DYNAMIC CRACK PROPAGATION IN A HETEROGENEOUS MATERIAL STRIP: STUDY OF THE BROBERG PROBLEM BY CONTINUUM AND ATOMISTIC METHODS

Huajian Gao, Shaohua Chen, Markus Buehler
Max Planck Institute for Metals Research, Heisenbergstrasse 3, D-70569 Stuttgart, Germany

ABSTRACT

Dynamic anti-plane shear crack propagation in an elastically stiff layer embedded in a soft matrix is investigated simultaneously by continuum mechanics and large-scale molecular dynamics simulation. The analytical solution predicts that the crack can move supersonically with respect to the soft material surrounding the layer. The stress amplitude ahead of the crack is influenced by the crack speed, layer width and elastic properties of both the layer and the matrix. The crack speed is found to depend on the ratio between the layer width and a characteristic length scale associated with energy transport in the vicinity of the crack. The corresponding atomistic simulation results are in good agreement with the theoretical predictions of continuum mechanics. This is a first quantitative study combining continuum-atomistic methods to confirm the recently proposed length scale for energy flux in dynamic fracture [9].

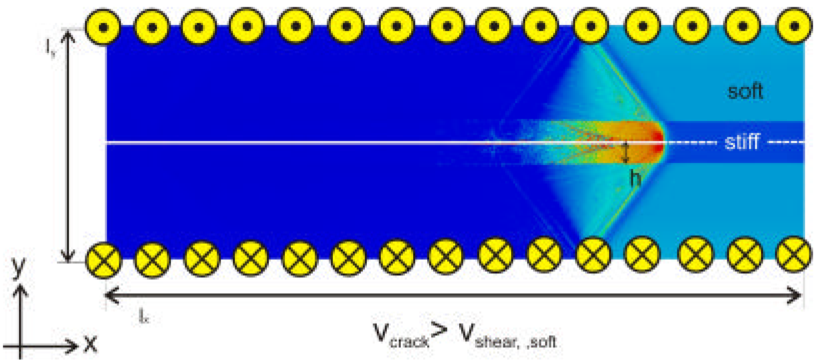

Fig. 1: Geometry of supersonic mode III crack propagation in a stiff layer surrounded by a soft matrix . The plot shows the potential energy field. The Mach cone due to supersonic crack motion is clearly visible in the soft matrix.

1 INTRODUCTION

One of the important questions of dynamic fracture mechanics is how fast a crack can propagate in a brittle solid [2,5,9]. For mode I cracks, the physically admissible stress singularity and energy release rate vanish for all crack velocities above the Rayleigh wave speed, and the Rayleigh wave speed is thus unambiguously identified to be the limiting speed for mode I cracks. For mode III cracks under antiplane shear loading, the shear wave speed C is the associated wave speed and the corresponding limiting speed. For mode II cracks, complications arise in that velocities below the Rayleigh wave speed and those between the shear and the longitudinal wave speed are both admissible. Between these two admissible regimes, there is an impenetrable velocity gap, giving

rise to the question which wave speed (Rayleigh or Longitudinal) should be the limiting speed for mode II cracks. Recent experiments and computer simulations have definitively shown that the mode II cracks can move at intersonic velocities [1-3,5] via a mother-daughter mechanism [5].
Super-Rayleigh mode I and supersonic mode II cracks have recently been reported in hyperelastic solids where the crack dynamic is governed by elastic properties at large strains [4,9]. The possibility for supersonic mode III crack in a solid with stiffening stress-strain relation has been investigated by Guo *et al.* [6] based on a continuum mechanics model. These studies have led to the conclusion that hyperelasticity can play an important role in dynamic fracture.
Buehler *et al.* [9] investigated the super-Rayleigh mode I crack motion by large-scale atomistic simulation. The authors discovered a new characteristic length scale that describes the region from which the crack needs to draw energy in order to sustain its motion. To further investigate the energy length scale, the authors considered the Broberg problem of a mode I crack propagating in a stiff layer embedded in a soft matrix as a model to understand locally subsonic and globally supersonic crack propagation. However, it has not been possible, even numerically, to study the solution obtained by Broberg [7] due to significant mathematical difficulties involved. Here we attempt to perform a combined atomistic and continuum study of the mode III Broberg problem, i.e. a locally subsonic and globally supersonic crack in a stiff layer surrounded by a soft matrix under remote anti-plane loading. The geometry of the problem is shown in Figure 1. The figure depicts the potential energy field near a supersonic mode III-loaded crack as obtained from a molecular-dynamics simulation. The mach cones due to supersonic crack propagation can clearly be observed.

