A Roadmap for the Assembly of Polyhedral Particles

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and connection strength distributions, find that the network is small-world, and identify its community (module) structure. They find overrepresented connectivity motifs among connected triplets of neurons, including feedforward motifs, which are also common in the hermaphrodite wiring diagram (*6*, *7*) and the mammalian cortex (*8*). The broad statistical similarity between these graphs and those reported for the mammalian cortex (*8*, *9*) suggests that fundamental principles of circuit operation gleaned from the worm may help us understand how mammalian brains generate behavior.

The challenge going forward is to convert the reconstruction into detailed knowledge of circuit function. First is the question of what the neurons (nodes) do. Of the 302 neurons of the hermaphrodite, functions are known for about 60%; 30% have also been characterized by functional calcium imaging, and 15% by electrophysiological recordings—a respectable fraction of the nervous system. For many male-specific neurons, functions remain to be assigned, and the neuronal activity patterns are unknown. Moreover, in the new reconstructions, two-thirds of the neurons that males share with hermaphrodites are strongly sexually dimorphic in their wiring, which suggests that the male worm is a new animal whose neurons cannot be assumed to have the same functions as those of his sisters (*10*).

At the circuit level, an anatomically reconstructed wiring diagram leaves many unanswered questions about synapses (edges). For example, electron micrographs do not reveal whether a chemical synapse is excitatory or inhibitory, or whether an electrical synapse is asymmetric or symmetric. Information about these properties and about neuronal dynamics is essential for understanding circuits, even for simple elements such as the feedforward motif. An anatomical map of synapses also fails to show neuromodulators that act at a distance, which play important roles in modifying functional connectivity between neurons. Which of these "nonanatomic" features are necessary to understand circuit function? The importance of the complete reconstruction is the ability to pose this question in a rigorous way. With advances in quantitative microscopy and genetically encoded sensors, it seems increasingly feasible to examine neuronal activity during mating behavior; such measurements would reveal whether attractor networks, perceptrons, and other models for circuit function are embodied in the male nervous system.

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MATERIALS SCIENCE

A Roadmap for the Assembly of Polyhedral Particles

How particles pack together as a solid can often be predicted just from their shape and how many neighbors they have in the fluid phase.

Joost de Graaf[1] and Liberato Manna[2,3]

Self-assembly of atomic, molecular, or artificial nanoscale units into superstructures is a prevalent topic in science. Advances in control over the synthesis of colloidal nanoparticles (*1*, *2*), in their organization into ordered structures (*3*–*7*), and in modeling of assembly (*8*–*10*) have boosted interest in this topic. Yet predicting what types of superstructures will be formed from specific building blocks according to the shape of the blocks and their interactions remains an open problem (*11*). Even if the shape is spherical and interactions between blocks do not depend on their mutual orientation, one cannot model the finite-pressure assembly on the basis of simple close-packing arguments; more elaborate approaches are required. On page 453 of this issue, Damasceno *et al*. (*12*) report the most extensive and systematic study thus far on the assembly behavior of polyhedral "hard" particles of many different shapes. The study exploits a large set of shapes to determine simple predictive criteria for assembly.

Modeling anisotropic hard-particle assembly began many decades ago. In 1949, Onsager predicted that hard cylinders with hemispherical caps (spherocylinders) spontaneously form a nematic liquid crystal past a threshold in volume fraction (*13*). The organization is driven by maximization of the configurational space that is made available to the particles (in other words, a maximization in the positional and orientational entropy of each cylinder). This assembly works best when spherocylinders are organized parallel to each other.

For hard particles with flat facets, entropy maximization favors mutual alignment of particles along these facets (*14*). This requirement translates into directional interactions of each particle with its neighbors [so-called "directional entropic forces" (*14*)]. The concept of directional entropic forces is similar to the directional bonding between atoms in solids, and the connection is exploited by Damasceno *et al*. to draw parallels between the results of their calculations for hard particles and the types of bonds found in solids.

Slow compression of particles from the fluid phase, as done in these calculations, mimics the assembly of colloidal nanoparticles by controlled evaporation of the solvent in which they are dissolved—a process that steadily increases the volume fraction of particles. The calculations show that, depending on their initial shape, hard polyhedra will assemble in one of four ways. They can form crystals (ordered structures in which units are positionally and orientationally blocked at their sites), plastic crystals (ordered structures in which units are free to rotate but remain positionally fixed at their sites), liquid crystals (structures that have positional disorder but have a strong orientational order), or fully disordered structures.

