NATURE|Vol 464|4 March 2010

MATERIALS SCIENCE

Mind the helical crack

Markus J. Buehler and Zhiping Xu

Catastrophic breakage of brittle materials such as ceramics is usually triggered by the rapid spreading of cracks. Computer simulations have now cracked the three-dimensional details of this process.

Earthquakes, the damage to biological tissues caused by disease, and the wear of materials in aeroplanes share an underlying feature — all eventually reach a point at which the breakdown of material constituents leads to the failure of a functional system. In brittle materials such as ceramics, rocks and glass, a fundamental mechanism of failure is the spreading of cracks, a phenomenon also seen in the shearing of tectonic plates in earthquakes[1]. Even though the phenomenon of fracture is seen throughout our world, the mechanisms by which cracks actually propagate remain largely unknown. On page 85 of this issue, Pons and Karma[2] describe a computational study that reveals the origin of segmented fracture surfaces, which are found widely in fracture phenomena in engineering and geology.

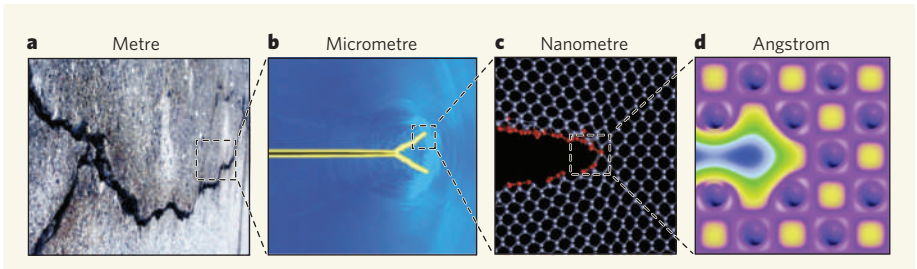
The cracking process is complex, and predicting the path a crack will take remains a challenge. Part of the difficulty is that cracking is a multiscale phenomenon — that is, it depends on mechanisms that operate across multiple length scales (Fig. 1). The spreading of cracks concurrently involves the overall material breakdown at the macroscopic scale, the evolution of crack fronts at intermediate micrometre scales, and the breaking of molecular or chemical bonds on nanometre or angstrom scales[3].

The complexity of the problem is further exemplified by the fact that, even in homogeneous materials, the mechanisms that underlie cracking depend on the speed at which a crack forms as well as the type of loading to which a material is subjected. For example, straight crack propagation becomes dynamically unstable when its speed exceeds a critical value, leading to the loss of smoothness and roughening of the crack's surface[1,3,4]. Similarly, a 'simple' change of a cracked specimen's loading condition from tension to shear (Fig. 2a, b) has a profound impact on the speed of cracking. Whereas, under tension, cracks tend to move slower than the speed of sound, under shear they have been observed to travel at close to and above the speed of sound[1,4,5].

Cracks subject to mixed loading conditions, such as a combination of tension and tearing (Fig. 2c), display a particularly intriguing behaviour. Experimental work by Smekar[6] in the 1950s showed that combined tension–tear loading leads to a distortion of the fracture surface, and that an initially planar crack breaks apart to form multiple daughter crack segments, or fracture 'lances' (Fig. 2c). Sommer[7] later showed experimentally that this phenomenon is due to a helical motion of crack fronts around the principal direction of crack propagation. In a pioneering contribution, Gao and Rice[8] subsequently proved theoretically that an initially planar crack must indeed rotate under combined tension–tear loading.

However, these analyses of cracking under combined tension–tear loading did not reveal the dynamic mechanisms by which fracture lances form. Pons and Karma's computer simulations[2] now describe the three-dimensional details of the crack-front evolution under such mixed loading. An intriguing finding of their analysis is that the spacing between fracture lances increases as the crack propagates, effectively resulting in a coarsening of the segmented surfaces as the crack moves. Notably, this coarsening is also seen in experimental studies of cracks under combined tension–tear loading. By taking material properties such as elastic constants for both glass and plexiglass (polymethylmethacrylate, or PMMA), the authors show that key geometric features predicted by their simulation, such as the initial spacing between the fracture lances and their rotation angles, agree well with experiments.

Pons and Karma's study of crack paths is based on the phase-field approach, a model that describes both macroscopic material properties and materials failure on intermediate microscopic scales. But the approach does not explicitly resolve the structure of materials at the atomic scale. Methods that provide higher resolution — for example, atomistic models[3,4] — may offer more insight. After all, fracture of materials involves the breaking of atomic or molecular bonds (Fig. 1), and therefore the



a, S. PUETZER/PHOTOLIBRARY.COM

Figure 1 | Multiscale cracking. Crack spreading in brittle solids such as rocks or ceramics involves mechanisms that span a vast range of scales: **a**, macroscopic metre-scale events, for example rock fracture caused by an earthquake; **b**, mesoscopic micrometre-scale evolution of cracks; **c**, atomistic nanometre-scale details of the geometry of the crack tip; and **d**, breaking of chemical bonds at the angstrom scale.

detailed mechanisms by which bonds break could be important for the formation and evolution of fracture lances.

