MATERIAL WITNESS

PARTICLE TRAPS

There was a time when a paper reporting a computer simulation might, in some fields (notably, molecular biology), be rejected purely on the grounds that it contained 'no experimental results' — simulation was seen as building castles in the air, disconnected from objective reality. Some now argue that, on the contrary, computer simulation is approaching the status of experiment, providing glimpses of what the real atoms and molecules in the corresponding material system are up to.

For non-practitioners, that latter view seems increasingly plausible. Surely the enormous increase in computing power must be enhancing the capabilities of simulation, allowing it to encompass bigger systems and to incorporate more of the nuances of molecular behaviour? It is sometimes whispered that we'll soon simulate a complete living cell or follow a crack all the way from atomic inception to the collapse of a bridge.

It's undoubtedly true that computer simulation can now handle systems of a complexity unimaginable when, for example, Nicholas Metropolis and his collaborators proposed a method in 1953 for sampling probability distributions in what became the Monte Carlo algorithm. But the allure of computational muscle for understanding molecules and materials has sometimes fooled researchers into imagining that sheer number-crunching offers a transparent and reliable predictive tool, a kind of virtual microscope for the molecular world.

Being misled by computer simulation is not necessarily a mark of naivety. Even experienced practitioners can be derailed by bugs, spotted only via an obstinate irreproducibility. But aside from coding glitches, simulations present a host of subtleties that may trip the unwary, as Daan Frenkel of Cambridge University explains in a recent preprint stemming from a summer school at Varenna in Italy (D. Frenkel, http://www.arxiv.org/abs/1211.4440).

Frenkel's examination of the pitfalls — as he puts it, the "dark side" — of simulation offers many warnings that fellow experts know well. But in aggregate, they create a timely reminder, as the possibilities of computer simulation seem poised on the threshold of almost limitless potential, of what this sort of modelling truly entails: to put it bluntly, a cartoon version of molecular interactions that are themselves often imperfectly understood, hedged around with compromises yet offered in a proliferation of varieties whose relative merits may be poorly known.

Even well-explored issues such as boundary conditions may remain slippery. For example, structured materials such as smectic liquid crystals might find themselves confined to an inadequate configuration space unless the boundary conditions enable lateral interlayer exchange of particles. And a classic algorithm such as the 'particle insertion' method for determining chemical potentials is complicated for crystalline systems in which vacancies play a central role. It's all too tempting to assume, meanwhile, that molecular dynamics provides actual rather than merely possible time trajectories — a distinction particularly important for, say, investigating protein-folding mechanisms.

Beyond technical details, Frenkel supplies a selection of the myths that any field is liable to accumulate: what boundaries and free-energy landscapes do and do not mean, for instance. Some of these myths are still matters of opinion, and Frenkel freely admits that a paper like this will contribute to them as well as explode them. ❐

PHILIP BALL

MECHANICAL FAILURE

Imaging cracks in hostile regimes

The evolution of microcrack damage in materials under hostile thermal and mechanical conditions has now been imaged in three dimensions by real-time *in situ* X-ray microtomography.

Philip J. Withers

Our understanding of the physical world has progressed hand in hand with our ability to observe it. For instance, computer tomography (CT) — which was originally developed for medical imaging — has been instrumental in the non-destructive testing of materials. In CT, a digital three-dimensional replica of the object under observation is reconstructed from hundreds or thousands of two-dimensional projections (radiographs) collected at different illumination angles using X-rays, neutrons or other penetrating wave beams. Because the images are collected non-destructively, CT can be applied repeatedly to follow how the structure of a material changes over time. In fact, it is now possible to

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study in real time and in three dimensions (3D) degradative processes of structural materials under realistic conditions — such as ceramic- and polymer-matrix composites for aerospace or nuclear-fusion applications — by using environmental rigs. However, designing rigs to study such materials under extremes of temperature and loading is a significant engineering challenge because the rigs must not significantly impede the view of the sample as it is rotated. As described in *Nature Materials*, Bale and co-authors have now developed an environmental rig suitable for real-time CT to probe, at the micrometre scale and in 3D, the progressive failure of ceramic matrix composites operating under load and at temperatures above 1,600 °C (ref. 1). Their method provides unprecedented insights on the failure of this class of materials, and should make it possible to quantitatively image the events leading up to failure for a wide variety of high-performance materials operating under hostile thermal and mechanical environments.

