

atoms in a square optical lattice created using two perpendicular standing waves of light. Initially, they arranged the system such that there was a known number of atoms per individual site, and they prepared the atoms in the same quantum state — the ground state, or band, of the lattice. If the neighbouring sites were already occupied, the repulsive interactions between the atoms suppressed tunnelling between lattice sites.

Next, by changing the intensity of one of the standing waves, the authors modulated the depth of the lattice sites. If the frequency of this modulation was tuned to exactly match the separation between the ground band and an excited band of the lattice, atoms could be excited to the higher band. In a similar situation to that for suppression of tunnelling between sites, if an atom was already excited to the higher band, the excitation of a second atom in the same site was suppressed as a result of the interactions. Because of this atom-number-sensitive OEB, the frequency needed to excite atoms depends on the number of atoms in the ground and excited bands. Atoms excited to the higher band could then be removed from the system. Bakr *et al.* demonstrated that OEB allows spectroscopic differentiation of sites with different numbers of atoms and control over the final number of atoms in a given site.

Having a lattice-trapped atomic system at finite temperature creates ‘defects’ in it. Instead of a uniform filling, defects exist in lattice sites at which either no atoms are present (holes) or there are extra atoms. OEB cannot be used to directly fill the holes, but by using atom-number-sensitive OEB, sites with extra atoms can be corrected, removing entropy from the system and so cooling it.

Bakr *et al.* achieved such atom removal in two experiments. In the first one, they initially loaded the lattice with atoms such that the system was in an insulating state — the ground state for the system — with a known number of between one and four atoms per site. Next, by sweeping the modulation frequency, they deterministically reduced the lattice occupation number to a single atom per site.

In the second experiment, the authors⁴ loaded the lattice such that the system was not in the ground state. Instead, they loaded a random number of atoms per site, and by sweeping the modulation frequency, they were able to remove all of the ‘extra’ atoms. After the frequency sweep, they adjusted the depth of the lattice sites so that the final state, an insulating state with a single atom per site, was close to the ground state. This cooling ‘algorithm’ is analogous to heat-bath algorithmic cooling, in which entropy is pumped out of a system into a heat bath. Heat-bath algorithmic cooling has previously been demonstrated using nuclear magnetic resonance of solid-state qubits⁹.

Bakr and colleagues’ technique allows entropy to be removed from the system. But it also allows individual lattice sites to be targeted, as has been shown previously¹⁰. The combination of these two features could facilitate the creation of a quantum register consisting of thousands of atoms, and provide a roadmap to scalable quantum computing using lattice-trapped atoms. Achieving picokelvin temperatures (1 picokelvin is 10^{-12} kelvin) for lattice-trapped atoms remains an important goal, which the authors’ technique could make achievable⁴.

In Bakr and colleagues’ experiments, the final entropy (and thus temperature) was limited by heating caused by the optical-lattice light beams, as well as by inefficiencies in the excitation of atoms to higher bands. Its value was $0.27k_B$ per particle (where k_B is the Boltzmann constant), which is comparable to previously reported values¹⁰. These limitations will need to be overcome if optimal cooling is to be achieved. But even without additional cooling, the use of OEB to deterministically

control the number of atoms in individual sites will be a valuable tool for future experiments. ■

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CONDENSED-MATTER PHYSICS

A fresh twist on shrinking materials

Unusual lattice vibrations have been discovered in scandium trifluoride — a simple compound that shrinks when heated. This finding may help to explain the phenomenon of negative thermal expansion.

