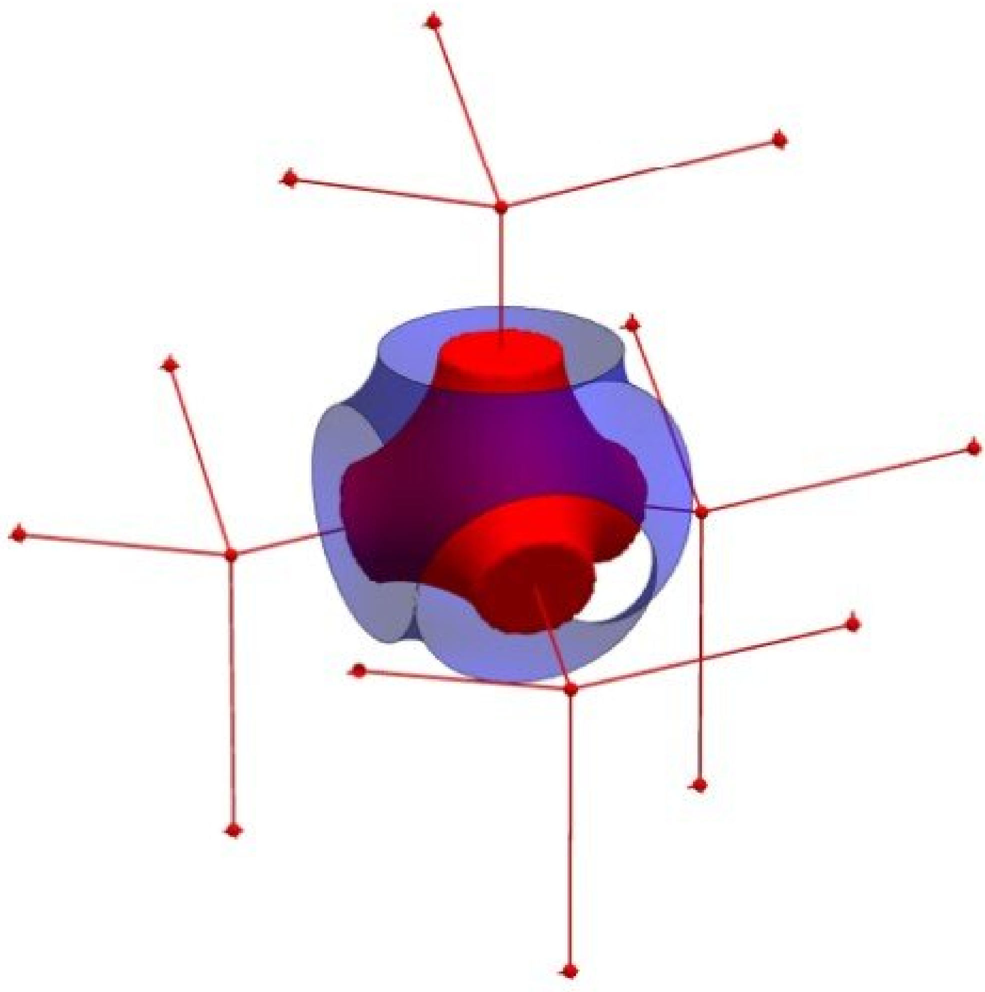
Evidence of new mesoatom shapes and symmetries that occur in a special twin boundary in soft matter

January 23 2023, by Raven Wuebker



Model of basic motif (i.e., f = 4 node or mesoatom) of the DD networks. The intermaterial dividing surface (IMDS) is rendered in red, and the triply periodic minimal surface (TPMS) is rendered in blue. The skeleton of the minority component domain is shown as red sticks. The basic motif occupies Wyckoff site 2a with site symmetry 43*m* in space group *Pn*3*m*. Credit: *Proceedings of the National Academy of Sciences* (2023). DOI: 10.1073/pnas.2213441120

New research published in the *Proceedings of the National Academy of Sciences* shows direct 3D experimental evidence of new mesoatom shapes and symmetries that occur in a special twin boundary in soft matter.

Dr. Ned Thomas, a professor in the Department of Materials Science and Engineering at Texas A&M University, studies twin boundaries, a type of planar defect. Twin boundaries occur in a soft matter block copolymer that forms a double diamond (DD) crystal from structural building blocks of polystyrene (PS) chains covalently linked to polydimethylsiloxane (PDMS) chains. Each mesoatom is comprised of thousands of PS-PDMS molecules and millions of atoms.

"A mesoatom is an intermediate atom. It's a new concept, which is at a much larger scale," Thomas said. "Atoms we know are the smallest kinds of individual chunks, usually represented by spheres and thought to be indivisible."

Mesoatoms in a soft DD crystal are analogous to single carbon atom building blocks in hard diamond (D) crystals. A DD mesoatom also has the same bonding, geometry and crystal structure as a carbon atom in single diamond.

"What we're interested in is the size of these mesoatoms because they're 1,000s of times bigger than atoms," he said. "It turns out these building blocks are on the order of the wavelength of light. So now we have an opportunity in the future to think about how to adjust the structure on the scale that matters to create novel light-defect interactions."

A twin boundary is a common low-energy planar defect in crystals, including those with an atomic diamond structure. Twins stand side by side and have a mirror plane halfway between them.

"We analyzed the defect and realized by looking at the data there's a mirror plane," Thomas said. "Then we wanted to figure out what the structure is. The single diamond red network has the same structure as the twin in your diamond ring. And it's like the atomic structure of hard atoms in the diamond has been reproduced by the mesoatom at a scale 1,000 times bigger."

The team discovered that there is more than one kind of mesoatom species.

"We don't have to build everything from the diamond tetrahedral symmetry. The structures form using trihedral and pentahedral symmetric mesoatoms," he said. "We're excited that we can make these new kinds of symmetries. Those are new shapes of mesoatoms that hadn't been noticed before."

These molecules reveal that they can form other shapes because they're soft and deformable, and given a certain environment, they will figure out the best shape to be in.

"The notion here for future work is the adaptability to create new structures," Thomas said. "We didn't know these things were new types of mesoatom structures and symmetries. Nobody predicted this."

Since crystals are periodic and have lots of symmetry, if you look at them from one place to another, they're identical. However, a twin is a defect with a smooth planar defect.

"We see these boundaries, these changes in the pattern all over the place," Thomas said. "We then do the research, taking a series of many 2D slices, and then we can create a reconstructed 3D image."

By creating defects, they can create new kinds of mesoatoms and the shape of the mesoatom is important to properties and the properties that the research team is interested in for properties of defects interacting with light waves.

"I think a little bit in the eye of the beholder, but for me, I'm pleased to see adaptability," he said. "Understanding how to manipulate matter is at the heart of that and is what materials scientists and materials engineers are all about."

More information: Xueyan Feng et al, Soft, malleable double diamond twin, *Proceedings of the National Academy of Sciences* (2023). DOI: 10.1073/pnas.2213441120

Provided by Texas A&M University College of Engineering