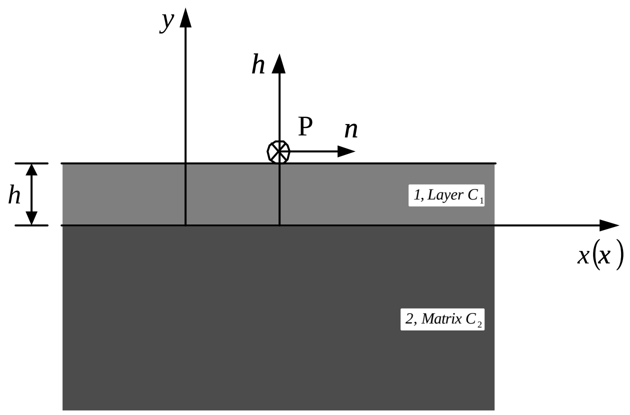

Fig. 2: Model of a concentrated force P moving with a constant velocity v acting on $y = h$

2 THEORETICAL ANALYSIS

Consider a linear elastic strip with thickness $2h$ embedded in an infinite elastic matrix. The strip is taken to be elastically stiffer than the surrounding matrix. A mode III crack is assumed to propagate in the strip with a velocity v slower than the shear wave speed of the strip material C_1 and faster than that of the matrix material C_2, i.e. $C_2 < v < C_1$. Here, subscript 1 denotes the layer and 2 denotes the solid. The relevant elastic properties are the shear modulus of the strip

m_1 and that of the matrix m_2.

First, we seek the auxiliary solution to the boundary value problem of a layered half space subjected to a point force P moving with velocity v, as depicted in Figure 2. Due to the anti-plane symmetry, the Broberg problem can be effectively converted to a mixed boundary value problem of such a layered half-space. Later we will integrate the moving force solution of Fig. 2 to describe the loading associated with the moving crack problem. We introduce a cartesian coordinate system (x, y) such that the lower crack face lies on the plane of $y = h$ and $x < vt$, where t denotes time. The solution to the crack problem will be obtained by the Wiener-Hopf method.

In terms of dimensionless coordinates moving with velocity v,

$$x = \frac{x - vt}{h}, \qquad h = \frac{y}{h}, \tag{1}$$

The equation of motion for the strip can be written as

$$a_1^2 \frac{\partial^2 w_1}{\partial x^2} + \frac{\partial^2 w_1}{\partial h^2} = 0 \qquad 0 \le h \le 1, \quad a_1 = \sqrt{1 - \frac{v^2}{C_1^2}} \tag{2}$$

and that for the matrix is

$$a_2^2 \frac{\partial^2 w_2}{\partial x^2} - \frac{\partial^2 w_2}{\partial h^2} = 0 \quad h \le 0, \qquad a_2 = \sqrt{\frac{v^2}{C_2^2} - 1}. \tag{3}$$

The equations of motion can be solved when the boundary and continuity conditions are considered. The displacement gradient on $h = 1$ for the point force is found to be

$$\left.\frac{\partial w_1}{\partial x}\right|_{h=1} = \frac{-P}{p a_1 m_1} \int_0^\infty \frac{N(a)}{D(a)} e^{iax} \mathrm{d}a\,, \tag{4}$$

where the two terms in the above equation are

$$N(a) = (l + i)e^{a a_1} - (l - i)e^{-a a_1}, \tag{5}$$

$$D(a) = (1 - l i)e^{a a_1} - (1 + l i)e^{-a a_1} \tag{6}$$

and

$$l = \frac{a_2 m_2}{a_1 m_1}. \tag{7}$$

For an arbitrarily distributed load $s_{yz} = f_1(x)$, the displacement gradient can be obtained by integration on the moving force solution as

$$\left.\frac{\partial w_1}{\partial x}\right|_{h=1} = \frac{-1}{p a_1 m_1} \int_{-\infty}^{\infty} f_1(a) \int_0^\infty \frac{N(a)}{D(a)} e^{ia(x-a)} \mathrm{d}a\mathrm{d}a\,, \tag{8}$$

Consider a moving crack with tip located at $(x = 0, h = 1)$ in the moving coordinates. For the crack problem, we decompose the crack face loading

$$f_1(x) = f(x)U(x) + h(x)U(-x) \tag{9}$$

into one part ahead of the crack and one part behind the crack, where $U(x)$ is the unit step function. The displacement gradient function

$$g^*(x) = -\int_{-\infty}^{\infty} f_1(a) \int_0^{\infty} \frac{N(a)}{D(a)} e^{ia(x-a)} \mathrm{d}a \, \mathrm{d}a \,, \tag{10}$$

associated with the crack should then satisfy

$$g^*(x) = \begin{cases} 0 & x > 0 \\ g(x) & x < 0 \end{cases} . \tag{11}$$

Two-sided Laplace transformations have been used to obtain the Wiener-Hopf equation for the problem. Using the standard Wiener-Hopf technique and inverse Laplace transform, the stress field ahead of the crack tip and the displacement gradient on the crack face can be obtained. The details are omitted here and we give the solution for the case of a homogeneous crack face loading, $h_0(x) = -s_{yz}$, in the (x, y) coordinate system as

$$f(x) = \frac{-s_{yz}}{\sqrt{p}\, a_1} \sqrt{\frac{h}{x - vt}} \sum_{n=0}^{\infty} \frac{1}{b_n^2 K_-(-b_n)} \qquad \text{as} \quad \frac{x - vt}{h} > 0 \tag{12}$$

Where

$$\begin{aligned} \ln K_-(q) &= -\frac{1}{2pi} \int_{-\infty}^{\infty} \left[\ln \frac{N(p)}{D(p)} \right]' \ln(p + iq) \mathrm{d}p + \frac{1}{2} \ln \frac{N(-\infty)}{D(-\infty)} \\ &= -\frac{1}{2pi} \int_{-\infty}^{\infty} \left[\ln \frac{N(p)}{D(p)} \right]' \ln(p + iq) \mathrm{d}p - \frac{pi}{4} \end{aligned} \tag{13}$$

and $D(p)$ possesses imaginary roots $p = ib_n$ ($b_n > 0$), $n = 0, 1, 2, 3, \cdots, \infty$.

