A MOTHER-DAUGHTER-GRANDDAUGHTER MECHANISM OF SHEAR DOMINATED INTERSONIC CRACK MOTION ALONG INTERFACES OF DISSIMILAR MATERIALS

Markus J. Buehler and Huajian Gao*

ABSTRACT

In this paper we report recent progress in large-scale atomistic studies of crack propagation along interfaces of dissimilar materials. We consider two linear-elastic material blocks bound together with a weak potential whose bonds snap early upon a critical atomic separation. This approach confines crack motion along the interface. In the two blocks, atoms interact with harmonic potentials with different spring constants adjacent to the interface. An initial crack is introduced along the interface and subjected to shear dominated displacement loading along the upper and lower boundaries of the sample. Upon initiation of the crack, we observe that it quickly approaches a velocity close to the Rayleigh-wave speed of the soft material. After cruising at this speed for some time, a secondary crack is nucleated at a few atomic spacings ahead of the crack. This secondary crack, also referred to as the daughter crack, propagates at the longitudinal-wave speed of the soft material. Shortly after that, a tertiary crack, referred to as the granddaughter crack, is nucleated and begins to move at the longitudinal wave speed of the stiff material. The granddaughter crack is supersonic with respect to the soft material and is clearly identifiable by two Mach cones in the soft material. Our results indicate that the limiting speed of shear dominated cracks along a bi-material interface is the longitudinal wave speed of the stiff material, and that there are two intermediate limiting speeds (Rayleigh and longitudinal wave speeds of the soft material) which can be overcome by the mother-daughter-granddaughter mechanism.

Key Words: dynamic fracture, interface crack, mother-daughter-granddaughter crack, molecular dynamics.

I. INTRODUCTION

Large-scale atomistic simulation is becoming an increasingly important tool to investigate fundamental aspects of dynamic fracture. Recent progress in this field includes systematic atomistic-continuum studies of fracture (Gao *et al.*, 2001; Abraham *et al.*, 2002; Buehler *et al.*, 2003a; 2003b; 2004a; 2004b), investigations of the role of hyperelasticity in dynamic fracture (Buehler *et al.*, 2003), instability dynamics of cracks (Abraham *et al.*, 1994), as well as the limiting speeds of mode II cracks (Abraham and Gao, 2000; Gao *et al.*, 2001).

Here we extend existing atomistic models of dynamic fracture in homogeneous materials (Gao *et al.*, 2001; Abraham *et al.*, 1994; 2002; Buehler *et al.*, 2003a; 2003b; 2004a; 2004b) to crack propagation along interfaces of elastically dissimilar materials. From the perspective of fundamental crack dynamics, an interesting question is how fast the interface crack can propagate. The crack limiting speed is associated with the elastic properties of the material. In homogeneous materials, extensive theoretical and numerical studies have been performed to address the question of limiting speed of cracks under different loading conditions (Gao *et al.*, 2001; Abraham *et al.*, 2002; Buehler *et al.*, 2003a; 2003b; 2004a; 2004b).

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*Corresponding author. (Email: hjgao@mf.mpg.de)

M. J. Buehler and H. Gao are with the Max Planck Institute for Metals Research, Heisenbergstrasse 3, D-70569 Stuttgart, Germany.

In the absence of nonlinear effects, the limiting speed of mode I cracks has been shown to be the Rayleigh-wave speed, while mode II cracks can attain velocities up to the longitudinal wave speed via a mother-daughter mechanism to overcome a forbidden velocity regime between Rayleigh and shear wave speeds (Abraham and Gao, 2000; Gao *et al*., 2001; Buehler *et al*., 2003a; 2004a). At bi-material interfaces, the situation is expected to be somewhat more complicated, as the elastic properties change discontinuously across the interface (e.g. Rice and Sih, 1965).

Cracking along interfaces is an important problem from the standpoint of technological applications. Interfaces in composite materials frequently serve as critical sites for failure initiation. Early theoretical studies focused on static interfacial cracks in dissimilar media (Rice and Sih, 1965; England, 1965; Rice, 1988; Hutchinson and Suo, 1992). One of the peculiar features of the elastic interfacial crack problem is the characteristic oscillating stress singularity found by Williams (1959). The oscillating solution implies that the crack faces would penetrate each other near the crack tip, illustrating some of the theoretical difficulties associated with modeling of dynamic fractures among dissimilar materials. It is generally difficult to predict the speed of an interfacial crack based on the Griffith condition (see, for instance, Rice, 1988; Liu *et al*., 1993a, 1993b; Lambros, 1995).

