

Clusters and Decagons

New rules for constructing a quasicrystal

By IVARS PETERSON

The view from inside a typical crystal is notably monotonous. One neat row of atoms succeeds another at regular intervals.

One can think of such an ordered solid in terms of stacked building blocks. The blocks of a particular crystal consist of identical arrangements of atoms. Constructing a crystal out of these unit cells is much like laying bricks to build a wall.

Until 1984, scientists thought that all ordered solids have such a simple, periodic arrangement. Then, during a project at the National Institute of Standards and Technology in Gaithersburg, Md., Dan Shechtman of the Israel Institute of Technology in Haifa was shocked to discover that an aluminum-manganese alloy, which appeared to be crystalline, did not obey the conventional rules of crystal structure (SN: 3/23/85, p. 188).

What set this material apart from normal crystals was the spacing of its rows of atoms. Instead of repeating throughout the structure at some regular interval, atoms of this so-called quasicrystal were spaced at either of two characteristic intervals, in a fixed ratio. The atoms appeared to be clustered in complex patterns that led to an unusual geometric arrangement.

Since Shechtman's startling discovery, researchers have synthesized a variety of alloys with similar structures, which they have grouped with the aluminum-manganese alloy into a new class of materials. They have also discovered that some quasicrystalline alloys are harder than crystalline materials having the same composition, some have a higher resistance to electricity at low temperatures, and some have surfaces that are particularly slippery.

Until recently, however, materials scientists could not explain how the atoms of these quasicrystals could assemble themselves into such a complex arrangement rather than the regularly repeating pattern of a crystal.

Now, physicists Paul J. Steinhardt of the University of Pennsylvania in Philadelphia and Hyeong-Chai Jeong of the University of Maryland in College Park have introduced a novel mathematical model that may shed light on the interactions responsible for quasicrystal formation. Their model requires only a single type of building block for constructing a two-dimensional quasicrystal.

Extended to three dimensions, this approach could provide a simple, unified picture of how both ordinary crystals and quasicrystals form, Steinhardt contends. The researchers report their findings in the Aug. 1 *NATURE*.

One convenient way to picture a two-dimensional quasicrystal is as an arrangement of structural units spread across a surface, like tiles on a bathroom floor. To get the nonrepeating pattern characteristic of quasicrystals, however, one can't use tiles shaped like squares or hexagons.

In 1974, mathematical physicist Roger Penrose of the University of Oxford in England discovered that he could construct a nonperiodic tiling by using two different tile shapes—a wide diamond and a thin diamond—with special rules for how neighboring tiles fit together. All the pieces join neatly to cover a flat surface, but the resulting pattern of tiles doesn't repeat itself at regular intervals.

The Penrose tiling embodied several features characteristic of quasicrystal structures. When quasicrystals were discovered, some researchers immediately looked to Penrose tiling

as a simple model of how quasicrystal atoms might be arranged. It suggested that the atoms of a quasicrystal organize themselves into two types of clusters, which act as building blocks, rather than into the single type of block typical of conventional crystals.

The trouble was that a Penrose tiling requires a set of rules that specify how the tiles must be placed. The tiles, marked for example with lines or arrows, must abut certain edges to yield the final pattern.

The scientists can't imagine how clusters of atoms in quasicrystals could interact in ways that mimic the complicated matching rules. Moreover, it's difficult for anyone to piece together, say, 100 Penrose tiles without error (SN: 7/16/88, p. 42). Yet perfect quasicrystals made up of 10^{23} atoms can form in minutes.

These inadequacies of the original Penrose tiling model prompted searches for alternative ways of describing quasicrystals. One possibility involved replacing Penrose's two shapes of diamond tiles with a single type of building block.

Mathematician Petra Gummelt of the University of Greifswald in Germany was one of the first to come up with such a scheme. She used a 10-sided, or decagonal, tile as her basic structural unit. Rather than abutting each other like the Penrose tiles, these decagons overlap in specific ways. The lumpiness one would get with bathroom tiles was not a problem, because her mathematical tiles were only two-dimensional.

When Steinhardt first heard of Gummelt's pattern, he was skeptical. "It wasn't clear from her paper that the construction actually worked," Steinhardt says.

However, he and Jeong ended up proving Gummelt correct, and they worked out a simpler version of her proof that illuminated the link between her decagons and Penrose's diamond tiles. They then proved that her overlap rules are equivalent to Penrose's matching rules.

These results show that the atomic structure of quasicrystals and ordinary crystals can be understood in terms of a single repeating unit, Steinhardt says.

A sensible way of interpreting the overlap rules in physical terms is as a sharing of atoms by neighboring clusters, rather than as two clusters penetrating into each other, he adds. Such a possibility is consistent with experimental data on the positions of clustered atoms in quasicrystals.

Steinhardt and Jeong also found a second, independent way of constructing a Penrose tiling suitable for modeling a quasicrystal. It eliminates the need for matching or overlap rules.

The physicists identified a small cluster of adjacent tiles that appears again and again within the Penrose tiling pattern. These clusters overlap, sharing tiles with their neighbors. The pattern that contains the maximum number of such overlapping clusters automatically generates a nonperiodic tiling.

"Maximizing the density of a chosen cluster of tiles suffices to produce a quasiperiodic tiling," the researchers say. The decagon scheme also meets this criterion.

This finding suggests that when atoms settle into clusters that have the lowest possible energy, the natural tendency is to form clusters of overlapping clusters. This lowers the energy further by maximizing the number of low-energy clusters present. "Cluster overlap plays an important part in this energy minimization," Steinhardt says.

In ordinary crystals, no overlap occurs, and the atomic unit cells pack into a repeating pattern, which gives the structure minimum energy.

"If the clusters can share atoms and have the proper geometry, then quasicrystals form," he notes. "The same basic picture explains both crystals and quasicrystals."

These results for two-dimensional nonperiodic tilings apply directly to certain stacked materials that researchers have synthesized. In this case, the quasicrystalline geometry is restricted to thin layers. No one has yet extended the ideas to three-dimensional structures.

“If these principles can be established [in three dimensions], they may enable the reliable prediction of new quasicrystals,” Steinhardt and Jeong conclude.

With a better understanding of why quasicrystals form, materials scientists may achieve improved control of the composition and structure of these materials, potentially leading to a variety of practical applications. □