

predict that its crystal structure will distort unexpectedly when subjected to the conditions at the centre of the Earth. Together with a model of the orientation of iron crystals in the inner core by Buffett and Wenk⁵ (see page 60), these results can explain the observed seismic anisotropy.

The inner core is believed to be made up of iron crystals in the hexagonal close-packed (h.c.p.) structure (Fig. 1b). So the observed seismic anisotropy must arise from differences in the elastic response of h.c.p. iron — that is, how fast compressional waves travel in different directions through the crystal. (Acoustic anisotropy is the rule for all crystal structures, rather than the exception.) To understand the microstructural origin of this elastic anisotropy requires knowledge of the properties of iron at extreme pressures (about 330 gigapascals) and temperatures (about 6,000 K). One problem dogging progress so far has been that these pressure and temperature conditions are hard to create simultaneously, whether in the laboratory or in theoretical calculations. An earlier attempt at computer simulation of elasticity from first principles, for example, had to ignore the effects of temperature altogether, settling for absolute zero⁶.

So why do the new calculations work? Steinle-Neumann *et al.*⁴ have produced a detailed theoretical prediction of the elastic properties of pure iron at core pressure and temperature that uses a quantum-mechanical treatment of the electrons in iron interacting both with the slower-moving atomic nuclei and with each other. This method, known as density-functional theory (DFT), has a long pedigree and has underpinned many accurate predictions of crystal structure and elasticity at low temperatures. But to calculate high-temperature properties, the thermal vibrations of the atomic nuclei must also be considered. The frequencies of these vibrations have a range that depends in turn on the quantum-mechanical forces exerted by the electrons. So a correct treatment of the nuclear motion is far more demanding than for nuclei assumed to be stationary at absolute zero.

Steinle-Neumann *et al.* solve this problem by resurrecting a technique known as the particle-in-a-cell method (used well over 30 years ago when atomic modelling was limited by the available computational power) and combining it with much more sophisticated electronic-structure methods. They have been able to include the effects of thermal vibration, and predict the effects of temperature on iron up to 8,000 K. Their work complements recent calculations on the high-temperature thermodynamics of iron at core conditions⁷.

The authors find that the high temperatures significantly increase the ratio of the lengths of the unit cell, known as c/a , of a single crystal of h.c.p. iron (Fig. 1b). This

change in c/a produces changes in the elasticity that in turn control the speed of seismic waves for different propagation directions in the crystal. At core temperatures of 6,000 K, compressional waves travel about 12% faster in the basal (a - b) plane of h.c.p. iron than along the c -axis (Fig. 1b). This elastic anisotropy is much stronger than expected and means that about 30% of iron crystals in the core need to be preferentially aligned, easing requirements suggested by previous calculations for almost 100% alignment. The calculation nicely explains the high Poisson's ratio — the ratio of material strain perpendicular and parallel to an extensional force — of the inner core.

But calculating the properties of a single iron crystal is not enough to determine the elastic properties of the whole inner core. It also needs a model describing the collective evolution of the orientations (texture) of many single crystals (grains) in the core. Texture can be generated by forces acting on and restructuring the core material, or it can be intrinsic to the crystal growth process. No mechanism has yet been proposed that satisfies all geodynamic criteria.

Buffett and Wenk⁵ offer a new mechanism: electromagnetic forces acting on the inner core that arise from generation of the Earth's magnetic field in the outer core. The authors generate a model of the flow response of the inner core under magnetic stress and calculate the induced plastic (irreversible) deformation. Their model includes a step-by-step statistical simulation of grain growth from an initial random orientation, and takes into account mechanisms by which planes of atoms slide over one another, and the potential recrystallization of iron at high temperature. Calculations of the average seismic wave speeds using this texture model and the updated elastic constants of Steinle-Neumann *et al.* produce a travel-time difference in agreement with seismic observations.

As Buffett and Wenk point out, many other geodynamic effects have yet to be incorporated into models of inner-core growth, and several physical parameters used in their model are not reliably known. Moreover, the observed variation of the seismic anisotropy with depth is hard to reproduce and reflects the difficulty of determining the rate of strain accumulation relative to inner-core growth. Including the effects of high-temperature recrystallization in the model also seems to lead to stronger anisotropy than is observed.

Nonetheless, high-pressure experiments have yet to catch up and provide comparable elasticity data for iron at core temperatures. Such experiments might address the assumption that a small deviation from an inner core of pure iron has a negligible effect on elasticity and grain growth. Coupled with the prospects for clearer three-dimensional images from seismology, it may then only be a matter of time before another round



100 YEARS AGO

"I returned, and saw under the sun, that the race is not to the swift, nor the battle to the strong," wrote the wise man. Writing in the same prophetic vein, M. J. de Bloch in the current *Contemporary Review*, and Mr. H. G. Wells in the *Fortnightly* for September, depict in graphic colours the transformation which the immediate future will witness in the methods of warfare. Both writers are convinced that the military tactics of the past are irretrievably dead. The effective soldier of the future will be a man whose capacity for individual action has been cultivated and developed... Mr. Wells takes into account the resources which modern science has made available for the business of war, and proceeds to anticipate the most likely directions that future advances will take. Of one thing he leaves his reader in no doubt, victory is bound to be with the nation that most sedulously attends to the education of its people in the scientific method. The great war of the future will be fought by citizens familiar with destructive instruments of precision, who have learnt to utilise all the accessory helps which science is gradually perfecting.

From *Nature* 5 September 1901.

50 YEARS AGO

According to Dr. Grantly Dick Read, the influence of fear on social structure is not well understood or appreciated... Practically the whole basis of human communal existence today, he suggests, is influenced by fear; man's mental and physical health vary as to his ability to remain balanced in the face of fear. Dr. Dick Read also suggests that children are not only emotionally influenced from the moment of their birth but even from the moment of conception. At fifteen weeks the reflexes of the foetus indicate individuality of behaviour. From birth the child is regularly subjected to stimuli which induce fear and lead to insecurity. According to its nature the child risks rebellion in violence or excessively anti-social behaviour, or resolves into that submissive state when even attempted activity of any sort, or any expression of its individuality, is paralysed by the deeply implanted fear of consequences. Dr. Dick Read believes that much of this unnecessary fear with its harmful effects on the individual and society would be eliminated if the fear of child-birth in women were eliminated.

From *Nature* 8 September 1951.