Table 1 Volume ratio of oxygen anion and several cations in 6 coordination

Ion	Ionic radius (pm)	Volume ratio (O = 1.0)
O^{2+}	140	1.00
Si^{4+}	40	0.02
Mg^{2+}	72	0.14
Fe^{2+}	78	0.17

Such simulations will be particularly useful for gaining a better understanding of phenomena such as amorphization or phase transition in liquids because the structural information for these materials obtainable through X-ray diffraction technique alone is simply insufficient.

The results by Huang and co-authors represent a clear example of how the rapid development of computer hardware and the consequent capability to handle more complex algorithms make computer simulation a very powerful tool to compensate for the limits of X-ray diffraction techniques. Could simulation ever replace experiments? Although it may be tempting to draw this conclusion, it is rather unlikely. Let us take, for example, the discovery of the post-perovskite phase in 2002, at 120 GPa and 2,000 K (ref. 7). This unexpected observation, which disproved the long-standing belief that the perovskite-type $MgSiO_3$ is the stable phase at the bottom of the Earth mantel, triggered several studies aimed at understanding the elastic and plastic properties of this phase[8,9,10]. In this case, the role of computer simulation is essential because experiments under such extreme conditions are extremely difficult, if at all possible. However, no theoretical work has ever predicted the existence of this post-perovskite. Computer simulations therefore stand as a very powerful aid to experiments, but cannot substitute them.

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MATERIAL WITNESS

Pulling a leg

Bone gets tough by relaying strain down its levels of hierarchical microstructure in diminishing amounts. So say Himadri Gupta of the Max-Planck Institute of Colloids and Interfaces in Potsdam, Germany, and colleagues (*Proc. Natl Acad. Sci. USA* doi:10.1073/pnas.0604237103; 2006). At each stage the load transferred gets smaller, which is why, when it gets to the mineral phase (hydroxyapatite), the crystals don't snap.

Hydroxyapatite is stiffer and stronger than the collagen matrix that surrounds it, but is also more brittle. That's why the tensile strength of bone plummets by more than an order of magnitude if the organic phase is removed.

So why use brittle mineral anyway? Tough, stiff materials can certainly be made from organic fabrics alone: look at wood, horn or insect cuticle. But protein is physiologically expensive, and an entire mammalian skeleton of it perhaps carries too high a price. Minerals offer stiffness, but at the cost of brittleness. The celebrated case of nacre reveals one solution: absorption of energy by crack deflection at the weak interfaces of an inorganic–organic laminar composite.

But bone is different. The mineral here isn't disposed in large sheets, but in oriented nanoscale platelets embedded within collagen fibrils. The fibrils themselves, about 100 nm across, are packed in parallel within an organic extrafibrillar matrix. There are higher levels of structural organization: concentric lamellar cylinders called osteons, which may themselves be woven into porous structures. There are many types of bone in different organisms and body parts, with different degrees of mineral content, porosity and structural organization.

Gupta and colleagues have investigated the archetypal form: cortical bone from the femur of an ox. They point out that, whatever the function of the higher-order structure, it must ultimately derive from the nanoscale behaviour.

Christine Ortiz and colleagues at MIT suggested that the compressive strength of bone comes from friction between the inorganic grains (*Nano Lett.* 6, 2520–2525; 2006), with the organic phase playing little part. But for the tensile stresses applied by Gupta *et al.*, it's another story. Using X-ray diffraction to monitor the strains in the fibril and mineral components of bone as it is stretched to breaking point, they find that the strain is passed down a hierarchical chain in ever-decreasing amounts.

The strain in the overall bone tissue is more than twice that in the fibrils, indicating that much of the deformation is taken up by the matrix between fibrils. Equally, the strain in the fibrils is 2.5 times that in the mineral platelets, the difference being accommodated by the collagen. This lets the various materials do what they do best: the mineral phase stiffens but does not experience strains that test its brittleness.

If that's right, bone is governed by different properties in tension and compression — the criterion that Julian Vincent of Bath University in the UK proposes as the signifier of a 'structure' rather than a true 'material'.

Philip Ball