latitudinal bands in the Sun's northern and southern hemispheres. Two distinct reversals can be seen, at radial distances of about 0.9 $R_\odot$ and 0.8 $R_\odot$. Such profiles imply a large-scale flow field consisting of two distinct circulation cells, as illustrated in figure 2b.

A two-cell meridional circulation doesn't come as a complete surprise. Other researchers have speculated on its existence from indirect experimental evidence and numerical simulations. "But this new evidence is currently the most compelling," says Mark Miesch of the National Center for Atmospheric Research in Boulder, Colorado.

The results could prove problematic for some solar dynamo theories. In particular, one popular class of models—the so-called flux-transport dynamo models—has long relied on a single circulation cell to explain phenomena associated with the 11-year solar activity cycle.[5] For instance, sunspots—cool, dark patches on the solar surface that form when magnetized plasma bubbles up from the convective zone's floor—appear at mid latitudes early in the cycle and at progressively lower latitudes as the cycle proceeds.

Flux-transport dynamo models attribute that equatorward migration to the meridional flow at the bottom of the convective zone. But in a two-cell pattern—or any even-celled pattern—that flow is toward the poles, not the equator.

A potential saving grace for the flux-transport models is the possibility of a third meridional cell squeezed in between 0.7 $R_\odot$, the radial distance of the convective-zone floor, and 0.75 $R_\odot$, the distance corresponding to Zhao and coworkers' deepest measurements. The HMI will continue collecting data for at least three more years, which should allow Zhao and his coworkers to extend their measurements deeper, perhaps to the convective zone's floor. If those studies don't reveal a third reversal, there may be little wiggle room left for flux-transport dynamo models of the solar cycle.

Ashley G. Smart

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Ceramic nanolattices hold up under pressure

At the right size scale, a brittle substance becomes strong and springy.

Apply a large enough stress to a piece of brittle material and it will break—most likely at a preexisting flaw or weak spot. Flaws thereby reduce the fracture strength of real materials relative to their theoretical maxima, sometimes by orders of magnitude. That reduction can be well predicted by the expected statistical distribution of flaw sizes, which depends on the sample's size.

Reduce the sample's dimensions below a micron or so and the picture changes. Submicron single crystals of metal or ceramic, whether they contain flaws or not, are much stronger than their bulk counterparts.[1] Furthermore, a submicron sample is no more likely to break at a flaw than anywhere else. The reasons for that size effect remain unclear. But it's been noted that fracture-resistant biomaterials—such as shells, bone, and tooth enamel—are made up of just such submicron mineral crystals embedded in a protein matrix.[2] (For more on the structure and properties of bone, see the article by Rob Ritchie, Markus Buehler, and Paul Hansma, PHYSICS TODAY, June 2009, page 41.) The secret of their strength may lie in the size effect.

Now Julia Greer and colleagues have taken a step toward exploiting the size effect to produce strong, lightweight materials.[3] They fabricated lattices with submicron dimensions, such as the one shown in figure 1, made up of hollow struts of titanium nitride, a brittle ceramic. Under deformation, the lattices exhibited material properties close to the theoretical limit for TiN.

Smaller is stronger

Two years ago researchers at HRL Laboratories in Malibu, California, and their collaborators (including Greer) developed a technique for building hollow metal lattices.[4] (See PHYSICS TODAY, January 2012, page 13.) Those lattices had some extraordinary material properties—most notably, their ultralow density. But their unit cells had dimensions of hundreds of microns to millimeters, far too large to exhibit the size effect.

Greer and colleagues used similar techniques to construct their TiN lattices, with some important modifications to allow them to reach a 100-times-smaller size scale. First, to produce a polymer scaffold using a negative photoresist (a liquid polymer that hardens when exposed to bright light), they programmed a computer-controlled focused laser to "draw" the desired three-dimensional structure in the liquid photoresist. Then they deposited alternating monolayers of titanium and nitrogen onto the scaffold to form a 75-nm layer of TiN. Finally, they etched away the polymer scaffold using an oxygen plasma treatment.

To test the strength of their TiN lattices, the researchers applied a compressive load while observing the sys-

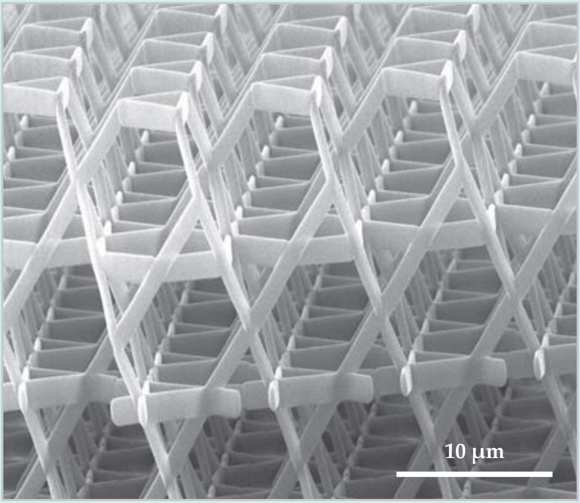

Figure 1. A hollow ceramic nanolattice with a three-dimensional kagome structure. Each of the several-micron-long struts is a tube with an elliptical cross section, 1 μm × 250 nm, and a wall thickness of 75 nm. (Courtesy of Lucas Meza and Lauren Montemayor.)

