Surprising discovery: X-rays drive formation of new crystals

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detect broken bones, tumors and dental cavities, analyze atoms in diverse materials and screen luggage at airports -- but who knew they could cause crystals to form?

A team of Northwestern University researchers has discovered that X-rays can trigger the formation of a new type of crystal: charged cylindrical filaments ordered like a bundle of pencils experiencing repulsive forces, which is unknown in crystals. Similar phenomena may occur naturally in biology, such as in the cytoskeleton filaments of cells, which control cell division and migration in cancer metastasis and many other processes.

The results, which will be published this week in the Jan. 29 issue of the journal *Science*, expand scientific knowledge of crystals, whether from nature, technological devices or the lab, and also open the door to using X-rays to control the structure of materials or to develop novel biomedical therapies.

Crystal formation is usually based on attractive forces between atoms or molecules, making the Northwestern discovery completely unexpected.

"This is a very intriguing and astonishing result," said Samuel I. Stupp, the paper's senior author and Board of Trustees Professor of Chemistry, Materials Science and Engineering, and Medicine. "The filaments are charged so one would expect them to repel each other, not to organize into a crystal. Even though they are repelling each other, we believe the hundreds of thousands of filaments in the bundles are trapped within a network and form a crystal to become more stable."

The discovery of the new crystals was serendipitous. Very early one morning at Argonne National Laboratory, the members of Stupp's research team applied synchrotron X-ray radiation to a solution of peptide nanofibers they were studying. (The peptides are small synthetic molecules that can be used to create new materials.) The researchers saw the solution go from clear to opaque.

"There was a dramatic change in the way filaments scattered the radiation," said first author Honggang Cui, a postdoctoral fellow in Stupp's lab. "The X-rays turned a disordered structure into something ordered -- a crystal."

The X-rays increase the charge of the filaments, and thus a repulsive electrostatic force drives the crystallization -- a hexagonal stacking of filaments. Trapped in a three-dimensional network, the charged bundled filaments are unable to escape from each other. The crystals disappear when the X-rays are turned off, and the material is not significantly damaged by the radiation.

As a result of repulsive forces, the filaments are positioned far apart from each other, with as much as 320 angstroms separating the filaments. This striking feature is not found in ordinary crystals where molecules are less than five angstroms apart.

"There are oceans of water inside the crystal," Stupp said. "More than 99 percent of the structure is water." The researchers also observed that when the concentration of the charged filaments in solution was higher, the same crystals formed spontaneously without the need to expose them to X-rays.

More information: The *Science* paper is titled "Spontaneous and X-Ray Triggered Crystallization at Long Range in Self-Assembling Filament Networks." In addition to Stupp and Cui, other authors of the paper are E. Thomas Pashuck, Yuri S. Velichko, Steven.

Provided by Northwestern University