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# Atomic structure of a glass imaged at last

### **Paul Voyles**

The positions of all the atoms in a sample of a metallic glass have been measured experimentally – fulfilling a decades-old dream for glass scientists, and raising the prospect of fresh insight into the structures of disordered solids. **See p.60** 

If the chemical element and 3D location of every atom in a material are known, then the material's physical properties can, in principle at least, be predicted using the laws of physics. The atomic positions of crystals have long-range periodicity, which has enabled the development of powerful methods that combine diffraction experiments with the mathematics of symmetry to determine the precise atomic structure of these materials. Moreover, deviations from periodicity that create defects in crystals can be imaged with sub-ångström resolution. But these methods do not work for glasses, which lack long-range periodicity. Our knowledge of the atomic structure of glasses is therefore limited and acquired indirectly.

On page 60, Yang *et al.*<sup>1</sup> report the experimental determination of the 3D positions of all the atoms in a nanometre-scale sample of a metallic glass.

The authors accomplished this feat using atomic-resolution electron tomography. In this method, 2D projections of the 3D atomic structure of a sample are acquired by passing a beam of electrons through the sample: a series of 2D images is produced by altering the orientation of the sample to the beam, and these images are then reconstructed into a 3D image of the whole sample. This technique has been used to determine the atomic structure of crystals for a decade<sup>2.3</sup>. However, most of the information required to construct the full 3D atomic structure of a crystal is contained in just a few of the 2D images, which are acquired when the sample is oriented in ways that cause the atoms to line up in rows, one behind the other, with empty space between them<sup>4</sup>. Unfortunately, such orientations do not exist for glasses.

Special orientations are also lacking for non-crystalline biomolecules. Electron microscopists have overcome this problem by studying millions of nearly identical copies of the same biomolecule, thereby achieving single-atom resolution in tomographic reconstructions<sup>5</sup>. By contrast, every cubic nanometre of a glass has a unique structure, which means that Yang et al. had to adopt a different strategy. They used a combination of state-of-the-art computational imaging techniques - including sophisticated methods to correct distortions and to reduce noise that obscures the image signal - to produce a series of high-quality 2D images that capture subtle variations in contrast when the glass is viewed in different orientations. They then used an original approach to reconstruct the final, atomically resolved 3D image (Fig. 1). Although the authors cannot specifically identify the element for each atom, they do assign each atom to one of three categories, each of which includes either two or four of the eight elements in the glass.

Theoretical descriptions of glass structure rely on long-standing principles that define motifs of atoms. For glasses in which the atoms are covalently bonded, such as commonplace window glass, the principle is preservation of bond lengths and angles, and the motif is a continuous random network of bonds<sup>6</sup> (Fig. 1a). The random-network motif has been elaborated to accommodate, for example, atoms that have varving numbers of bonds<sup>7</sup>.

For glasses in which the atoms exhibit metallic bonding, the principle is to achieve dense,



**Figure 1** | **The atomic structure of glasses.** Knowledge of glass structure has been based on long-standing models developed from simple physical principles. **a**, For glasses in which the atoms are covalently bonded, a continuous random network of atoms has been proposed to form<sup>6</sup>, in which bond lengths and angles between atoms are preserved. **b**, For metallic glasses, the structure was thought to involve the dense random packing of spherical atoms<sup>8</sup>. **c**, Yang *et al.*<sup>1</sup> have used a method called atomic-resolution electron tomography to determine the position of every atom in a nanometre-scale sample of a metallic glass. Although the authors could not specifically identify the element for each atom, they did assign each atom to one of three types, each including either two or four of the eight elements in the glass. The availability of fully resolved atomic data for glasses represents a step change in understanding compared with **a** and **b**.

## News & views

random packing of spherical atoms<sup>8</sup> (Fig. 1b), and the motifs are clusters of atoms that define the vertices of various polyhedra (such as the polyhedra defined in ref. 9). The principle of dense random packing has been elaborated to include the chemical propensity of some elements to bond preferentially to other elements<sup>10</sup>. Experiments have confirmed various aspects of these descriptions of metallic-glass structure<sup>11</sup>, but only computer simulations have been able to determine the unique position and element for every atom (see ref. 12, for example). Unfortunately, simulations can model the motions of atoms only at short timescales, and therefore can't really account for the very slow motions of atoms that occur in glasses and glass-forming liquids - thus limiting their ability to predict the atomic structure of glasses.