Rapid developments in CT allow for a wide range of structural scales in 3D to be probed. Imaging resolutions from hundreds of micrometres on metre-sized samples to tens of nanometres on micrometre-sized samples are achievable with today's laboratory or synchrotron sources. Also, processes that occur over a wide range of timescales can be followed. For example, creep or corrosion, which typically occur over weeks or months, are well suited to studies using laboratory sources, whereas the subsecond frame rates achievable at synchrotron sources (at present as fast as 10 milliseconds per dataset in 3D) can provide insights into faster events, such as hot cracking[2,3] (also known as hot tearing), which occurs in casting during the final stages of metal solidification when the solid fraction becomes high (Fig. 1a).

There has been a progression in the capabilities of environmental rigs that can be accommodated on CT instruments. Small self-contained environmental rigs[4] that can sit on the rotation stage of tomography scanners have provided access to a broad range of thermal, corrosion and mechanical environments *in situ*, and allowed, for example, hot tearing to be studied (Fig. 1a). Recent extensions to more hostile thermal conditions have required the development of more complex rigs, such as those used to study the cracking of frozen soil[5] (Fig. 1b). To gain access to extremely high temperatures, laser-heating arrangements have been used[1,6]. Such developments are shedding light on a whole range of processes that could not previously be observed in 3D, such as failure processes of high-performance engineering materials operating under extreme conditions.

Although the high-temperature stability of many engineering ceramics makes them attractive for applications in hostile conditions (such as those in a turbine engine), the characteristically low toughness of these materials has limited their widespread use. Still, toughness — and thereby the resistance to catastrophic cracking — can be enhanced through tailored microstructural complexity. For this, the competition between the intrinsic damage mechanisms occurring ahead of the crack and the extrinsic shielding mechanisms that limit local crack growth need to be understood and controlled. Although there are many microstructural mechanisms available to control crack growth that can be observed and quantified by X-ray tomography (Fig. 2), not all of them can be exploited at high temperature. The usual approach for high-temperature ceramics has been to take advantage of weak or sliding interfaces to absorb energy, and to bridge or deflect the crack using laminated or fibrous composite systems. However, it has been difficult to quantify the efficacy of these mechanisms at the extremes of temperature at which these materials are designed to be used. For instance, in certain cases interfacial friction may decrease with increasing temperature, leading to reduced strength and energy absorption, whereas chemical reaction can cause other interfaces designed to be relatively weak to become too strong at high temperature[7]. In this regard, the thermomechanical environmental rig described by Bale and colleagues promises to provide information that will guide and accelerate the development of tough, high-temperature ceramics with engineered interfaces. In fact, in addition to providing data on crack paths, crack bifurcation and crack-opening displacements (the latter can be used to quantify crack-tip shielding and the local crack driving force[8]) the authors have shown that CT measurements can

