COMPUTATIONAL MATERIALS SCIENCE

Substitution with vision

A method has been developed for predicting the stability and elasticity of certain alloys for millions of atomic configurations of the materials. This approach should help to identify materials with optimized properties. SEE LETTER P.740

GUS L. W. HART

Early civilizations began alloying copper with arsenic, tin or zinc nearly 6,000 years ago[1], ushering in the Bronze Age. Even when more-abundant iron became a mainstay during the Iron Age, substitutional alloys of copper — in which some of the copper atoms were replaced with atoms of a different metal — were superior materials. So Roman foot soldiers were equipped with wrought-iron weapons, whereas Roman officers had swords made of bronze. Similarly, at the turn of the twentieth century, French scientists developed a steel that substituted some iron with vanadium. This alloy, which had three times the tensile strength of competing steels, became an essential ingredient of the venerable Ford Model T (and of early French luxury cars).

Materials substitution — the replacement of some of the atoms of a material with those of another (Fig. 1) — continues to be a key strategy for developing the materials of tomorrow, but predicting the properties of new alloys is remarkably difficult. On page 740 of this issue, Maisel *et al.*[2] report a method for calculating from first principles both the elasticity and the thermodynamic stability of alloys*.

The difficulty of developing improved materials is a bottleneck — perhaps the main bottleneck — to advances in new technologies. In 2011, to increase the pace of materials development, and to leverage impressive advances in computational materials science, US President Barack Obama announced the Materials Genome Initiative, a project that aims to create an infrastructure of informatics and experimental tools for materials development in the United States[3]. Materials substitution is central to this initiative and has also been specifically referred to in recent calls for research proposals from US federal funding agencies.

Many computational approaches have been developed to take advantage of the materials-substitution strategy, but Maisel and colleagues' report brings something new to such efforts. Their work is noteworthy because it demonstrates a clear correlation between the thermodynamic and elastic properties of alloys known as face-centred-cubic intermetallics, and because their approach can easily be applied to other alloy types. It therefore not only provides a fundamental understanding of the physical properties of materials, but also opens up opportunities for materials engineering. Using the authors' method, it may be possible to tune the elastic stiffness of alloys using materials substitution. For example, alloys could be softened to make compounds for orthopaedic implants that integrate well with bone, in order to avoid the difficulties that arise when bone and implant materials have disparate elastic properties.

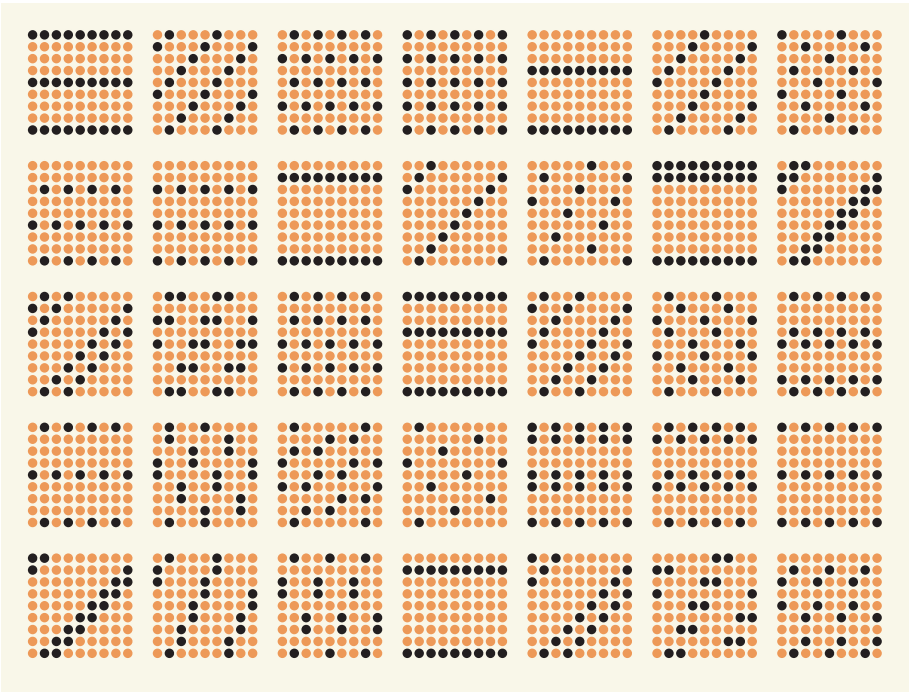

Figure 1 | Atomic configurations. Substitutional alloys are formed when a fraction of the atoms of a metal are replaced with different atoms. Several atomic configurations of possible alloys are depicted here for a hypothetical case in which the atoms of the main metal (orange) form a square lattice. Substituted atoms are shown in black. Maisel *et al.*[2] report a computational technique that allows rapid prediction of both the elastic stiffness and the thermodynamic stability of different atomic configurations of certain alloys.

The authors' technique extends a computational methodology known as cluster expansion that is often used to calculate the properties of substitutional alloys. Cluster expansion involves two basic steps: first, calculate the target property for a number of different atomic arrangements using quantum mechanics; and second, map this information onto a simple model that accounts for the effects of atomic substitutions. In this way, one essentially 'trains' a computational model, which is then used to calculate the target property for any atomic configuration — instantly and with quantum-mechanical accuracy. Because computation of the target quantity is so efficient, cluster expansion can be used to simulate thermodynamic and kinetic properties of atomic ensembles from first principles, and to screen hundreds of millions of atomic configurations for a specific property.