The dynamics of moving cracks along dissimilar interfaces has attracted some attention in the past decade. For instance, the asymptotic stress field near dynamic cracks at bimaterial interfaces has been studied in detail (Yang *et al*., 1991; Liu *et al*., 1993a; 1993b). The analysis discussed by Yang *et al*. (1991) assumed steady-state crack propagation and provided the spatial structure of square-root singular stress field very close to the dynamic crack tip. Later, the steady-state assumption was relaxed and higher order terms were included (Liu *et al*., 1993a; 1993b). Additional theoretical, numerical and experimental studies were carried out to address steady-state intersonic crack propagation along bimaterial interfaces (Wang *et al*., 1998; Huang *et al*., 1998).

Experiments on interfacial cracking (Lambros and Rosakis, 1995a; 1995b; Rosakis *et al*., 1998; Rosakis, 2002) include cracks propagating along interfaces between PMMA and metals. Lambros and Rosakis (1995a; 1995b) focused on the development of a criterion for interface crack growth and compared experimental results with theoretical predictions of the stress field near the crack tip. Crack speeds that exceeded the shear wave speed of PMMA were observed in these studies.

Existing theory and experiments showed that the limiting speed of tension-loaded cracks at bimaterial interfaces can exceed the Rayleigh-wave speed of the soft material (Yang, 1991; Liu, 1993a; 1993b). For shear dominated interface cracks, supersonic crack motion with respect to the soft material has been experimentally observed (Rosakis *et al*., 1998; Wu *et al*., 2000), although the underlying mechanism has not been fully investigated.

In contrast to experimental and theoretical progresses, few atomistic simulations of dynamic fracture along bimaterial interfaces have been reported. One example is recent molecular-dynamics simulation of a mode II crack propagation along an interface between a material defined by a harmonic potential neighboring a material defined by a tethered LJ potential (Abraham *et al*., 2002). The two materials have identical elastic properties under small deformation but behave differently under large deformation. In the setup, one material was modeled by the harmonic potential and the other by a tethered LJ potential with material behavior stiffening with strain (Abraham *et al*., 2002). The simulation revealed a mother-daughter-granddaughter mechanism by which the crack finally approached a velocity faster than the longitudinal wave speed of the harmonic material (Abraham *et al*., 2002). Although this setup constituted an interface of different materials, the small-strain wave speeds associated with each half space were identical.

The present study investigates the limiting speed of a shear-dominated interface crack via molecular dynamics simulations. We adopt a set-up similar to Abraham *et al*.'s (2002), but focus on two linear elastic dissimilar materials with unique elastic wave speeds. We develop an atomistic model to show that, under sufficiently large loading, the crack approaches the longitudinal wave speed of the stiffer of the two materials via a mother-daughter-granddaughter mechanism, thus generalizing the observation made by Abraham *et al*. (2002) to a broader class of bimaterial systems. The mother-daughter-granddaughter mechanism may be quite a general phenomenon for interfacial crack motion.

II. ATOMISTIC MODELING OF CRACKING ALONG A BIMATERIAL INTERFACE

To model a crack along an interface between two elastically dissimilar materials, we study two crystal blocks described by harmonic interatomic potentials with different spring constants $k_2 > k_1$. For simplicity, we consider two-dimensional triangular lattices with isotropic elastic properties. The harmonic potential is defined as

$$\phi(k_i) = \frac{1}{2} k_i (r - r_0)^2 , \qquad (1)$$

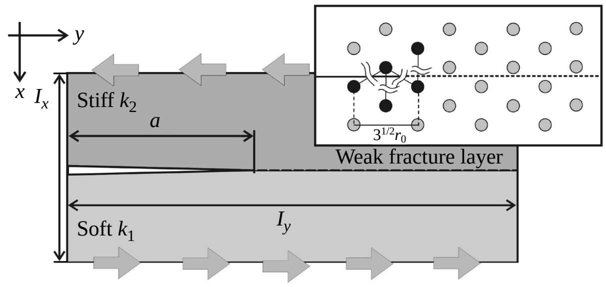

Fig.1 Simulation geometry and lattice orientation for the study of interfacial cracking. The figure shows the slab under shear loading. The crack moves in a two-dimensional triangular lattice and is confined to propagation along a weak interface (see the blowup of the crystal orientation). An initial crack of length $a \approx 750$ serves as the initial flaw. The lower part slab is relatively soft (with harmonic spring constant k_1) compared to the upper slab (with harmonic spring constant $k_2 > k_1$)

