# Crystal mysteries spiral deeper, chemists find

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New York University chemists have discovered crystal growth complexities, which at first glance appeared to confound 50 years of theory and deepened the mystery of how organic crystals form. But, appearances can be deceiving.

Their findings, which appear in the latest edition of *Proceedings of the National Academy of Sciences*, have a range of implications—from the production of pharmaceuticals and new electronic materials to unraveling the pathways for kidney stone formation.

The researchers focused on L-cystine crystals, the chief component of a particularly nefarious kind of kidney stone. The authors hoped to improve their understanding of how these crystals form and grow in order to design therapeutic agents that inhibit stone formation.

While the interest in L-cystine crystals is limited to the biomedical arena, understanding the details of crystal growth, especially the role of defects—or imperfections in crystals—is critical to the advancement of emerging technologies that aim to use organic crystalline materials.

Scientists in the Molecular Design Institute in the NYU Department of Chemistry have been examining defects in crystals called screw dislocations—features on the surface of a crystal that resemble a spiraled ham.

Dislocations were first posed by William Keith Burton, Nicolás Cabrera, and Sir Frederick Charles Frank in the late 1940s as essential for crystal growth. The so-called BCF theory posited that crystals with one screw dislocation would form hillocks that resembled a spiral staircase while those with two screw dislocations would merge and form a structure similar to a Mayan pyramid—a series of stacked "island" surfaces that are closed off from each other.

Using atomic force microscopy, the Molecular Design Institute team examined both kinds of screw dislocations in L-cystine crystals at nanoscale resolution. Their results showed exactly the opposite of what BCF theory predicted—crystals with one screw dislocation seemed to form stacked hexagonal "islands" while those with two proximal screw dislocations produced a six-sided spiral staircase.

A re-examination of these micrographs by Molecular Design Institute scientist Alexander Shtukenberg, in combination with computer simulations, served to refine the actual crystal growth sequence and found that, in fact, BCF theory still held. In other words, while the crystals' physical appearance seemed at odds with the long-standing theory, they actually did grow in a manner predicted decades ago.

"These findings are remarkable in that they didn't, at first glance, make any sense," said NYU Chemistry Professor Michael Ward, one of the authors of the publication. "They appeared to contradict 60 years of thinking about crystal growth, but in fact revealed that crystal growth is at once elegant and complex, with hidden features that must be extracted if it is to be understood. More importantly, this example serves as a warning that first impressions are not always correct."

**More information:** Illusory spirals and loops in crystal growth, www.pnas.org/cgi/doi/10.1073/pnas.1311637110

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