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Brittle Fracture Mechanism breaks the Sound Barrier

Materials scientists discover the conditions under which cracks can propagate supersonically in brittle solids

Glass breaks, rubber bursts—there are numerous ways in which materials can fail under extreme conditions. Many of the atomic mechanisms of materials failure however still remain a mystery. Some materials harden when they are stretched, others soften under large deformation. This phenomenon is referred to as hyperelasticity. Scientists from the Max Planck Institute for Metals Research in Stuttgart and IBM Almaden Research Center in San Jose, California study the dynamics of cracks using the world's most powerful computers, whereby the motion of every single atom in the material is calculated according to Newton's laws of motion. Combining theoretical considerations and large scale molecular dynamics simulations, the scientists derived the conditions under which hyperelasticity governs dynamic fracture. The researchers discovered that cracks can propagate supersonically when hyperelasticity, the elasticity at large strains, becomes dominant within a zone of high energy transport near the crack tip. This is important in understanding the dynamics of earthquakes or nucleation and propagation of cracks in aircrafts and space shuttles (Nature, November 13, 2003). The results are in clear contrast to classical theories in which the speed of elastic waves was considered the limiting speed of fracture, analogous to the speed of light in the theory of relativity.

Historically, the classical physics of continuum has been the basis for most theoretical and computational tools in engineering, and theories relying on numerous phenomenological assumptions have been used. Over the last decades, there has been a new realization that atomic scale behavior is crucial to achieving a more fundamental understanding of how materials fail. There is also the challenge created by the increasing trend to miniaturization in technology as relevant length scales of materials approach the nanoscale. At nanoscales which the continuum description of materials becomes questionable. Scientists use atomic simulations to study how materials behave under extreme conditions. The simulations yield fundamental "ab-initio" information about the mechanisms of deformation and failure at length and time scales unattainable by experimental measurement and unpredictable by continuum theories. With today's supercomputers, systems up to billions of atoms can be simulated, approaching materials size on the order of micrometers! Such length scales are of immediate interest to engineers. It is estimated that the billion-atom simulations will become routine in a few years, underlining the enormous potential of atomistic methods for technological innovations in materials science.

In a recent article in Nature, a team of scientists from Max Planck Institute for

Max Planck Society
for the Advancement of Science
Press and Public Relations Department

Hofgartenstraße 8
D-80539 Munich

PO Box 10 10 62
D-80084 Munich
E-mail: presse@mpg-gv.mpg.de
Internet: www.mpg.de

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Metals Research in Stuttgart and IBM Almaden Research Center in San Jose, California study the dynamics of brittle crack propagation with large-scale atomic simulations. In this article the scientists report the discovery of an important missing feature in the existing theories of dynamic fracture: The elasticity of solids depend on their state of deformation. Metals will weaken, or soften, and polymers may stiffen as the strain approaches the state of materials failure. "It is only for infinitesimal deformation that the elastic moduli can be considered constant and the elasticity of the solid linear," says Prof Dr Huajian Gao, Director at the Max Planck Institute for Metals Research in Stuttgart, Germany. "However, many existing theories model fracture using linear elasticity, and neglect the considerable difference in material behavior at small and large strains. Certainly, this can be considered questionable since materials fail at the tip of a dynamic crack because of the extreme deformation." The scientists hence postulated that hyperelasticity, the elasticity at large strains, can play a governing role in dynamic fracture.

In their studies, the scientists show that hyperelasticity, the elasticity at large strains, can dominate the dynamics of fracture. Cracks moving in solids absorb and dissipate energy from the surrounding material. "We discovered a new length scale characterizing the zone near the crack tip from which the crack draws energy to sustain its motion," says Gao. "When materials are under extreme stress, this length scale extends only a few dozens nanometers."

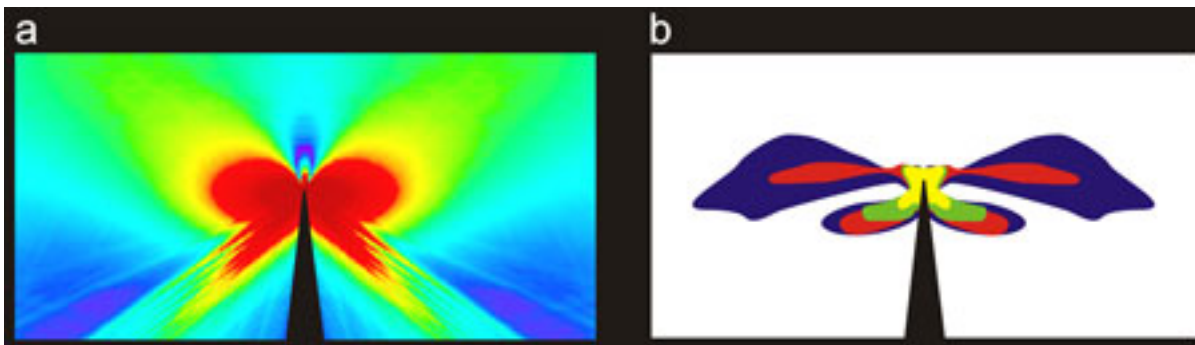


Fig. 1: Plot (a) shows the color map of the magnitude of the local energy flux near a crack tip. The zone colored in red defines a characteristic length scale for energy transport. Plot (b) displays regions of nonlinear (hyperelastic) material response near the crack tip. Hyperelasticity dominates crack dynamics when the size of the hyperelastic region becomes comparable to the characteristic energy length. In this case, the elastic properties associated with large strains dominate energy transport. Therefore the speed of energy transport is modified and the crack speed may become higher or lower. In this case, many phenomena unpredicted and unexplainable by classical theories, such as supersonic fracture, become possible.