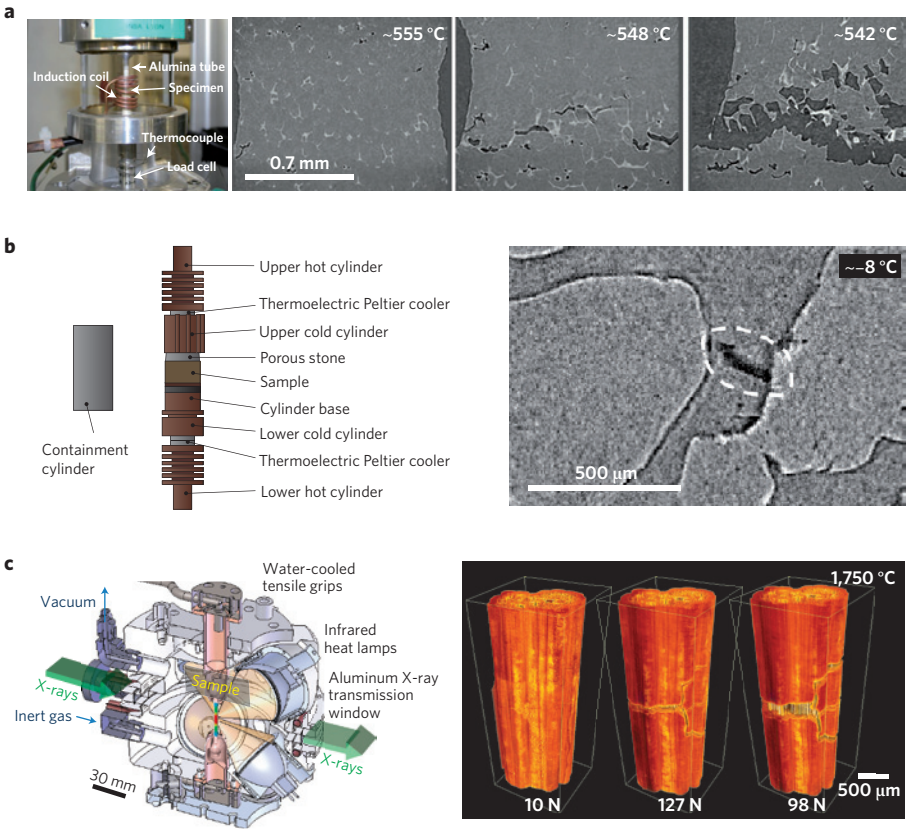

Figure 1 | By combining computer tomography with environmental rigs (leftmost image in all panels) new regimes of damage can be imaged. **a**, Hot tearing in an Al-8 wt% Cu alloy deformed at a strain rate of 2×10^{-4} s^{-1} while cooling at a rate of about 1.2 °C min^{-1}. **b**, A crack (circled) formed in the ice between two particles of sand at −8 °C. **c**, SiC–SiC single-tow failure at very high temperature (1,750 °C) showing the pull-out of fibres as the displacement of the microcrack opening increases. Image reproduced with permission from: **a**, ref. 3, © 2012 Springer; **b**, ref. 5, © 2012 Wiley; **c**, ref. 1, © 2012 NPG.

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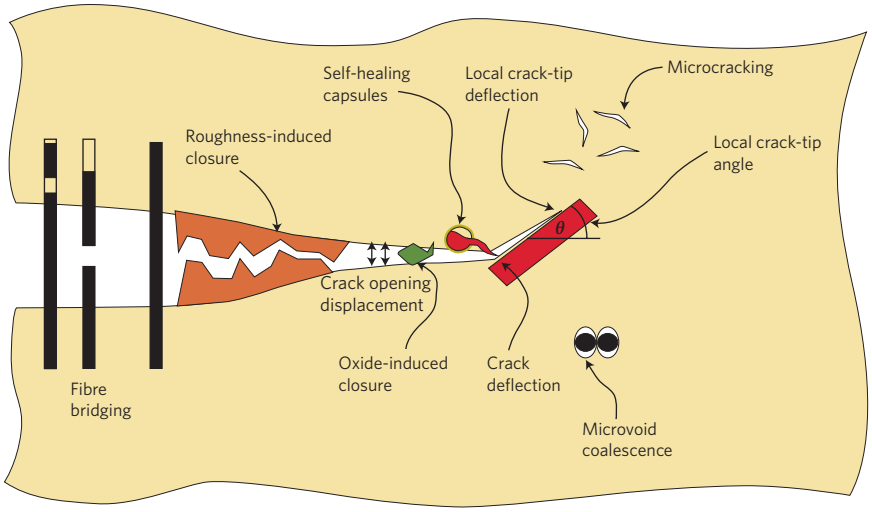

Figure 2 | A wide range of toughening mechanisms can be observed and quantified by X-ray computed tomography, many of which are critical to the toughening of high-temperature ceramics. Image reproduced with permission from ref. 9, © 2012 AR.