J. PAUL ATTFIELD

The term might sound like a euphemism for misfortune, as in ‘negative equity’ or ‘negative patient-care outcome’, but materials that exhibit negative thermal expansion (NTE) are interesting and sometimes useful exceptions to the general rule that substances expand when heated. Negative or zero thermal expansion arises from electronic effects in some metal alloys, such as the iron–nickel alloy Invar ($\text{Fe}_{0.64}\text{Ni}_{0.36}$). Many materials in a second ‘structural’ class, in which NTE is associated with vibrations that bend an atomic network, have been discovered in the past 20 years. Deviations of the materials’ lattice vibrations from the simplest (harmonic) behaviour are expected to contribute to NTE, but most of these materials have structures that are too complex for detailed vibrational analysis. Writing in *Physical Review Letters*, Li *et al.*¹ provide an elegant demonstration of a non-harmonic (anharmonic) twisting vibration of a simple structural NTE material, scandium trifluoride (ScF_3), that helps to explain the origin of NTE in this class.

Scandium trifluoride contains a simple network of corner-sharing ScF_6 octahedra (Fig. 1). Other fluorides and oxides with the same structural arrangement do not show significant negative expansion, so it came as a surprise when a large NTE effect was discovered² in ScF_3 across a wide range of temperatures, from 10 to 1,100 kelvin. Previously reported materials with a comparable NTE, such as zirconium tungstate (ZrW_2O_8), have more complex crystal structures³, so ScF_3 has proved an ideal material in which to explore the subtle features of lattice vibrations (phonons) that can give rise to NTE.

Li and colleagues¹ used a combination of inelastic neutron-scattering experiments and phonon calculations to investigate ScF_3 . The experiments provided the phonon density-of-states, a detailed spectrum of lattice vibrations. The measurements showed that, as ScF_3 was heated, a phonon with an initial energy of about 25 millielectronvolts (meV) underwent an unusual shift to higher energies (stiffening), which is a signature of anomalous behaviour such as NTE. By comparing the measurements with the phonon calculations,

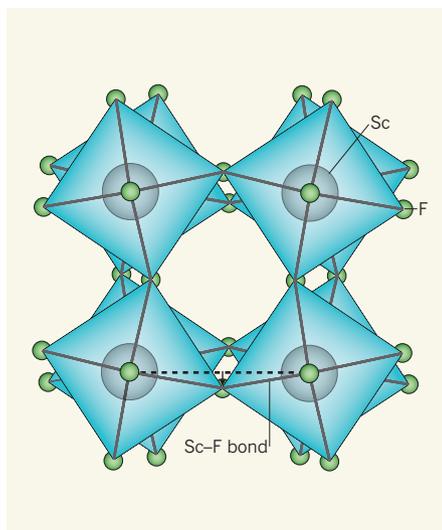


Figure 1 | Twisting vibration in the network structure of scandium trifluoride. Scandium atoms (Sc, grey) are at the centres and fluoride atoms (F, green) at the six shared corners of each of the eight ScF_6 octahedra seen here in projection. When the Sc–Sc distances are fixed (dotted line), twisting vibration stretches the Sc–F bonds. If these bonds stretch harmonically, the potential energy of the motion varies with x^4 , where x is transverse fluoride displacement (as indicated by the arrow). Li *et al.*¹ discovered that this form of vibration makes an important contribution to the phenomenon of negative thermal expansion in scandium trifluoride. (Modified from ref. 1.)

the authors demonstrated that the 25-meV vibration originates from a twisting mode of ScF_6 octahedra (Fig. 1).

A key question on structural NTE materials has been whether polyhedra such as the ScF_6 octahedra distort during twisting vibrations. If the octahedra remain rigid during the vibrations, this ‘rigid unit mode’ has a harmonic potential: the potential energy of the motion varies with the square of the amplitude (x), like the stretching of a mechanical spring. This vibration would bring the scandium atoms at the centre of the octahedra together, shrinking the lattice. However, if the Sc–Sc distances instead remain fixed so that the Sc–F bonds have to stretch during the twisting motion, the potential energy has a quartic (x^4) variation — an example of anharmonicity. Li and colleagues’ analysis¹ of ScF_3 reveals that the twisting vibration has an almost ideal quartic potential. They validate their analysis by showing that both the initial energy and the stiffening of the 25-meV phonon are consistent with the quartic potential for this twisting mode.