where $r_0 = 2^{1/6} \approx 1.12246$ is the nearest neighbor distance. We choose $k_1 \approx 28.57$ with the corresponding Rayleigh-wave speed $c_r \approx 3.4$, shear wave speed $c_r \approx 3.68$ and longitudinal wave speed $c_l \approx 6.36$. The difference in Young's modulus of the two materials can be related to the ratio $\Xi = k_2/k_1 > 1$. The wave speeds of the two materials thus differ by a factor $\sqrt{\Xi}$ (e.g., Freund, 1990). Atomic bonds across the weak interface have spring constant k_1 and break upon a critical separation $r_{break} = 1.17$.

The simulation slab is subjected to an applied shear strain rate $\dot{\gamma} = 0.0005$ and a smaller tensile strain rate $\dot{\varepsilon} = 0.00005$ along the upper and lower boundaries, as shown in Fig. 1. The system size is given by $l_x = 2{,}298$ and $l_y = 4{,}598$. Further details on modeling fracture based on harmonic potentials, as well as a detailed analysis on the elastic and fracture properties can be found elsewhere (Gao *et al.*, 2001; Abraham *et al.*, 1994; 2002; Buehler *et al.*, 2003a; 2003b; 2004a; 2004b). In homogeneous materials, it has been shown that the simulated results of limiting crack speeds, the energy flow fields and the stress fields near rapidly propagating cracks are in good agreement with continuum mechanics predictions (Gao *et al.*, 2001; Abraham *et al.*, 1994; 2002; Buehler *et al.*, 2003a; 2003b; 2004a; 2004b).

The geometry of our atomistic model, the loading as well as the crystal orientation of crack propagation is described in Fig. 1. The upper block of the simulation slab is relatively stiff with higher Young's modulus and higher wave speeds than the lower block.

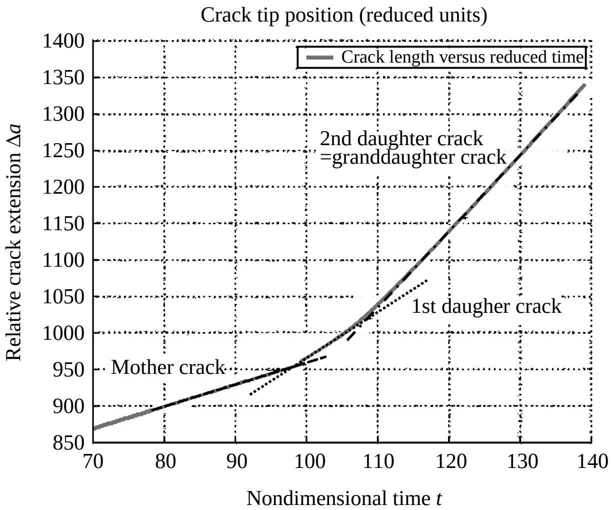

Fig.2 Crack tip history for a shear loaded crack propagating along an interface with stiffness ratio $\Xi = 3$. The crack tip history plot reveals a mother-daughter-granddaughter mechanism: After a critical time, a secondary crack (the daughter crack) is nucleated ahead of the mother crack. Shortly afterwards, a tertiary crack (the granddaughter crack) is nucleated. The transition in crack speed from the daughter to the granddaughter is more continuous compared to that from the mother to the daughter (see also the velocity history plot depicted in Fig. 3).

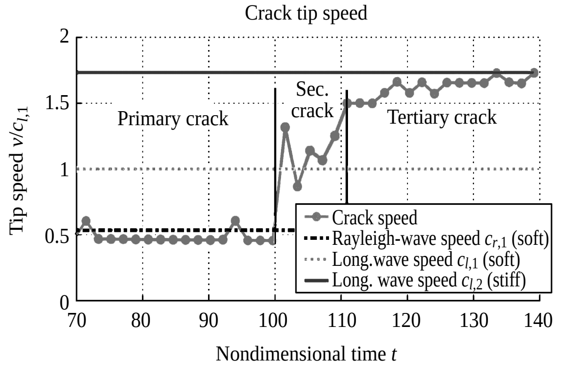

Fig.3 Crack tip velocity history during the mother-daughter-granddaughter mechanism for a shear loaded crack propagating along an interface with stiffness ratio $\Xi = 3$. The plot is obtained by numerical differentiation of the crack tip history shown in Fig. 2. The crack speed changes abruptly at the nucleation of the daughter crack, and rather continuously as the granddaughter crack is nucleated.

