3D Icosahedral Aperiodic Packings of Spheres of Different Diameters from Discrete Icosahedral Crystals

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A 6-d icosahedral discrete crystal is constituted by a 6-d periodic assembly of colored points obeying a 6-d icosahedral space group. 6-d atoms are here of dimension 0, and this is compatible with deWolff's (1977) and Janner and Janssen's (1977) approaches. We assume that the 6-d discrete crystals which can be built according to different ways from approximant crystals (for instance (Verger-Gaugry, 1990; Verger-Gaugry and Tamura, 1990)) are "close" to such 6-d ideal icosahedral crystals. These 6-d ideal icosahedral crystals provide a 3-d icosahedral quasiperiodic skeleton for the icosahedral phase. From this skeleton, small (3-d) sites displacements are controlled by the way the 6-d discrete crystal is built and the result is here called the *i*-phase (Verger-Gaugry and Tamura, 1990); the *i*-phase can then be seen as a unique icosahedral skeleton endowed with a collection of coherent aperiodic small displacements on the centers of icosahedral atomic clusters and the clusters themselves. Many possibilities of displacement fields exist and the problem is to establish an energy function to be able to decide which is (or are) more likely to exist. To first order, the diffraction properties of the *i*-phase are essentially those of the cluster term together with a transparency function associated with the cluster skeleton (Verger-Gaugry *et al.*, 1990).

The problem amounts now to restoring 3-d atoms in physical space when the atomic surfaces are not of maximal dimension, namely 3 in the 6-d formalism (perpendicular space dimension). For this, we assume that H is the 6-d icosahedral space group of the 6-d icosahedral crystal (with point group $m\bar{3}5$) and we propose the following general scheme when atoms are 0-dimensional (Verger-Gaugry, 1990): we dualize the discrete 6-d icosahedral crystal by paying attention to the collection of Voronoi cells deduced from the 6-d atomic positions, which is H -invariant. Each 6-d Voronoi domain takes the color of the central atom it contains. If v is such a cell, we can tile physical space E (embedded in $\mathbb{R}^6$ as an irreducible $\mathbb{R}[m\bar{3}5]$ -module) by the collection $\{v \cap E, \text{color of } v\}$. Assume for instance $H = Pm\bar{3}5$, then this set is $m\bar{3}5$ -invariant. This infinite set of colored tiles is now replaced by the infinite set of atoms where one atom is positioned at the centroid of the tile $v \cap E = c(v \cap E)$.

The color of the atom is that of the tile $v \cap E$ which contains it. We obtain a quasiperiodic packing of spheres of different diameters in E whose Fourier transform is almost $m\bar{3}5$ -invariant. The minimal interatomic distances are satisfied once a change in scale in E is made.

Taking the locus of all the centroids of the (3-d) cells $v \cap E_\alpha$ in $\mathbf{R}^6$ (with $E_\alpha = E + \alpha$) when α varies in E_{perp} that is $\bigcup_v \bigcup_\alpha c(v \cap E_\alpha)$, we obtain a collection of colored (continuous, open at their extremities) *atomic lines* (1-d). This requires a good knowledge of the second moments of 3-d Voronoi cells (Conway and Sloane, 1988), while their walls have a crystallographic meaning arising from the atomic position parameters and the 6-d Wyckoff positions of the 6-d discrete icosahedral crystal. This is the analogue of the 3-d atomic surfaces for volumic 6-d atoms (for instance, Cornier-Quiquandon *et al.*, 1991). We investigate the analogy with Katz's polyhedra and the way to generalize a 3-d dynamics on the Laguerre mouss formed by the collection $\{v \cap E\}$, following Telley (1989).

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