also be used to evaluate the pull-out of SiC fibres from single SiC–SiC composite tows at 1,750 °C (Fig. 1c), thereby establishing the interfacial frictional sliding stress for pull-out (0.4 MPa versus 2 MPa at room temperature) and hence the capacity for energy absorption[1]. Indeed, the authors' X-ray microtomography approach and the wealth of information it can generate should speed up the optimization of the interfacial properties of materials under static and fatigue loads to further tailor their high-temperature toughness. ❐

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References

1. Bale, H. A. *et al. Nature Mater.* **12,** 40–46 (2013).
2. Puncreobutr, C., Lee, P. D., Hamilton, R. W. & Phillion, A. B. *JOM* **64,** 89–95 (2012).
3. Suéry, M. *et al. JOM* **64,** 83–88 (2012).
4. Buffiere, J. Y. *et al. Exp. Mech.* **50,** 289–305 (2010).
5. Bhreasail, A. N. *et al. Permafrost Periglac.* **23,** 170–176 (2012).
6. Fife, J. L. *et al. J. Synchrotron Radiat.* **19,** 352–358 (2012).
7. Hung, Y-C. & Withers, P. J. *Acta Mater.* **60,** 958–971 (2012).
8. Withers, P. J., Lopez-Crespo, P., Kyrieleis, A. & Hung, Y-C. *Proc. R. Soc. A* **468,** 2722–2743 (2012).
9. Withers, P. J. & Preuss, M. *Annu. Rev. Mater. Res.* **42,** 81–103 (2012).

NANOSCALE HEAT TRANSFER

Single hot contacts

Measurements of heat transport across polished nanoscale contacts formed between the tip of a scanning thermal microscope and a surface support the notion that their true contact area consists of discrete atomic contact points.

Yifei Mo and Izabela Szlufarska

What does the interface between two solid objects in close contact look like on a molecular scale? What physical and chemical processes take place at such an interface? And how are forces, heat or electric currents transferred across it? The fact that these questions remain for the most part unanswered underlines the fundamental difficulties in understanding nanoscale friction, which in great part arise from the lack of well-developed experimental techniques that would allow imaging of individual atoms and molecules when they are buried in between two surfaces in close contact. Writing in *Nature Materials*, Bernd Gotsmann and Mark Lantz show that measurements of the pressure dependence of heat transfer across polished nanoscale contacts agree with a model that assumes quantum thermal transport across individual atomic contact points[1]. Their findings provide indirect evidence on the nature of nanoscale roughness.

At the macro- and microscales, the true or real contact area between two solid bodies — which governs most physical behaviour at the interface, including friction and heat transfer[2,3] — consists of a large number of discrete contact points (Fig. 1a,b). At the nanoscale, however, the nature of the true contact area, or even whether the contact area can be well defined, are still a matter of debate[4–6]. On the basis of molecular simulation results, it has been proposed that in many situations nanoscale contacts cannot be treated as smooth (Fig. 1c), but instead they can be viewed as consisting of discrete atomic contact points that behave analogously to real contacts at larger length scales[4] (Fig. 1d). Still, limitations in experimental characterization techniques have precluded experimental verification.

The work of Gotsmann and Lantz is a strong voice in this debate. Using a scanning thermal microscope (Fig. 2a), the researchers found that the thermal conductance across single-asperity contacts that are tens of nanometres in size increases linearly with the applied normal pressure (Fig. 2b). Strikingly, this dependence is inconsistent with the common assumption that a nanometre-sized contact is atomically smooth and continuous. A straightforward explanation is that the contact is rough, and hence that only a small fraction of the interfacial area contributes to the heat transfer. Furthermore, the researchers discovered that existing theories of thermal transport, which assume that thermal conductance is not quantized, predict a much weaker dependence of heat conductance on pressure than the dependence measured experimentally. By comparing their experimental results to different contact models, Gotsmann and Lantz concluded that the true contact area of a nanoscale contact comprises individual discrete atomic contact points

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