III. MODE II CRACKS AT BIMATERIAL INTERFACES: OBSERVATIONS IN MD SIMULATION

While noting that the basic observations seem to hold for a range of elastic mismatch ratios, we mainly discuss the results at $\Xi = 3$. The primary crack is observed to initiate at time $t \approx 34$ and quickly approaches the Rayleigh speed of the soft material $v \to c_{r,1} \approx 3.4$.

Figure 2 shows the history of crack tip location, and Fig. 3 that of the crack tip velocity. Both curves are shown over a time interval close to the nucleation of secondary and tertiary cracks. We observe a discontinuous jump in the crack velocity at $t \approx 100$, as the daughter crack is nucleated in front of the mother crack. The daughter crack forms at a distance $\Delta a \approx 10$ ahead of the mother crack and quickly approaches the longitudinal wave speed of the soft material $v \rightarrow c_{l,1} \approx 6.36$. The mechanism of nucleation of the daughter crack is reminiscent of the mother-daughter mechanism of mode II cracks in homogeneous materials (Abraham and Gao, 2000; Gao *et al.*, 2001).

Shortly after the daughter crack is nucleated, another change in propagation speed is observed at time $t \approx 108$ (see Figs. 2 and 3). This is due to initiation of a tertiary granddaughter crack ahead of the daughter crack. The nucleation of the granddaughter crack occurs a short time ($\Delta t \approx 8$) after nucleation of the daughter crack (Figs. 2 and 3).

The transitions from mother to daughter and daughter to granddaughter cracks are quite sharp, and the crack motion stabilizes after the granddaughter crack is nucleated. Fig. 4 shows a few snapshots of the potential energy field from the initial configuration until the birth of the granddaughter crack. In Fig. 5, we show a blowup plot of the potential energy field close to the crack tip, with crack surfaces highlighted with “larger” atoms in red color. The mother (A), daughter (B) and granddaughter (C) cracks can be clearly identified.

The result suggests that shear dominated cracks along a bimaterial interface can reach the longitudinal wave speed of the stiffer material and can become supersonic with respect to the wave speeds of the soft material. Similar observations have been made in experiments. Rosakis *et al*. (1998) reported crack speeds exceeding the longitudinal wave speed of the softer material and, at least on one occasion, reaching the longitudinal wave speed of the stiffer material. In another experimental study by Wu and Gupta (2000), a crack at Nb-saphire interface was found to approach the longitudinal wave speed of the stiff material. Our results suggest three critical wave speeds for shear dominated interface cracks: The Rayleigh-wave speed of the soft material, the longitudinal wave speed of the soft material and the longitudinal wave speed of the stiff material.

Atomistic studies are particularly suitable for studying the details of processes close to the crack tip. Fig. 6 shows a time sequence of the shear stress field very close to the crack tip during the nucleation of the secondary and tertiary cracks. The results suggest that a peak (concentration) in shear stress ahead of the crack causes nucleation of the daughter and granddaughter cracks. The shear stress peak ahead of the mother crack moves with the shear wave speed of the softer material and is indicated by the arrow in Fig. 6 (b). In Fig. 6 (c), the daughter crack has just nucleated, but there appears another peak in shear stress a few atomic spacings ahead of the daughter crack moving close to the shear wave speed of the stiffer material. In Fig. 6 (d), the granddaughter crack has appeared, as indicated by two shock fronts in the softer material. These observations are, at least qualitatively, in agreement with the mother-daughter mechanism observed for mode II cracks in homogeneous materials (Abraham and Gao, 2000; Gao *et al.*, 2001). The corresponding times of the snapshots are given in the caption of Fig. 6, and can be compared with the crack tip history and crack speed history shown in Figs. 2 and 3. We also encourage the reader to view a movie showing the details of nucleation of the secondary and tertiary crack. The movie may be downloaded from www.markus-buehler.de/slides/modeIIinterface.avi.