Image: Max Planck Institute for Metals Research

This characteristic length scale is found to be proportional to the fracture surface energy and elastic modulus, and inversely proportional to the square of the applied stress. Contrary to the common belief, the crack does not need to transport energy from regions far away from its tip, rather only from a small local region described by the characteristic length scale. Figure 1(a) shows a color map of the magnitude of the local energy flux near the crack tip. The region of significant energy transport shown in red color defines the characteristic length scale. Figure 1(b) displays the region of nonlinear hyperelastic material response.

The assumption of linear elasticity, and hence the classical theories, fails if the hyperelastic zone shown in Fig. 1(b) becomes comparable to the local energy flux zone shown in Fig. 1(a). This is because in soft materials energy is transported slower, in stiff materials faster. Correspondingly, the crack velocity becomes slower or larger once the hyperelastic region is sufficiently large. If the region around the crack tip becomes stiff due to hyperelasticity, more energy can flow to the crack tip in shorter time. On the other side, energy transport gets slower when there is a local softening zone around the crack tip.

Therefore, the scientists conclude that hyperelasticity is crucial for understanding and predicting the dynamics of brittle fracture.

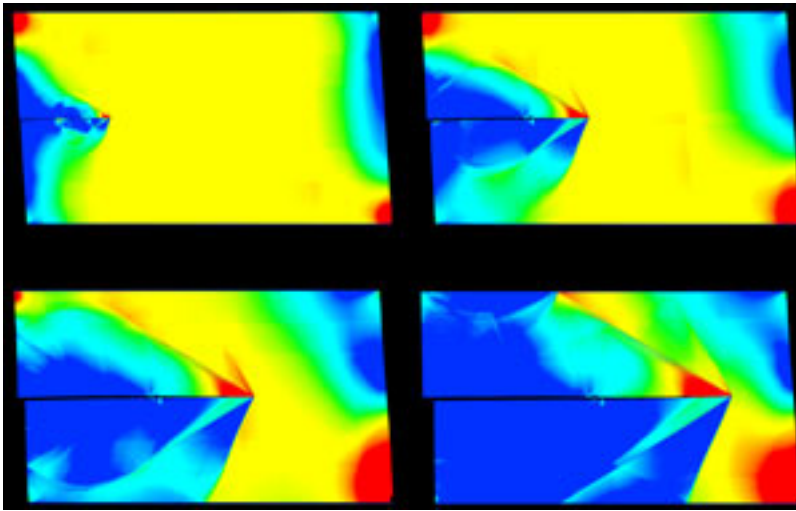


Fig. 2: *Supersonic crack motion. The plot shows the snapshots of a shear dominated crack (similar to an earthquake in California) propagating at a velocity faster than the longitudinal wave speed of the solid. The two Mach cones or shock fronts (analogous to the shock front or sonic boom around a supersonic jet airplane) indicate supersonic crack motion. This phenomenon can not be understood using the classical theories of fracture and is now explained by hyperelasticity models.*

Image: Max Planck INstitute for Metals Research

When hyperelasticity dominates, cracks can move faster than all elastic waves. This is in clear contrast to the classical theories in which it is believed that the longitudinal elastic wave speed is an impenetrable upper limit of crack speed. Figure 2 shows snapshots of a computer simulation where the crack breaks through the sound barrier and propagates at a supersonic velocity (in glass, for instance with a speed higher than 5.300 m/sec, which is greater than 19,000 km/h). Such phenomenon can only be understood through hyperelasticity.

Hyperelasticity dominates fracture energy transport when the size of the hyperelastic zone approaches the energy characteristic length. Under normal experimental conditions, the magnitude of stress may be one or two orders of magnitude smaller than that under atomic simulations. In such cases, the characteristic length is relatively large and the effect of hyperelasticity on effective velocity of energy transport is relatively small. At about one percent of elastic strain, the energy characteristic length is on the order of a few hundred atomic spacing and significant hyperelastic effects are observed. It seems that hyperelasticity can play the governing role especially in nanostructured materials such as thin films, or under high-impact conditions where huge stresses occur, so that the region from which the crack needs to draw energy is small.

The computer simulations reported in the Nature article to prove the concepts of hyperelasticity and energy characteristic length need to attain sufficiently large system sizes, and are hence very resource demanding. These simulations have been performed at the Max Planck Society's Supercomputer Center in Garching, which is among the most prominent scientific computer centers in the world.

Related Links:

[1] [Department Gao, Max Planck Institute for Metals Research, Stuttgart](#)

[2] [Movie of the simulation \(low resolution\)](#)

[3] [Movie of the simulation \(high resolution\)](#)

Original work:

M.J. Buehler, F.F. Abraham, and H. Gao

Hyperelasticity governs dynamic fracture at a critical length scale

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Contact:

Prof. Huajian Gao

[Max-Planck-Institute of Metals Research, Stuttgart/Germany](#)

Tel.: +49 711 689-3510

Fax: +49 711 689-3512

E-mail: hjgao@mf.mpg.de

Markus J. Buehler

[Max-Planck-Institute of Metals Research, Stuttgart/Germany](#)

Tel.: +49 711 689-3579

Fax: +49 711 689-3512

E-mail: m.buehler@mf.mpg.de