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COMPUTATIONAL MATERIALS SCIENCE

Two-dimensional tellurium

Materials that consist of just one or a few layers of atoms could have a range of useful applications. Computer simulations now show that the element tellurium might form three such phases, and that they have potentially useful properties.

EVAN J. REED

The discovery of graphene[1], a material that consists of a single layer of carbon atoms, triggered intense research effort and garnered the 2010 Nobel Prize in Physics. Graphene's remarkable properties suggested that it could be used for a diverse range of scientific and engineering applications, ranging from studies of exotic forms of quantum 'tunnelling' behaviour of particles, to the development of touchscreens and composite plastics. Writing in *Physical Review Letters*, Zhu *et al.*[2] suggest that almost atomically thin materials can also be made from tellurium atoms. The potential existence of these two-dimensional materials was revealed by computational simulations, reflecting the increasingly powerful role of such methods in guiding the search for new materials.

Tellurium ordinarily forms a crystal structure consisting of atomic chains that spiral along one of the axes of the crystal lattice — it is essentially a bundle of one-dimensional wires, in which each atom exhibits two-fold coordination, bonding to two other atoms (Fig. 1a).

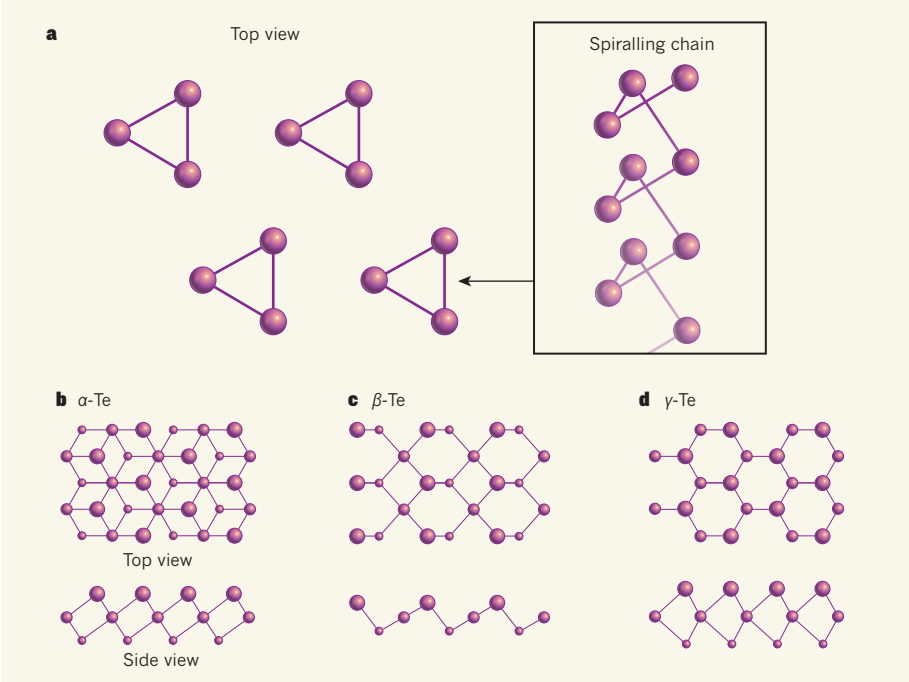

Figure 1 | Observed and predicted phases of tellurium. **a**, The element tellurium ordinarily forms a crystal structure consisting of atomic chains that spiral along one of the axes of the crystal lattice. The tellurium atoms show two-fold coordination — that is, each atom bonds to two other atoms. **b**–**d**, Zhu and colleagues' computational simulations[2] reveal that tellurium might be able to form solid phases just three atoms thick. The top and side views of the atomic arrangements in each phase are shown. In the α-Te (**b**) and γ-Te (**d**) phases, the atoms exhibit a mixture of three- and six-fold coordination, whereas the β-Te (**c**) phase exhibits a mixture of three- and four-fold coordination. The authors suggest that these 2D phases of tellurium have electronic properties suitable for applications in electronic devices. (Adapted from Fig. 1 of ref. 2.)