VI. DISCUSSION AND CONCLUSIONS

The study reported in this paper shows that cracking along a bimaterial interface is a rich phenomenon. We show that the limiting speed of an interfacial crack is the longitudinal wave speed of the stiffer material. A shear-dominated interface crack can propagate supersonically with respect to the softer material. We find that the crack speed changes discontinuously as the loading is increased, with more detailed analysis revealing a mother-daughter-granddaughter mechanism to achieve the ultimate limiting speed (see Figs. 2 and 3). A clear jump in crack velocity can be observed when the daughter crack is nucleated. However, the nucleation of the granddaughter crack occurs with a more continuous velocity change.

A mother-daughter-granddaughter mechanism in shear dominated cracks has been reported in previous MD simulations of crack propagation along an interface between a harmonic material and an anharmonic material having the same elastic wave speeds under small deformation (Abraham *et al.*, 2002). In the present study, we show that the mother-daughter-granddaughter mechanism not only occurs in nonlinear materials but also for linear elastic bimaterial interfaces. The fact that the mother-daughter-granddaughter mechanism occurs in both systems suggests that the phenomenon is robust and may occur under a wide range of conditions.

The elastic field of an interface crack can be very different from that of a homogeneous crack (Freund, 1990; Buehler *et al.*, 2004a; 2004b). If crack propagation is supersonic with respect to one of the materials, multiple shock fronts are expected. The shock fronts shown in Fig. 5 indicate that crack propagation is supersonic with respect to the soft material. A more detailed comparison of continuum theory and MD simulation is left to future work due to the known

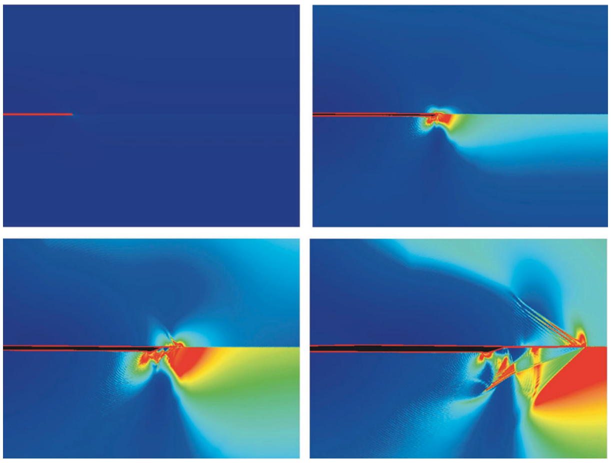

Fig. 4 The plot shows the potential energy field near a shear loaded interface crack with stiffness ratio Ξ=3 (color code: red corresponds to high potential energy and blue corresponds to the potential energy of atoms in a perfect lattice). The plot shows a small section around the crack tip. The crack surfaces are highlighted red. In the upper left plot, the initial configuration with the starting crack is shown. As the loading is increased, the mother crack starts to propagate, eventually leading to secondary and tertiary cracks. Two Mach cones in the soft solid and one Mach cone in the stiff solid can be observed in the lower right figure, suggesting supersonic crack motion with respect to the soft material and intersonic motion with respect to the stiff material.

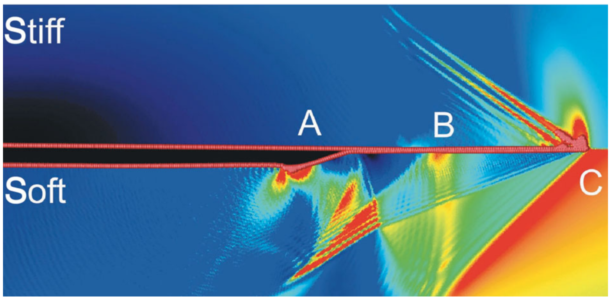

Fig. 5 The plot shows the potential energy field in the vicinity of the crack tip, shortly after nucleation of the granddaughter crack (color code: red corresponds to high potential energy and blue corresponds to the potential energy of atoms in a perfect lattice). The mother, daughter and granddaughter cracks can be identified. In the blow-up on the right, the mother (A), daughter (B), and granddaughter (C) are marked. The mother and daughter cracks are represented by waves of stress concentration in the soft material. For the daughter crack (B), the Mach cone associated with the shear wave speed in the soft material can clearly be observed. The granddaughter crack (C) carries two Mach cones in the soft material.

difficulties related to the oscillatory character of the continuum mechanics solution.