Maisel and colleagues report two major advances in cluster expansion. First, they have expanded its use to calculate multiple properties in a single model; and second, they have used it to identify a specific relationship between those properties. Specifically, they combined two cluster expansions to predict both the thermodynamic stability and the mechanical stiffness of any atomic

*This article and the paper under discussion[2] were published online on 21 November 2012.

configuration in their target alloys. This revealed that the more thermodynamically stable the configuration, the stiffer the resulting material.

Many researchers use computation to identify atomic structures of a given material that have desirable properties, often with little regard for whether those structures are feasible to make (thermodynamically stable). Maisel and co-workers' approach shows that, at least in the case of elastic stiffness, hunting for metastable structures that have better properties than stable structures — whether known or predicted — is essentially futile, and that researchers should focus on other materials instead. That said, being able to predict both the stability and another target property of a material will allow scientists to efficiently scan through sets of hypothetical materials and 'see' promising candidates, lending vision to an established computational approach. It is in this discovery mode that Maisel and colleagues' work could contribute greatly to efforts such as the Materials Genome Initiative.

It remains to be seen how many other materials' properties will be studied using the new approach. In principle, any property that directly depends on atomic configuration is within reach, but many properties of relevance to engineering are still difficult to compute in practice. Furthermore, some of the most important properties of materials depend not only on the atomic configuration of a fixed lattice, but also on microstructural elements — such as boundaries between microscopic crystals (grains), grain sizes and extended crystal defects. These remain beyond the reach of quantum-mechanical calculations.

Still, high-throughput approaches[4,5] for sifting through thousands, or tens of thousands, of candidate materials are poised to make a substantial contribution to society's needs by generating large databases of information that will be of use to researchers[6,7]. These databases will be more effective if the information they contain about physical properties is used to build computational models that, in turn, could search for thermodynamically stable materials to meet a particular need[8]. Maisel and colleagues' work, coupled with automated model-building methods[9], might help us to achieve that goal. ■

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PLANT ECOLOGY

Forests on the brink

An analysis of the physiological vulnerability of different trees to drought shows that forests around the globe are at equally high risk of succumbing to increases in drought conditions. SEE LETTER P.752

BETTINA M. J. ENGELBRECHT

Water is the most limiting factor for ecosystem diversity and productivity worldwide. But the global climate is changing, and both warming and shifts in rainfall patterns are projected, which will leave large areas of the planet with less rain and a higher likelihood of extreme drought events[1,2]. These changes will almost certainly affect forests, which cover more than 30% of the world's land surface. Understanding these effects is imperative: forests play an integral part in carbon and water cycles, they provide timber and other products, and they are home to a vast diversity of plants, animals and microorganisms. But forests occur in a wide range of climatic conditions, so it is a challenge to predict how the vulnerability of trees to changes in water availability compares between different biomes. In this issue, Choat *et al.*[3] (page 752) use a combination of physiological measurements of the vulnerability of trees to drought and of the drought stress they actually experience in their natural habitats to show that forests worldwide are at high risk*.

We might expect that trees in forests currently exposed to seasonal or multi-annual droughts, such as in 'Mediterranean-type' systems, are already well adapted and will therefore suffer less from an increase in drought conditions than trees in wet forests. Conversely, but equally reasonably, we could predict that trees in dry areas are already at their physiological limits and would therefore be more vulnerable to increased drought than trees in wet forests. To investigate these questions, Choat and colleagues compared the vulnerability of the tree water-transport system to drought in different species worldwide.

In plants, water is transported through a tubing system, a tissue called xylem that is made up of a multitude of conduits. Loss of water vapour (transpiration) through stomata (pores) in the plants' leaves generates suction that pulls water in the xylem from the soil through the roots and stem to the leaves — much like sucking water through a straw. On its way, the water provides crucial services to the plant: it is the medium for metabolic reactions, it transports nutrients and other substances, and it provides stability. However, the powerful suction that pulls water through the xylem brings with it the risk of pulling air through small holes, called pit pores, in the sides of the conduits. These air bubbles can block the xylem and impair water transport, just like sucking air into a broken straw. This process is called xylem embolism, and the higher the suction in the conduit, the more embolism occurs.

The link between this physiology and drought conditions comes from the fact that suction increases with increasing transpiration and/or decreasing water availability in the soil. Plants can regulate their stomata to delay the increase in suction, but if water is not replenished, more and more conduits will become clogged, leading to hydraulic failure and the eventual death of the plant. However, different plant species have different xylem structures, so the vulnerability of a plant's xylem conduits to embolism, and therefore its ability to tolerate drought, are variable.

The authors compiled data on the xylem vulnerability of 480 tree species from 183 sites worldwide, covering the broad range of climatic conditions in which forests occur. They included both angiosperms (flowering trees, such as oak and maple) and gymnosperms (such as pine and cedar), which vary substantially in their xylem structure. Wherever the data were available, they also included the maximum suction occurring in the trees in their natural habitats. Combining these data enabled Choat *et al.* to explore how the suction that induces hydraulic failure in a given species compares with the suction that it actually experiences. If these values are close together, this represents a small 'safety margin' with respect to hydraulic failure and indicates that the species is at risk; if they are far apart, the species is likely to be able to withstand more intense drought conditions.

The data show that, as expected, trees growing in more arid conditions around the globe

*This article and the paper under discussion[3] were published online on 21 November 2012.