The study of how materials fail is crucial to our ability to engineer better ones — for example, to create lighter, stronger and tougher materials. The emergence of instability fracture mechanisms such as those studied by Pons and Karma tend to make it more difficult for cracks to spread because they increase the energy required for a crack to move forwards, thereby enhancing a material's overall resistance to catastrophic failure. The design of novel materials by deliberately invoking instability fracture mechanisms — perhaps through the creation of material structures that induce local combined tension–tear loading — could provide a powerful strategy to increase a structure's resistance to failure without the need to introduce additional material components, instead relying solely on structural changes.

An intriguing direction in which Pons and Karma's idea could be taken is the study of failure in biological materials — for example, spider silk, nacre and bone. In these materials, better resistance to fracture is achieved not through the addition of stronger materials but rather by reliance on a hierarchy of structures, in which each hierarchical level has its own fracture mechanism. The synergistic effect of fracture mechanisms at all levels, attained through a seamless merger of structure and material, achieves an overall performance that vastly exceeds that of each individual level. Although we rely on strong element bonding in the design of most engineered materials — such as covalent bonds in glass or polymers, or metallic bonds in steel — bonding in biological materials is often weaker. For example, spider silk is one of the strongest materials known (stronger than steel), yet its strength lies in the cooperation of extremely weak hydrogen bonding between protein molecules[9]. The effective use of multiple structural levels enables biological materials such as silks to achieve high performance without relying on strong bonding.

From a slightly different viewpoint, the breakdown of biological materials' capacity to effectively withstand fracture can lead to injury and disease, as observed, for example, in osteogenesis imperfecta (brittle-bone disease). As such, the study of fracture could also help us to understand the mechanisms that underlie severe diseases and perhaps provide new pathways for treatment.

Pons and Karma's work[2] shows that a computational approach, validated by experiment, is a powerful tool in explaining fundamental issues in materials failure. The emergence of computational materials models that involve multiple scales[10], from the atomic to the macroscopic, holds great promise in elucidating the complex facets of how materials fail, and could lead to exciting breakthroughs in our understanding of material breakdown in engineering, geology and biology. ■

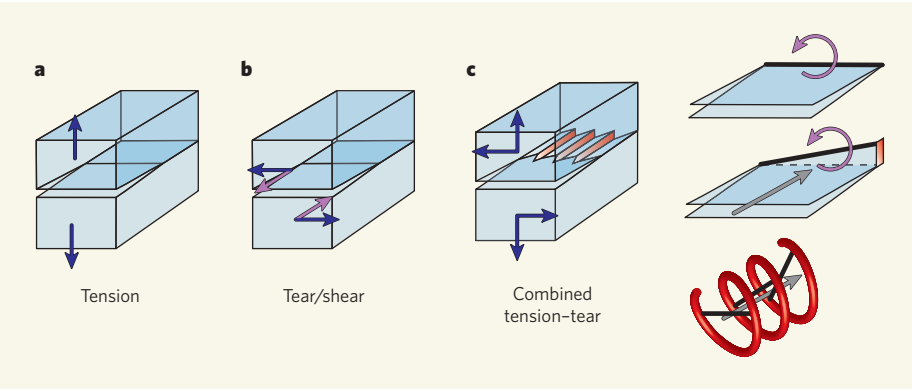


Figure 2 | Cracked specimen under different types of loading. a, Tension. **b**, Tear/shear (dark blue arrows for tear, pink arrows for shear). **c**, Combined tension–tear; under mixed tension–tear loading, an initially planar crack splits into several daughter cracks, or fracture 'lances' (red). This splitting is caused by a helical rotation of the crack front (thick black lines in right panel) around the principal direction of crack propagation (grey arrow). Pons and Karma's computational study[2] describes the three-dimensional details of crack-front evolution under such mixed tension–tear loading.

Markus J. Buehler and Zhiping Xu are at the Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering, and the Center for Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA.
e-mail: mbuehler@mit.edu

1. Freund, L. B. *Dynamic Fracture Mechanics* (Cambridge Univ. Press, 1990).
2. Pons, A. J. & Karma, A. *Nature* **464,** 85–89 (2010).
3. Fineberg, J. & Marder, M. *Phys. Rep.* **313,** 1–108 (1999).
4. Buehler, M. J. & Gao, H. *Nature* **439,** 307–310 (2006).
5. Sekiguchi, H. & Iwata, T. *Bull. Seismol. Soc. Am.* **92,** 300–311 (2002).
6. Smekar, A. *Oesterr. Ing. Arch.* **7,** 49–70 (1953).
7. Sommer, E. *Eng. Fract. Mech.* **1,** 539–546 (1969).
8. Gao, H. & Rice, J. R. *ASME J. Appl. Mech.* **53,** 774–778 (1986).
9. Keten, S., Xu, Z., Ihle, B. & Buehler, M. J. *Nature Mater.* doi:10.1038/nmat2704 (in the press).
10. Liu, W. K., Karpov, E. G. & Park, H. S. *Nano Mechanics and Materials: Theory, Multiscale Methods and Applications* (Wiley, 2006).