Yang and colleagues' results (Fig. 1c) are a major step towards experimental confirmation of current models of metallic-glass structure. The authors' structural analysis provides support for a model in which solute atoms (those that occur in small quantities in the glass) are found at the centres of clusters of solvent atoms (which account for the majority of the atoms). The clusters act as 'super atoms' that pack together densely at length scales greater than the atomic scale to form the glass structure<sup>13</sup>. Yang et al. show that, in their glass, some of these clusters are densely packed, but others are not. The observed loose packing of some clusters might be a product of the extremely rapid cooling that was used to synthesize the studied glasses, but it could also point to important gaps in current models.

The next experimental challenges are to identify the specific element for every atom, which should be possible for glasses that have a simpler composition than that of the glass in the current study, and to improve the precision of the determined atom positions. Yang et al. report a random uncertainty of 21 picometres in the atomic positions (1 pm is  $10^{-12}$  metres). That is a tiny distance, but it represents about 8% of the most common interatomic distance in the glass. Shifts in position of that scale would cause significant changes in the energy of the bonds between the atoms and in the geometries of the super-atom clusters. The uncertainty might also explain why the abundances of polyhedra observed in the current study differ from those predicted by previously reported simulations<sup>12</sup> – if the atoms in the simulations were all randomly shifted by up to 21 pm, the resulting polyhedra distributions could be more similar to those reported by Yang and co-workers. It remains to be seen whether the authors' characterization of the structure (the specific way in which they partitioned atoms into super-atoms, and the packing of those super-atoms) is the best theoretical description of the studied system, and whether solute-centred clusters will become the most useful general description of metallic-glass structures.

Advanced electron tomography promises to substantially advance glass science. The acquisition of complete atomic-structure data for more metallic glasses could provide insights that aid the development of methods for discovering new glass-forming alloys, and could improve our understanding of unusual materials such as polyamorphous<sup>14</sup> and structurally anisotropic<sup>15</sup> glasses. It could also open the way to techniques for characterizing structural defects in glasses; such characterization is currently restricted to defects that have a spectroscopic signature. Technologies such as superconducting quantum bits (used in quantum computers) and the LIGO gravitational-wave observatory are limited by glass defects known as two-level systems<sup>16,17</sup>, which can be detected only by their effects, not by their structure. Having the ability to identify defect structures could be a first step towards engineering better materials for various applications. In the meantime, Yang et al. have achieved something that glass scientists have dreamt of for at least 90 years<sup>6</sup> - measuring the positions of all the atoms in a glass.

## **Molecular biology**

## A new phase in meiotic cell division

## **Kevin D. Corbett**

The exchange of DNA between pairs of chromosomes is key to sexual reproduction. It emerges that one step in this process – the introduction of DNA breaks by the enzyme Spo11 – relies on condensation of proteins into liquid-like droplets. **See p.144** 

Our cells carry two copies of each chromosome, known as homologous chromosomes or homologues, with one inherited from each parent. Sexual reproduction requires the formation of germ cells that have only one copy of each chromosome; the fusion of two germ cells during fertilization restores the original chromosome number in the next generation. Germ cells are formed by a specialized cell division called meiosis, an early step of which involves the segregation of homologues into separate daughter cells. Errors in meiotic chromosome segregation can produce germ cells that have too many or too few chromosomes - a condition called aneuploidy that underlies disorders such as Down's syndrome and is a major cause of miscarriage. On page 144 Claeys Bouuaert et al.<sup>1</sup> highlight a key role for a process called liquid-liquid phase separation in the molecular events underlying

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this crucial biological pathway.

Accurate chromosome segregation in meiosis requires that each chromosome first identify and physically link to its homologous partner. These steps depend on a DNA-repair pathway called homologous recombination, which begins with programmed DNA breakage at a few randomly chosen sites along each chromosome. The broken DNA ends seek out similar sequences on other chromosomes, eventually identifying their homologous partner and establishing physical links called crossovers. Crossovers also enable the exchange of genetic information between homologous chromosomes, ensuring genetic variation between parents and offspring.

The molecular mechanisms that control homologous recombination in meiosis have been studied for more than two decades, since the identification of a set of ten proteins in the