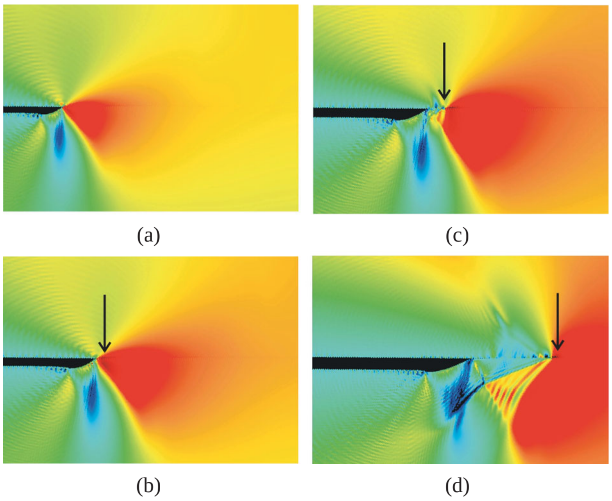

Fig. 6 Shear stress field during the transition from the mother crack (subplot (a)) to propagation of the granddaughter crack (subplot (d)). The analysis of the deformation field suggests that the large shear deformation ahead of the mother crack causes nucleation of the daughter crack. The peak in shear stress is indicated by the arrow in subplot (b), and appears in dark red color. In subplot (c), the daughter crack has nucleated, and there is still a peak shear stress ahead of the crack leading to initiation of the granddaughter crack (subplot (d)). In subplot (d) the granddaughter crack has appeared propagating at the longitudinal wave speed of the stiff material, while leaving two shock fronts in the soft material. Subplot (a)-(d) are taken at times t=82.2, t=98.76, t=104.4, and t=115.2 respectively.

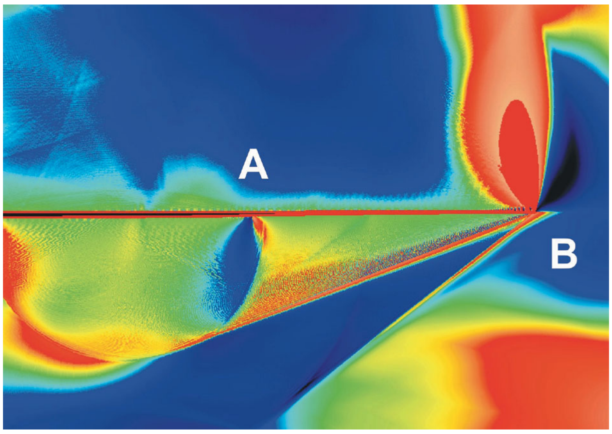

Fig. 7 A tension loaded crack along a bimaterial interface can move at the Rayleigh wave speed of the stiff material. The mother crack is marked "A" and the daughter crack is marked "B". The mother crack transformed into a Rayleigh-surface wave after the nucleation of the daughter crack. The daughter crack propagates at the Rayleigh-wave speed of the stiff material, and moves supersonically with respect to the soft material under the large elastic mismatch (Ξ=10).

We have also carried out similar studies for a tension loaded crack along a bimaterial interface. In this case, we observed a mother-daughter mechanism but not the mother-daughter-granddaughter mechanism. This is surprising to us since mode I cracks in homogeneous materials do not involve secondary daughter cracks (Abraham and Gao, 2000; Gao *et al.*, 2001). Fig. 7 shows the deformation field near a tension loaded interface crack. The crack “A” refers to the mother crack (which transforms into a Rayleigh-surface wave after the birth of the daughter crack), and crack “B” is the daughter crack. The daughter crack propagates at the Rayleigh-wave speed of the stiff material, and moves supersonically with respect to the soft material due to the large elastic mismatch (Ξ=10).

Our results suggest that successive generations of cracks via mother-daughter or mother-daughter-granddaughter mechanisms may be an important aspect of interface cracking. The detailed mechanisms should be subjected to more rigorous mathematical analysis and interpretation. This is left to a forthcoming paper to be published elsewhere.

The present study illustrates that atomistic simulations are feasible for modeling the dynamics of crack propagation along bimaterial interfaces. Combining large-scale atomistic simulations with continuum mechanics is a powerful approach in modern studies of dynamic fracture mechanics.

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