Some of the individual results of the simulations are unexpected. For example, square pyramids first assemble into cubes and then into sheared cubic lattices—a case of hier-

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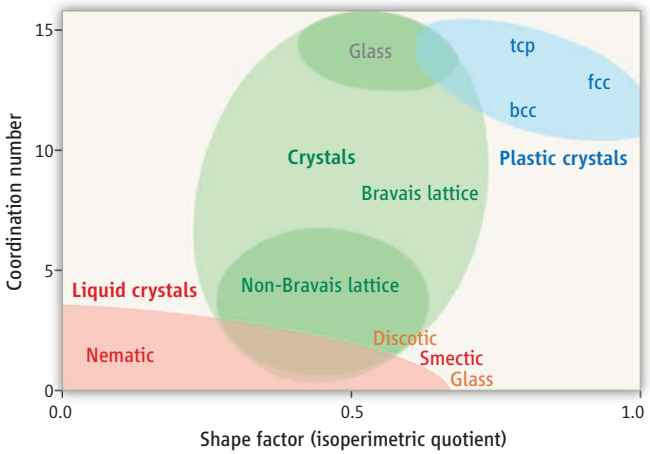

An assembly map. Damasceno *et al*. have charted the types of superstructures into which polyhedral particles can assemble using only two readily determined parameters, a shape factor and a coordination number. For any given polyhedron, the map predicts its assembly category (one of the shaded areas in the map). In a Bravais lattice, all lattice points are equivalent, which is not the case for a non-Bravais lattice. Abbreviations: fcc, face-centered cubic; bcc, body-centered cubic; tcp, topologically close-packed.

archical assembly. However, a unified view is found when results are mapped in terms of two parameters: the "coordination number" in the fluid phase (that is, the number of nearest neighbors surrounding each polyhedron in the fluid) and the isoperimetric quotient, which depends on the particle shape and measures the deviation of the shape from the sphere. Damasceno *et al*. determined that highly faceted polyhedra, which are almost spherical and also have a high coordination number, will assemble into plastic crystals. Polyhedra that are highly nonspherical, with a smaller number of facets and a low coordination number, tend to form liquid crystals. Nonspherical polyhedra that have an intermediate coordination number will assemble into crystals. Almost the entire set of polyhedra that crystallized, according to simulations, fell into one of these three major regions (see the figure).

The coordination number in the fluid phase and the coordination number in the ordered phase were nearly identical in almost all cases. Thus, the packing category for a new type of nanoparticle (whether synthesized in the laboratory or computer-generated) can be determined using the map drawn by Damasceno *et al*., given its coordination number in the fluid and its shape parameter (both easily determined).

A conspicuous number of polyhedra formed glassy states, and there are overlapping regions where two or even more types of structures could arise from the same polyhedra. The frequent formation of glassy states, possible improvements in mapping, and the investigation of other cases not yet probed by systematic calculations all require further research. In addition, particles with more complex shapes—for example, with concave surfaces or branches—are more likely to become trapped into locally "jammed" configurations and to form disordered assemblies when the volume fraction is increased. These types of particles can, however, still spontaneously assemble into ordered superstructures if they follow hierarchical assembly schemes like those adopted by biomolecules, in which complicated building blocks sequentially organize into assemblies of growing complexity.

An example is the organization of DNA into symmetric supramolecular structures, which do not require high volume fractions of units to form (*15*), but where favorable kinetic and thermodynamic paths drive organization even at very low volume fractions of the units. A nanoparticle analog of hierarchical self-assembly was recently reported for colloidal branched nanocrystals (*16*), which did not form close-packed structures but nonetheless self-organized in a hierarchical way. Many more examples can be expected as the synthesis of monodisperse colloidal nanoparticles with unconventional shapes progresses. For now, a comprehensive framework for predicting the assembly of any particle based only on the shape and interparticle forces is still out of reach (*17*).

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NEUROSCIENCE

dSarm-ing Axon Degeneration

Xiaomeng Milton Yu and Liqun Luo

An axon self-destruction program may underlie neurodegeneration in injury and diseased states.

Plucked from the tree, a leaf withers. Such a loss of vitality upon removal from the whole appears so natural that one may take it for granted as a passive and unstoppable process. But is it? Although cell death was long thought to be a passive process, we now know that at least one form of cell death, apoptosis (from Greek "falling away"), is an active process that can be blocked by inhibiting a specific signaling pathway (*1*). On page 481 of this issue, Osterloh *et al*. (*2*) find that the death of a portion of a nerve cell, the axon, after it is severed from the cell body, can be dramatically slowed by the inactivation of just one gene. The discovery has important implications for understanding the molecular mechanisms of axon degeneration, as well as for developing drugs against neurodegenerative diseases.

An axon is a long, polarized extension from the neuronal cell body that transmits a neuron's output signals to downstream cells. When an axon is acutely injured, the segment distal to the lesion site undergoes morphological changes that lead to its fragmentation and clearance within a few days (see the figure). This process of "Wallerian degeneration," named after Augustus Waller who described it in 1850 (*3*), was traditionally viewed as passive deterioration due to the lack of cell

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