Zhu *et al.* performed calculations using density functional theory to investigate the stabilities of different structures. These calculations suggest that films of tellurium three atoms thick might be mechanically stable and sufficiently close in energy to the ordinary phase to be produced in the laboratory.

The calculations show that tellurium could potentially adopt three different structures to form 2D crystals (Fig. 1b–d). Two of these structures (the α-Te and γ-Te phases) exhibit a mixture of three- and six-fold coordination, whereas the third phase (β-Te) exhibits a mixture of three- and four-fold coordination, indicating that tellurium has multiple possible bonding configurations. The α-Te and γ-Te phases are respectively equivalent to the 1T and 2H structures[3] commonly adopted by 2D materials known as transition-metal dichalcogenides, which have a general formula of MX_2 (where M is a transition metal and X is a chalcogen, the group of elements that includes tellurium). α-Te and γ-Te can therefore be thought of as transition-metal dichalcogenides in which the transition metal has been replaced by tellurium — a remarkable substitution.

Graphene can be obtained by peeling (exfoliating) a single layer of carbon atoms from graphite, but the proposed 2D forms of tellurium are not found within a known 3D crystal structure. This means that the 2D tellurium phases will have to be prepared by growing them on a substrate. Zhu and colleagues speculate that instabilities in thin films of the bulk 1D-wire phase of tellurium might spontaneously convert into the 2D forms. They also carried out experiments in which a tellurium film was grown on a graphite surface. Preliminary analysis of the film, including measurements of the distances between the atoms, suggest that it consists of β-Te.

Much of the early research into 2D materials was fuelled by the ready availability of bulk forms of the materials from which single layers could be exfoliated, and by the chemical stability of the single layers in air. Tellurium probably exhibits neither of these properties, and exemplifies the fact that the going might get harder for future research into 2D materials in general. But the challenges might be offset by the potentially advantageous properties of such materials. Zhu and co-workers' simulations of the electronic properties of α-Te and β-Te indicate that these phases are semiconductors, and that the effective masses of their charge carriers are three to four times smaller than that of molybdenum disulfide, the most commonly studied 2D semiconductor. This suggests that 2D tellurium could find applications in electronic devices that offer higher performance than those that use molybdenum disulfide.

There has been much focus on the mechanical stability of free-standing layers of 2D materials, but this property might not be relevant for many applications in which the material is placed on a substrate or embedded within another bulk material. If 2D materials do not need to be stable, free-standing structures, then how do they differ from ordinary thin films? The answer to this existential question probably depends on who you ask, but many researchers would point out that the chemical interactions between 2D materials and their environment are relatively weak, thus enabling the materials to retain their properties down to nearly atomic thicknesses and when placed in contact with a range of other materials. These properties allow the electronic behaviour at interfaces in devices to be engineered, and potentially enhance the 2D material's chemical stability.

In the early days of graphene research, substantial efforts were invested in modifying the material's properties for specific applications — for example, by endowing it with an electronic property known as a bandgap to improve the efficiency of transistors[4,5]. But the research focus shifted with the realization that many other nearly atomically thin materials exist, including some that already possess bandgaps or other desirable properties. The list of 2D materials is rapidly expanding, and more than 1,000 such materials are now known[6–8], encompassing the full spectrum of electronic and other properties. These materials were identified by mining data from publicly available materials databases, which illustrates the broad utility of such databases for applications that might not have been envisaged originally.

Zhu and co-workers' discovery is therefore certainly interesting scientifically, but it remains to be seen whether 2D tellurium compounds will become the materials of choice for engineering applications, particularly if they are challenging to work with. Nevertheless, the work undoubtedly shows that computational approaches are playing a crucial part in addressing important problems in materials science. ■

Evan J. Reed *is in the Department of Materials Science and Engineering, Stanford University, Stanford, California 94305, USA.*
e-mail: evanreed@stanford.edu

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