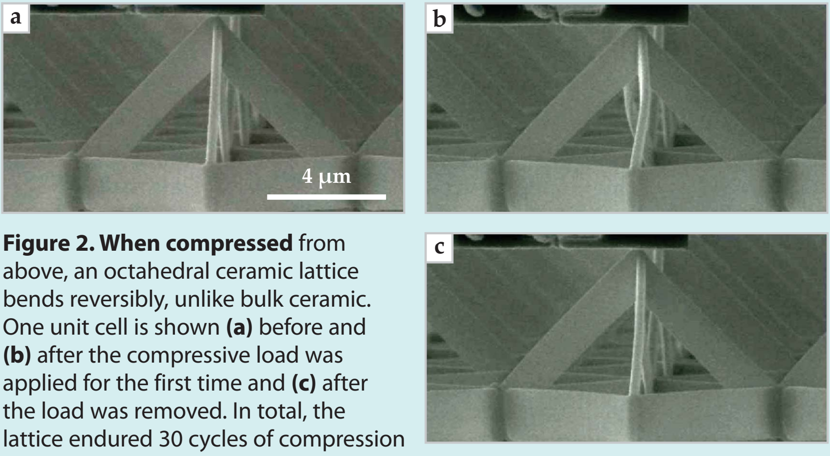

Figure 2. When compressed from above, an octahedral ceramic lattice bends reversibly, unlike bulk ceramic. One unit cell is shown **(a)** before and **(b)** after the compressive load was applied for the first time and **(c)** after the load was removed. In total, the lattice endured 30 cycles of compression and still recovered nearly its original shape. (Adapted from ref. 3.)

tem with a scanning electron microscope, as shown in figure 2. When an octahedral lattice was distorted until it broke, it exhibited a tensile strength of 1.75 GPa. (Even though the lattice as a whole was compressed, the failure occurred in a component that was under tension.) In comparison, the theoretical tensile strength for flawless TiN is estimated to be 3.27 GPa. Typical real bulk samples of TiN and other brittle ceramics have tensile strengths in the tens to hundreds of megapascals.

Furthermore, unlike bulk TiN, the lattices could bend significantly without breaking and spring back nearly to their original shape, even after 30 cycles of deformation. “Ceramics are not supposed to do that,” says Greer. “Imagine a piece of chalk that was bending and deforming and never breaking!”

The Caltech researchers are continuing to experiment with different lattice structures and materials, but so far their lattices are just 100 μm or so on a side. Drawing the lattice into the photoresist with a single focused laser gives them a lot of flexibility in the structures and dimensions they can achieve, but it doesn’t lend itself to mass production. As Greer explains, “That is the biggest roadblock” to developing engineering materials that capitalize on the size effect. “What someone needs to do now is develop a manufacturability route.”

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A powerful quantum chemical method tackles a protein

Previously limited to systems with a mere dozen or so atoms, coupled-cluster theory can now manage hundreds.

The fundamentals of theoretical chemistry are straightforward. A molecule’s electrons and atomic nuclei interact via a Coulomb potential. Nuclei can usually be treated as stationary classical particles, and electrons can often be assumed to be nonrelativistic. Solving the Schrödinger equation thus yields a molecule’s electronic structure and energy, from which one can derive reaction energies, spectroscopic properties, and other aspects of chemical behavior.

But the many-electron Schrödinger equation is too difficult to solve exactly. Computational chemists must develop simplifications that sacrifice some accuracy for the sake of efficiency. One approach, suitable for especially large or dynamic systems, is to treat just part of the molecule quantum mechanically and to simulate the rest classically. For their pioneering work on those quantum–classical hybrid models, Martin Karplus, Michael Levitt, and Arieh Warshel were awarded the 2013 Nobel Prize in Chemistry, which will be covered in detail in the December issue of PHYSICS TODAY.

Even when the entire system must be treated quantum mechanically, some approximations can still be made. (See the article by Martin Head-Gordon and Emilio Artacho, PHYSICS TODAY, April 2008, page 58.) One favorite approximation, coupled-cluster theory, is regarded as the gold standard for computational chemistry: It can compute relative energies to within 0.04 eV—accurate enough for most purposes—using just a tiny fraction of the computing time required for an exact solution.[1] But for large molecules, standard coupled-cluster theory is still far too computationally intense; one must typically resort to less accurate methods.

Frank Neese and colleagues at the Max Planck Institute for Chemical Energy Conversion have now developed an approach to coupled-cluster theory that reduces the difficulty of the calculation by a factor of 10^6 or more, while sacrificing little accuracy.[2,3] With it, they can compute coupled-cluster energies of molecules with several hundred atoms in a matter of days or weeks. Standard coupled-cluster calculations on the same molecules would take many thousands or even millions of years.

Hartree–Fock

The simplest useful computational chemistry method, and the one on which many others are based, is the Hartree–Fock method. In Hartree–Fock’s predecessor, the Hartree method, the N-electron wavefunction Ψ is approximated as the direct product of N single-electron wavefunctions, or orbitals, φ_i: $\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_N) = \varphi_1(\mathbf{x}_1)\varphi_2(\mathbf{x}_2) \ldots \varphi_N(\mathbf{x}_N)$, where $\mathbf{x}_i$ is the spatial position of the ith electron. The molecular orbitals φ_i are solved self-consistently: Each electron feels the electric field of all the other electrons, averaged over their respective wavefunctions. In modern implementations of the Hartree and other methods, the φ_i are written as linear combinations of a finite, predetermined set of basis functions, usually based on atomic orbitals. One aims to choose a basis that is large enough to be reasonably complete.

The Hartree method accounts for electron–electron repulsion in a rudimentary way. But in the true N-electron wavefunction, the electron positions are correlated in a way that can never be reproduced by the product of N single-electron wavefunctions. For one thing, electrons are identical fermions, no two of which can be in the same place at the same time. The Hartree–Fock method improves on the Hartree method by antisymmetrizing the wavefunction to account for the electrons’ Fermi statistics. For a two-electron system, the Hartree–Fock wavefunction is proportional to