A blueprint for a nanoscale pump

A computational study shows how a precise arrangement of charges on the surface of a nanotube can push water molecules in single file from one end to the other.

The system they consider is a short single-walled carbon nanotube of which both ends are embedded in a graphite sheet and exposed to a water reservoir (Fig. 1a). With repeated simulations, Fang and colleagues ‘test’ a number of charge arrangements to see which one produces a maximum pumping effect. The optimal configuration they find consists of three charges — two that are fractional charges of 0.5e and one with a charge of 1e, where e is the charge of an electron — placed asymmetrically about the vertical centre of the carbon nanotube. Positioned like this, the charges force the dipole moments of water to align near one of the carbon nanotube entrances, preferentially moving the water molecules in one direction over the other.

Nature, of course, dislikes perpetual motion scenarios and it is important to point out that molecular dynamics simulations are performed on short timescales and do not explore equilibrium conditions. Just as protein channels must expend chemical energy to maintain water flow, energy would be necessary to keep the the nanotube pump shown in Fig. 1 operating. (An analogy would be the mechanical pumping that is required during water purification to overcome osmotic pressure.) Although this initial report does not look at what pressure build-up would counteract the charge-induced pumping effect, the estimated force on each charge is several hundred piconewtons.

The report serves as a guide to experimentalists on how far the charges should be placed from the carbon nanotube surface to rotate the dipoles of the water molecules. Fang and colleagues find the water ordering effect is most pronounced when the charges are about 1 Å from the centre of the nearest carbon atom in the nanotube.

Although the fractional charges needed to operate the nanotube pump may appear odd, they can be achieved with ‘resonant’ charge structures, such as carboxylate ions, in which the charge is spread equally over two adjacent oxygen atoms, or by increasing the relative distance of the charge to the tube centre. To obtain a well-controlled spatial placement of charge along the length of...
the carbon nanotube, it would be feasible to ‘wrap’ it with a well-designed charged molecule. However, it may be difficult to overcome the repulsive van der Waals force of carbon ions and place such a functional molecule as close as 1 Å from the nanotube surface.

The concept behind the molecular dynamics simulations could be tested in large area membranes of carbon nanotubes embedded in a polymer matrix\(^1\), some of which have exposed tips\(^2\) (Fig. 1b). With these platforms, it is possible to apply the same mechanism that cells use to control chemical transport to large, manmade films.

This would have important bulk scale applications in chemical separation, water purification, sensing and drug delivery. Similarly, if the polymer matrix of such modified nanotube membranes is dissolved\(^3\), nanotubes with modified tips could, in principle, be dispersed into solution and subsequently incorporated into cellular micelles to become artificial membrane channels themselves.

A good deal of experimental work remains before the simulations presented by Fang and co-workers can lead to these types of applications. Even so, showing that manmade systems can give selective fluid flow in one direction and at a high rate by controlling the dipole orientation of water is both exciting and intriguing.

Published online: 21 October 2007.

References

NANOMAGNETISM

Probing magnetism at the nanoscale

Two groups have used scanning tunnelling microscopes to explore the behaviour of magnetic materials in exquisite detail with a view to developing new approaches to data storage.

Harald Brune
is in the Laboratory of Nanostructures at Surfaces,
Ecole Polytechnique Fédérale de Lausanne,
CH-1015 Lausanne, Switzerland.
E-mail: harald.brune@epfl.ch

The increase in the bit density of magnetic storage devices over recent decades has been more dramatic than that achieved by semiconductor memories, although it is less celebrated. When new magnetic storage media are being developed, two properties are crucial — the magnetic moment and the magnetic anisotropy energy. The first of these is the sum of all the magnetic moments (or spins) in the system, and the second is the energy gained by having the moments point in a certain direction. For small structures, the spins of the constituent atoms all point in the same direction to form a macroscopic moment or ‘macrospin’. If the anisotropy energy is large enough, the direction of this macrospin will be sufficiently stable to build a non-volatile memory. However, if the anisotropy energy is not much larger than the thermal energy, the macrospin can reverse direction spontaneously and is said to be superparamagnetic.

It is clear that measuring both the magnetic moment and the magnetic anisotropy with good — ideally atomic — resolution could be very useful. Writing in Science, Andreas Heinrich of IBM’s Almaden Research Center in San Jose and co-workers report that they have now done exactly this\(^4\). They have measured the anisotropy energy and spin of individual iron and manganese atoms adsorbed on a copper nitride surface. With a low-temperature scanning tunnelling microscope, they can look at electronic excitations at the iron or manganese site that correspond to a change in the magnetic state of the ions (Fig. 1). By analysing how the energy of these excitations depends on the direction and magnitude of an externally applied magnetic field, they can deduce the probability of the spin pointing in each of five possible directions and determine which direction is most energetically favourable.

It has thus become possible to find out how the magnetic properties of atoms and various test objects — such as metal dimers, trimers and tetramers — depend on their environment. Varying the size and shape of the test objects would give insights into coordination effects; combining different elements would provide new information about magnetic alloys; and varying the distance between the atoms could tell us more about magnetic interactions. Measuring the magnetic moments and anisotropy energies of such simple and well-defined model systems makes comparison with theory straightforward, which will lead to a better theoretical understanding of these systems and increased predictive power.

For a magnetic nanostructure with just one preferred axis of magnetization — known as the ‘easy’ axis — the macrospin points along (or almost along) this axis for a considerable time, before flipping to point in the opposite direction, again for a considerable time. The amount of time the macrospin points in one direction and the process by which it flips to the other can be measured with a spin-polarized scanning tunnelling microscope (STM) — that is, an STM with a magnetic tip that makes the majority of the spins in the tunnelling current point in the same direction. Now, as Stefan Krause, Roland Wiesendanger and co-workers at the University of Hamburg report in another Science paper, it is possible to influence the lifetimes of the two magnetic states by injecting a spin-polarized current\(^5\). This is not the same as switching the magnetization in the conventional sense because it does not produce a transition from one stable state to another. However, it makes one orientation of the magnetization more likely than the other and therefore comes close to switching.

In most magnetic memory devices, a magnetic field is used to write data, and the giant magnetoresistive effect (for which Albert Fert and Peter Grünberg have just been awarded the Nobel Prize in Physics) is used to read it. However, magnetic random access memories (MRAM) may well take a different approach to writing data in the not too distant future. The cells in an MRAM device consist of two magnetic electrodes separated by a thin