upon its projected area on the screen plane.

Figure 3 shows a typical shadow pattern. The diameter of the spot does correspond to the known stress intensity factor, but the numerical uncertainties are of order five to ten percent in the static case. Attempts to carry out the same analysis for dynamically moving cracks lead to larger errors, of order 50%. The dynamic pattern shown in the figure indicates a sound wave emanating from the crack tip.

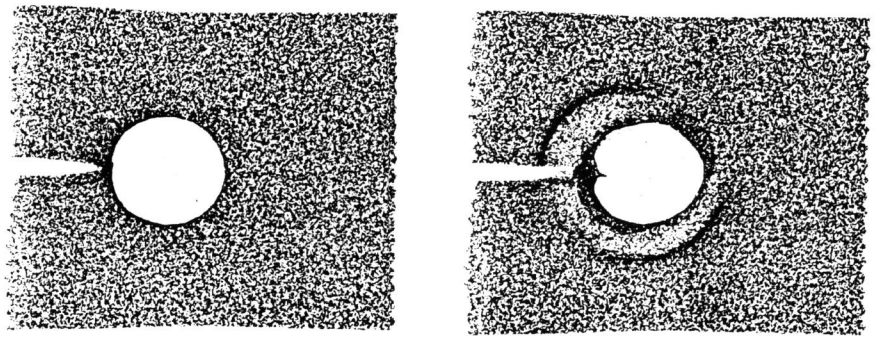

Fig. 3. Shadow patterns generated for static(left) and dynamic(right) cracks. The pattern size on the left corresponds to the known static stress intensity factor. The dim circle seen at the right is a sound wave emanating from the crack tip. A recognizable dynamic shadow pattern can be seen here.

Having obtained satisfactory shadow patterns, we developed a method to quantify our caustic diameter in the following steps:

(1) Find a polygonal path that passes through the maximum light intensity region in the caustic image plane. To produce smooth paths, we restrict the dot product of two vectors colinear with any two consecutive sides to be positive.

(2) Find the area of the enclosed polygonal path.

(3) Find an equivalent circular path, with the same area, with the center of the circle located at the average value of the polygonal-path nodal coordinates.

(4) Fit the light intensity in three concentric rings, using a parabola, so as to locate the maximum-intensity radius.

There are two kinds of difficulties in the numerical simulation of shadow patterns: First, as Knauss (1966) has shown, very large strips are required if the region large enough to produce a shadow spot is to be free of boundary influences. Second, in the dynamic case the thermal motion tends to increase the fluctuations, making the simulation of a well defined caustic shape rather difficult.

DISCUSSION

We developed and perfected a numerical recipe to simulate and quantify shadow patterns. The uncertainty in the simulated caustic diameter is limited because only a few zones in the near field region are close enough to the tip to be unaffected by the boundaries and yet far enough from the tip to be unaffected by its discrete nature. In the large crystal limit, the size of this region is linearly proportional to the size of the specimen and thus to the square root of the number of nodes. We found that using our recipe in 40-atom-wide strips, the uncertainty in the simulated caustic diameter is within seven percent in the static case. Further improvements can be made by fitting the shadow pattern to the theoretical caustic shape instead of a circle. In the dynamic case, the uncertainty in the caustic diameter is within 50%. Further improvement can be made by superposing several patterns generated from slightly different starting conditions.

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