A Quasicrystal Construction Kit

Picturing complex alloy structures as overlapping atomic clusters

By IVARS PETERSON

The unexpected discovery of quasicrystals in 1984 presented scientists with a new, puzzling class of materials.

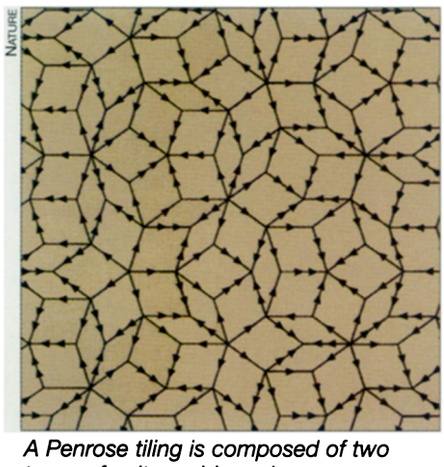
The atoms of these unusual metal alloys are neither arranged in neat rows at regularly spaced intervals—as they would be in a crystal—nor scattered randomly—as they would be in a glass. Instead, they exhibit a complicated but predictable pattern, described by mathematicians as quasiperiodic.

"Although a quasicrystal is nonperiodic, its structure still follows a subtle construction plan," remarks Knut W. Urban of the Institute of Solid State Physics at the Helmholtz Research Center-Jülich in Germany.

Until recently, however, materials scientists couldn't convincingly visualize how atoms turned that construction plan into reality, assembling themselves into complex, quasiperiodic patterns rather than regularly repeating arrangements.

Moreover, "you see transformations between quasicrystals and crystalline compounds that are close in composition," says Alan I. Goldman of Iowa State University and Ames Laboratory. "You would like to understand on a physical basis how you go from one to the other."

In 1996, Paul J. Steinhardt, now at Princeton University, and Hyeong-Chai Jeong of Sejong University in Seoul, South Korea, proposed a novel mathematical model that promised to shed light on the interactions responsible for quasicrystal formation (SN: 10/12/96, p. 232).



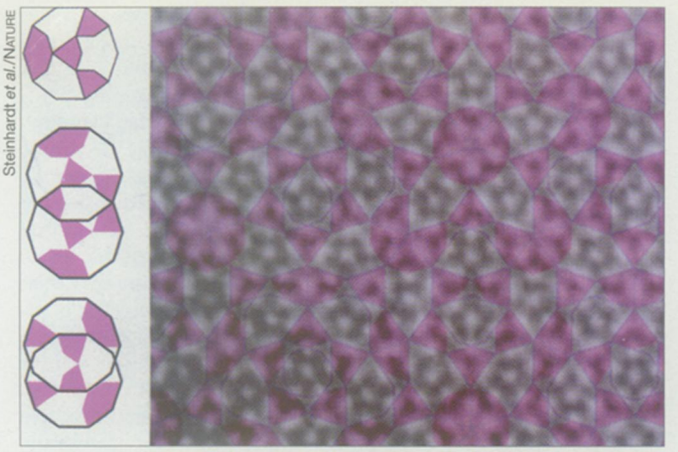
A Penrose tiling is composed of two types of units—wide and narrow diamonds—having edges of equal length. To create a quasiperiodic pattern, two tiles can join edge-to-edge only if the number and direction of arrows along the adjacent edges match.

Conventional crystals consist of repeated copies of a single geometric arrangement of atoms—a unit cell—stacked together like bricks. A quasicrystal, Steinhardt and Jeong suggested, can also be built up from a single type of atomic cluster, with the crucial difference that adjacent clusters overlap, sharing atoms with their neighbors.

Now, Steinhardt and his coworkers have obtained striking experimental evidence supporting their proposed model. "This is a beautiful demonstration of the power of the new picture of quasicrystals in terms of a single quasi-unit cell," Steinhardt says. The researchers report their findings in the Nov. 5, 1998 NATURE.

Quasicrystalline materials typically consist of aluminum mixed with metals such as manganese, cobalt, and nickel.

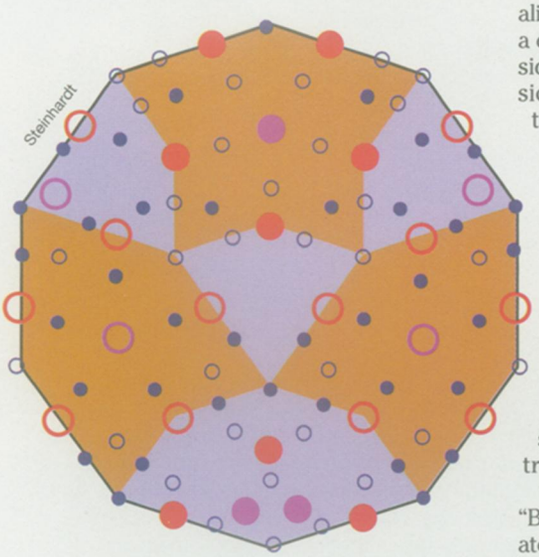
Images of X rays or electron beams deflected by these alloys show well-defined spots rather than a blurred pattern, indicating that the material has an orderly atomic structure. The geometric arrange-



A diagram of a set of decagonal units (top left), which can overlap in two different ways (middle and bottom left), is superimposed on a black-and-white electron microscope image of an aluminum-nickel-cobalt alloy (right) to reveal a good match between the mathematical model and atomic positions in a quasicrystal.

ment of the spots in these diffraction patterns, however, has a symmetry not found among patterns produced by conventional crystals.

