Researchers use DNA to make crystals that can switch configurations

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(Phys.org)—Beyond serving as the backbone of modern biology, DNA has come to be a molecule of great interest to engineers. That a DNA sequence will naturally bind only with a complementary sequence could make it part of a configurable, and potentially programmable, building material.

Researchers at the University of Pennsylvania's School of Engineering and Applied Science have now used DNA to make a crystal that can switch into a more stable configuration under the right temperature conditions, much like heat-treated steel.

The research was conducted by associate professor John Crocker and professor Talid Sinno, alongside graduate students Marie Casey, Raynaldo Scarlett, W. Benjamin Rogers and Ian Jenkins, all of the Department of Chemical and Biomolecular Engineering.

Their work was published in Nature Communications.

"The great thing about DNA is that it will only bind to other DNA that has the complementary sequence," Crocker said. "So engineers have long thought that we could make a whole library of parts, put the appropriate sequences on the outside, then put them in a test tube and they would self-assemble."

While this concept has yet to be fully realized, Crocker's group made an important step toward that goal in 2005, when it was the first to make a crystal using this method. Crystals are simply solids that are composed of parts arranged in a repeating 3D pattern. In the case of natural crystals, those parts are atoms, but in that experiment Crocker and his colleagues made crystals out of microscopic plastic spheres coated with specific DNA strands.

Making a crystal in this way was an important proof-of-concept for DNA-coated building materials. In their recent study, Crocker and his colleagues took this technique a step further.

"When I make an atomic crystal, I can do metallurgy; I can make the crystal bigger or smaller, reshape it or change its structure," Crocker said. "In this experiment, we wanted to show it's possible to do those sorts of things with these colloidal DNA crystals, and we did. We demonstrated that they do a trick that iron atoms do when you heat-treat steel."

This experiment involved coating plastic spheres, 400 nanometers wide, with strands of DNA. The researchers began by coating one group of particles with a particular DNA sequence and another group with that sequence's complement. They added different colored fluorescent dye to each group of particles so they would be easier to track and differentiate.

In this arrangement, there could only be "unlike" attraction; red particles could only stick to green particles, as if one was covered in Velcro hooks and the other was covered with the corresponding loops.

When put into a hot solution that was gradually cooled, this arrangement produced crystals that mimicked the pattern of cesium chloride, or CsCl. This means that each particle is at the center of eight neighbors. A green particle would have eight red particles around it, arranged like the corners of a cube.

The next step involved putting both kinds of DNA strands on each particle in different ratios, as if both red and green particles had both hooks and loops in varying amounts. This enabled "like" attractions—two particles of the same color could now bond—and, by making the ratio more even, the researchers could increase the strength of these "like" attractions.

"We might start by coating the red particles with 90 percent original and 10 percent complement and coating the green particles in 10 percent original and 90 percent complement. That way, when the red and green particles come together, there's a 90 percent as strong 'unlike' attraction making them still very likely to bond. But if two green particles were to come together, there is still a 10 percent as strong attraction as well."

The researchers found that a different kind of crystal formed when they used particles with both original and complement DNA strands on their exteriors. They had the pattern of copper gold crystals, or CuAu, and appeared in greater quantities as the researchers increased the strength of the "like" attractions between the particles.

In the CuAu crystal, a green particle has the same eight red neighbors as in the CsCL crystal. However, those red particles on the corners are flattened out to make room for four more particles — all of which are green — that are arranged on the faces of the cube.

The researchers could not directly see the CsCl crystals transforming into CuAu crystals but, bolstered by computer simulations developed by professor Talid Sinno and graduate student Ian Jenkins, they had a theory for what was occurring as the solution cooled.

"The CsCl crystal is floppy; it's made of squares rather than triangles, which makes it deformable," Crocker said. "This means it is always undergoing various shape fluctuations. It sheers and stretches and occasionally deforms enough that two 'like' particles can touch. But if there's no 'like' attraction, those particles just pull back again."

In the heat-treated-steel analogy, the additional energy allows the steel's iron atomic crystals to change orientation; it is temporarily like the floppy CsCl crystal. When the steel is rapidly cooled, its atoms lock into a stronger configuration. In this case, "like" attractions enable a similar locking mechanism.

"All it takes is one of those 'like' particle pairs to latch together, and then the entire crystal structure grows around that pattern," Crocker said. "It goes from that floppy, jiggling crystal to a solid, stiff crystal. Just like that harder steel, it's got more triangles in it because it has 12 neighbors instead of eight. As we make the like interactions stronger, we get more of those stiff crystals and less of the floppy ones."

To move from theory to proof, Crocker and his colleagues needed more evidence that this was indeed the process responsible for creating the CuAu crystals. Once again taking a cue from metallurgy, they found their evidence in a handful of naturally occurring crystals that formed both CsCl and CuAu patterns.

"If you do this experiment with iron atoms, you can make a piece of steel that has both kinds of crystals in separate regions," Crocker said. "Where those two types of crystals meet, they always do so at a certain characteristic angle, which the metallurgists call 'habit planes.'"

Crocker's student, Marie Casey, hunted through hundreds of crystals and categorized them as to whether they were CsCl or CuAu. She found seven that were both, which allowed the team to determine the habit plane that forms when the CsCl crystal pattern naturally turns into CuAu.

"The DNA particle crystals we looked at all had the exact same habit plane structure which matched that seen in iron, as well," Crocker said. "You didn't just see the two kinds of crystal just stuck together randomly; you would always see a nice ball where it looked like someone had drew a line in it, where one half was CsCl and the other was CuAu."

Understanding the mechanisms that allow the transition between these two crystal states will be helpful for creating more complex structures out of these DNA-based building blocks.

Provided by University of Pennsylvania

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