the perfect structure by elementary processes, that is, without global reconstruction? And, of course, its corollary: Can they be relaxed by elementary processes?

The answers to these questions are important both for the mathematical theory of tilings and for the understanding of real quasicrystalline structures. An affirmative answer implies that all local configurations can and will be found in icosahedral random tilings. It would also contribute to the explanation of the occurrence of nearly perfect quasicrystals without the necessity of obeying perfect matching rules during their growth.

Right from the start, we conjectured that at least a wide class of defective vertices in all aperiodic tilings would fit into the perfect patterns and could be created by simpleton (phason) flips. In many cases, this is obvious and we could prove it for the known 2D patterns. This was alluded to but not elaborated by Ben-Abraham (1993) and by Baake, Ben-Abraham, Klitzing, Kramer & Schlottmann (1994). Since we have not found a formal proof for the possibility of embedding and elementary creation of arbitrary vertices in the primitive icosahedral structure, we chose to approach the problem by a computer experiment.

We wrote a program that takes a finite patch of the perfect tiling, keeps the boundaries fixed (and hence takes care of a perfect neighborhood) and performs, according to a Monte Carlo algorithm, random flips within the patch. The updated patch is scanned in the search for newly created vertices, which are registered and checked against the known vertex list. For reasons of efficiency, we took an approximately round patch with a radius of six rhombohedral edge lengths.

The results fulfilled our expectations. Starting from the perfect primitive icosahedral tiling, we found that all possible 5450 vertices were reached through successive simpleton flips. In this sense, the whole configuration space of the tiling turned out to be ergodic. At the same time, this result provides a mutual consistency check of both the randomization algorithm and the vertex list previously established by an altogether different algorithm.

Our results open an avenue to numerical studies of models for quasicrystallline structures with prescribed interaction energies, such as calculations of entropies, elastic constants and specific heats. They also provide a key to the reconciliation of random growth patterns with the existence of nearly perfect quasicrystals.

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Right and left in chiral crystals.

By Jack D. Dunitz, *Organic Chemistry Laboratory, Swiss Federal Institute of Technology, ETH-Zentrum, CH-8092, Zurich, Switzerland*

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Abstract

Contrary to statements in the recent crystallographic literature, there is no ambiguity about which of two opposite faces of a chiral crystal is which.

Statements in the recent crystallographic literature (Colella, 1994; Spence, Zuo, O'Keefe, Marthinsen & Hoier, 1994) may give the impression that there is an ambiguity in the sign of Miller indices such that one cannot distinguish between the $\mathbf{H}(hkl)$ reflection of a given chiral crystal and the $-\mathbf{H}(-h,-k,-l)$ reflection of its enantiomorph in the absence of anomalous dispersion. There is no such ambiguity. Once one accepts the conventional (but binding) distinction between a right and a left hand, the crystal lattice can always be defined by a right-handed vector triple $\mathbf{a},\mathbf{b},\mathbf{c}$; the $\mathbf{H}(hkl)$ and $-\mathbf{H}(-h,-k,-l)$ planes are then unambiguously differentiated. What we do not know in the absence of additional information is whether the atomic coordinates are $\mathbf{x}_i$ or $-\mathbf{x}_i$. Thus, there is never any question about which of the two opposite $\{hkl\}$ faces is which, only the uncertainty about the sense of chirality of the atomic coordinates – a matter that can be settled by anomalous dispersion (Bijvoet, Peerdeman & van Bommel, 1951), by multiple diffraction measurements (Hummer, Weckert & Bondza, 1989), by experiments involving crystallization in the presence of 'tailor-made' additives (Addadi, Berkovitch-Yellin, Weissbuch, Lahav & Leiserowitz, 1986) or by *a priori* knowledge of the absolute configuration of the molecules. Analogous considerations apply to the specification of the sense of polarity of a polar axis in a crystal; polarity is just one-dimensional chirality.

For a discussion of this topic from a somewhat different point of view, see the recent comment by Burzlaff, Lange & Zimmermann (1995).

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