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Entropy alone creates complex crystals from simple shapes, study shows

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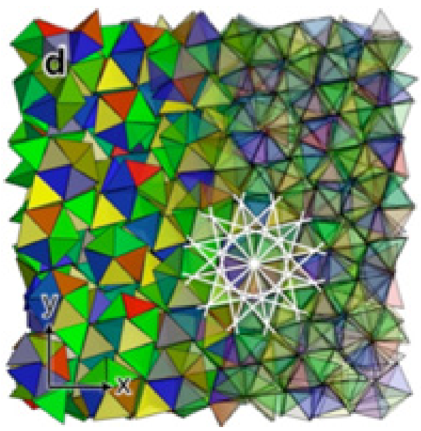

Researchers uncovered a way to pack tetrahedra more densely than ever before. Experiments and computer simulations, like the one shown here, helped the team to obtain the highest packing fraction of 85.03 and discover the formation of quasicrystals when the tetrahedra were compressed.

(PhysOrg.com) -- In a study that elevates the role of entropy in creating order, research led by the University of Michigan shows that certain pyramid shapes can spontaneously organize into complex quasicrystals.

A quasicrystal is a solid whose components exhibit long-range order, but without a single pattern or a unit cell that repeats.

A paper on the findings appears in the Dec. 10 issue of *Nature*. Researchers from Case Western Reserve University and Kent State

University collaborated on the study.

Entropy is a measure of the number of ways the components of a system can be arranged. While often linked to disorder, entropy can also cause objects to order. The pyramid shape central to this research is the tetrahedron---a three-dimensional, four-faced, triangular polyhedron that turns up in nanotechnology and biology.

"Tetrahedrons are the simplest regular solids, while quasicrystals are among the most complex and beautiful structures in nature. It's astonishing and totally unexpected that entropy alone can produce this level of complexity," said Sharon Glotzer, a professor in the University of Michigan departments of Chemical Engineering and Materials Science and Engineering and principal investigator on the project.

The finding may lead to the development of a variety of new materials that derive properties from their structure, said Rolfe Petschek, a physics professor at Case Western Reserve who helped with the mathematical characterization of the structure. "A quasicrystal will have different properties than a crystal or ordinary solid," Petschek said.

The scientists used computer simulation to find the arrangement of tetrahedrons that would yield the densest packing---that would fit the most tetrahedrons in a box.

The tetrahedron was for decades conjectured to be the only solid that packs less densely than spheres, until just last year when U-M mathematics graduate student Elizabeth Chen found an arrangement that proved that speculation wrong. This latest study bests Chen's organization and discovered what is believed to be the densest achievable packing of tetrahedrons.

But Glotzer says the more significant finding is that the tetrahedrons can unexpectedly organize into intricate quasicrystals at a point in the computer simulation when they take up roughly half the space in the theoretical box.

In this computer experiment, many thousands of tetrahedrons organized into dodecagonal, or 12-fold, quasicrystals made of parallel stacks of rings around pentagonal dipyramids. A pentagonal dipyramid contains five tetrahedrons arranged into a disk. The researchers discovered that this motif plays a key role in the overall packing.

This is the first result showing such a complicated self-arrangement of hard particles without help from attractive interactions such as chemical bonds, Glotzer said.

"Our results go to the very heart of phase transitions and to the question of how complex order arises in nature and in the materials we make," Glotzer said. "We knew that entropy on its own could produce order, but we didn't expect it to produce such intricate order. What else might be possible just due to entropy?"

Other approaches to solving the tetrahedron packing problem have not involved computer simulations. Researchers instead tried out different arrangements to arrive at the densest structure. That was the approach taken by Chen, who achieved a packing fraction of more than 77 percent, which means the shapes took up more than 77 percent of the space in the box. (Cubes have a 100 percent packing fraction in a cubic box, while spheres pack at only 74 percent.)

Rather than "posit what they might do," this computer simulation allowed the tetrahedrons to figure out the best packing on their own according to the laws of statistical mechanics and thermodynamics, said Michael Engel, a postdoctoral researcher at U-M and co-first author of the paper with U-M chemical engineering graduate student Amir Haji-

Akbari.

In the simulation, the tetrahedrons organized into a quasicrystal and settled on a packing that, when compressed further, used up 83 percent of the space. Engel then reorganized the shapes into a "quasicrystalline approximate," which is a periodic crystal closely resembling the quasicrystal. He found an arrangement that filled more than 85 percent of the space.

The researchers are excited about the possible applications of the new structure.

"Made of the right materials, this unexpected new tetrahedron quasicrystal may possess unique optical properties that could be very interesting and useful," said Peter Palffy-Muhoray, a professor in the Liquid Crystal Institute at Kent State University and a collaborator on the work. Possible uses include communication and stealth technologies.

More information: "Disordered, quasicrystalline and crystalline phases of densely packed tetrahedra." *Nature*.

Source: University of Michigan (news : web)

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