Because the unusual spacing evident in quasicrystals cannot result from a simply repeating unit cell, researchers turned to alternative structural models. To simplify matters, they started with two-dimensional units spread across a surface, like tiles on a bathroom floor.



In this diagram of a possible arrangement of atoms within a layered quasicrystal's decagonal unit cell, large circles represent nickel (red) or cobalt (yellow) and small circles represent aluminum (purple). The material has two types of layers. Solid circles show atomic positions in one sort of layer; open circles show their positions in the other.

One early candidate for a model of quasicrystals was based on a tiling discovered in 1974 by mathematical physicist Roger Penrose of the University of Oxford in England. Penrose found that he could construct a nonperiodic tiling by using two different tile shapes—a wide diamond and a narrow diamond—with strict matching rules specifying how neighboring pieces fit together to generate a faultless structure.

The tiles join neatly to cover a flat surface completely, but the resulting pattern doesn't repeat itself at regular intervals. Inspired by that example, some researchers suggested that the atoms of a quasicrystal organize themselves into two distinct types of clusters, which join together in a prescribed way to form the solid.

It wasn't at all obvious, however, how atoms would know where to go to create a defectfree structure with just the right proportion of the two kinds of clusters and the proper matching between adjacent clusters.

In 1991, mathematician Sergei E. Burkov of the Landau Institute of Theoretical Physics in Moscow realized that it was possible to create a quasiperiodic tiling by using 10-sided, or decagonal, tiles as the basic structural unit, provided that the tiles could overlap. Later, Petra Gummelt of the Ernst Moritz Arndt University of Greifswald in Germany proved mathematically that Burkov's overlapping decagons are indeed equivalent to a quasiperiodic Penrose tiling.

Steinhardt and Jeong extended Gummelt's work and postulated that three-dimensional quasicrystals form from a single type of building block, where neighboring clusters share atoms rather than actually penetrate each other.

"It's an attractive model," Goldman says. "By allowing the clusters to share specific atoms, you eliminate the need for matching rules." In other words, the clusters don't have to follow the precise rules of the Penrose tiling. It's then easier to imagine how atoms interact with their neighbors to create the necessary structure.

Steinhardt and Jeong went on to demonstrate theoretically that a quasiperiodic packing, where clusters can overlap by sharing atoms, produces a denser array of atoms than any periodic packing pattern, where the clusters sit side by side.

"That emerges naturally as a way to get the lowest-energy structure," Steinhardt notes. The lowest-energy structure of a crystal is its most stable.

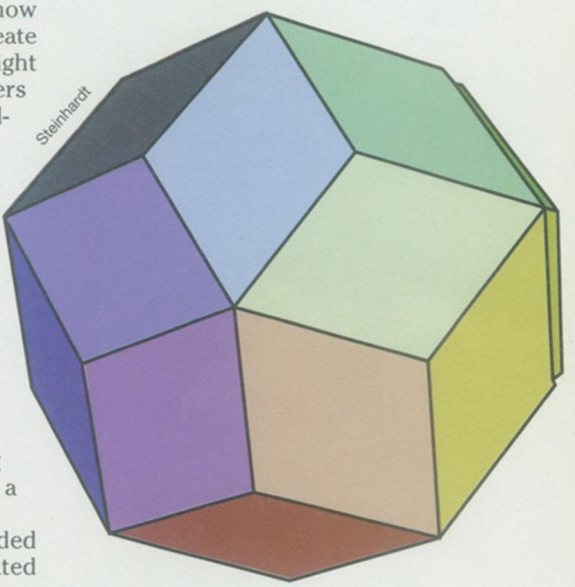
To test their model, Steinhardt and Jeong obtained electron-microscope data unveiling the surface structure of a quasicrystalline alloy composed of aluminum, nickel, and cobalt. This particular material arranges itself in thin, neatly stacked layers, so the quasicrystalline geometry is restricted, in effect, to two dimensions, as in a tiling.

The researchers obtained a remarkably precise correspondence between the atomic-scale features visible on the quasicrystal's surface and a model pattern of overlapping decagons.

"That the entire structure reduces to a single repeating unit means that quasicrystals have a simplicity more like that of crystals than previously recognized," Steinhardt contends.

Just as for crystals, determining the structure of a quasicrystalline solid comes down to figuring out the distribution of atoms in a single unit cell of clustered atoms, which is then repeated throughout the entire structure.

"It becomes a matter of how you attach these units together," Goldman says. "In the case of crystals, you have attachments at the boundaries of the unit cells. In the case of quasicrystals, you have some sharing of atoms."



A triacontahedron.

The still evolving model provides clues about what may be going on at the atomic level to produce the distinctive quasicrystalline structures.

Whether the same sort of model works in three dimensions isn't known yet. Nonetheless, "this gives a possible path to a general solution," Goldman says.

Steinhardt and his colleagues are now trying to work out how three-dimensional analogs of decagons—a polyhedron with 30 faces, known as a triacontahedron—might overlap and fit together to generate other kinds of quasicrystals. □