The corresponding energy release rate can be calculated by standard methods [8], and the Griffith energy balance gives

$$G = \frac{s_{yz}^2 h}{m_1 a_1^3} \left[\sum_{n=0}^{\infty} \frac{1}{b_n^2 K_-(-b_n)} \right]^2 = 2g \,. \tag{14}$$

Following [8], we define a characteristic length scale for energy transport

$$c = b \frac{g m_1}{s_{yz}^2} \tag{15}$$

where b is a parameter to be fitted with the atomistic results. These results suggest the following relationship between the ratio h/c and the crack velocity v,

$$\frac{h}{c} = \frac{2a_1^3}{\left[\sum_{n=0}^{\infty} \frac{1}{b_n^2 K_-(-b_n)} \right]^2} . \tag{16}$$

3 ATOMISTIC SIMULATIONS

The continuum solution of eqn (16) predicts crack velocity as a function of the ratio h/c, i.e. $v = v(h/c)$. To compare with continuum solution, we have performed MD simulations to calculate the curve $v(h/c)$. Details of the MD simulation procedure will be published in a forthcoming paper [10]. Note that the aspect ratio of the slab is $l_x / l_y = 3$ in the simulations (see also Figure 1).

The crack speed should only depend on the ratio of the layer width h to the characteristic energy length scale c for a given pair of strip and matrix materials. The characteristic energy length scale is defined such that h/c equals one when the increase in crack speed is 50 percent of the difference between the shear wave speeds of soft and stiff material.

Figure 3 depicts the results of a set of calculations for the mode III Broberg problem. The continuous line corresponds to the continuum mechanics solution as discussed in the previous section, and the data points are MD simulation results obtained for different simulation conditions. In the MD simulations, the loading s_{yz}, the fracture surface energy g as well as the slab width are changed independently. These calculations suggest that the velocity scaling law predicted by eqn (16) is satisfied.

From comparison of MD results to the continuum solution, we find $b \approx 11$ and therefore $c = bgm_1 / s_{yz}^2$. When the inner layer width h approaches this length scale, the crack speed reaches halfway between the soft and stiff shear wave speeds. We note that the value of b may also depend on the properties of the strip and matrix materials. Discussion on this point will be included in a forthcoming paper [10].

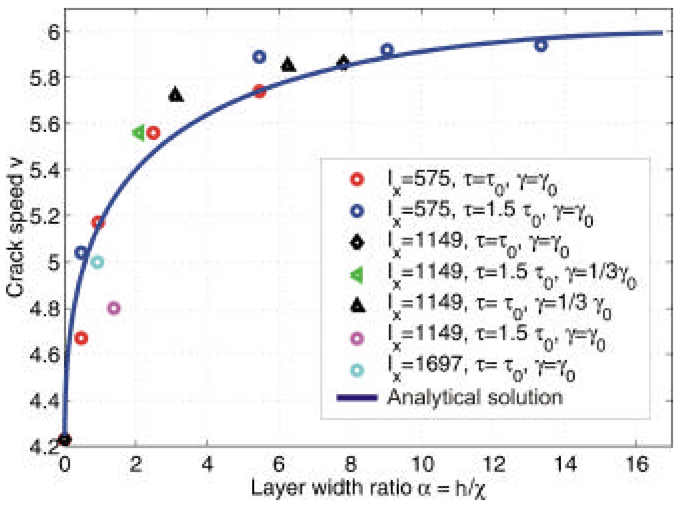

Fig. 3: Comparison of MD simulation results with the analytical solution to the mode III Broberg problem.

4 CONCLUSIONS

We report a first quantitative study combing atomistic and continuum descriptions of the mode III Broberg problem of a globally supersonic and locally subsonic crack propagating in a stiff strip embedded in a soft matrix. The problem is significant for understanding the mechanism of energy flux near a dynamically propagating crack and, more generally, crack propagation in nonlinear elastic solids where, due to large local strains, the material property near the crack tip might become significantly different from that far away from the crack.

In the continuum analysis, the solutions have been used to predict crack velocity as a function of the layer width scaled by a characteristic length scale associated with energy transport near the crack tip. The most significant result is the crack velocity scaling law derived in eqn (16), which is numerically solved and plotted in Fig. 3. Such velocity scaling law was discovered previously for the mode I case [9] based on a dimensional analysis. This paper is aimed at a quantitative study of the scaling law and energy length scale combining continuum and atomistic mechanics.

5 ACKNOWLEDGEMENTS

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