After modifying the phonon calculations slightly by allowing the stretched Sc–F bonds to pull the scandium atoms together, the authors demonstrate that this anharmonic model predicts NTE that agrees well with the observed thermal behaviour for ScF_3 (ref. 2).

This result shows that the non-rigidity of the ScF_6 octahedra makes an important contribution to NTE. However, this does not signal the end of the rigid-unit-mode approach: Li *et al.*¹ acknowledge that both harmonic rigid unit motions and quartic anharmonic effects are likely to be needed to provide a full explanation for NTE. With continuing improvements in inelastic neutron spectroscopy and in the computer power available for the supporting phonon calculations, the role of quartic anharmonicity in structural NTE is likely to be clarified further through future studies of more complex materials.

Finally, I note that the discovery² of NTE in ScF_3 marks another step in the seemingly unstoppable rise of perovskite-type materials. Perovskites, named after the mineral form of the calcium titanium oxide CaTiO_3 , have structures like that of ScF_3 but with an additional atom such as calcium that occupies the holes formed between groups of eight octahedra (Fig. 1). They are already

known to have excellent electronic and magnetic properties. Very large electronically driven NTE at ambient temperatures has been discovered in materials that are based on two perovskites, ZnNiMn_3 (ref. 4) and BiNiO_3 (ref. 5); now the ‘empty perovskite’ ScF_3 has been confirmed as a fundamental member of the structural NTE family. ■

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PHYSIOLOGY

On time metabolism

In mammals, molecular clocks regulate transcription and glucose homeostasis. One way they do so is by controlling glucocorticoid–receptor signalling, which suggests that clocks are embedded in liver metabolism. SEE LETTER P.552

JOSEPH BASS

The idea that genes program behaviour dates back to the 1970s, when researchers discovered that heritable mutations in fruitflies alter the daily, or circadian, sleep–wake cycle. At a molecular level, the clock machinery, which is composed of an autoregulatory transcription feedback loop¹, is present in almost all cell types and generates oscillations in the expression of at least 10% of the genes transcribed^{2,3}. Such observations led to an intensive search for the clock’s physiological functions. Lamia *et al.*⁴ describe one such function on page 552 of this issue. They report that the clock protein cryptochrome acts as an on/off switch for the nuclear receptor of glucocorticoids — hormones that are involved in glucose and lipid metabolism⁵. The finding expands our understanding of how metabolism is coordinated with geophysical time.

The impact of circadian clocks on organismal energetics and survival has been investigated in photosynthetic organisms. In cyanobacteria⁶ and plants⁷, alignment of the period length with the environmental light cycle (a defining property of the clock) influences growth and reproduction. This suggests that ‘resonance’ of internal oscillators with the environment may provide a selective

advantage during evolution. In these organisms, the clock machinery also separates oxygen- and nitrogen-fixation processes, averting accumulation of cytotoxic free radicals and preventing futile energetic cycles⁸.

In mammals, circadian rhythms operate at the behavioural, physiological and molecular levels. But studying the link between circadian cycles and metabolism in organisms with a nervous system is complicated. This is because the light response originates from the brain’s pacemaker neurons, whereas nutrient sensing occurs in other neurons and throughout many peripheral tissues. The discovery that fibroblasts maintained in culture exhibit self-sustaining circadian oscillations that show signature properties of a circadian clock⁹ was crucial because it hinted that peripheral clocks can function autonomously. Normally, however, brain and peripheral timepieces seem to communicate to give rise to coherent metabolic outputs. Indeed, genetic studies suggest that the brain and peripheral clocks participate in weight regulation and in glucose and lipid metabolism³.

Circadian oscillations in hormone levels are certainly crucial for metabolic health, and disturbances in these have been used in clinical diagnosis for decades. For instance, high blood levels of the glucocorticoid hormone cortisol