**Sizes and Series of $m\overline{35}$ -Atomic Clusters in
Icosahedral Quasicrystals and in $m\overline{35}$ -
Approximant Crystals. Theory and Examples**

J.-L. Verger-Gaugry and N. Tamura

*LTPCM/ENSEEG/INPG (CNRS UA 29), BP 75, Domaine Universitaire, 38402 Saint
Martin d'Hères, France*

The present study covers simultaneously several areas about icosahedral order in crystallized matter. In (3-d periodic) crystals, the question of how icosahedral local order can propagate around some sites is extremely relevant, since it does exist in some crystals, and the structure of the icosahedral phase is intimately linked to this problem: indeed, the first modeling of quasicrystals was effectively started from the knowledge of the approximant crystal α -AlMnSi (Guyot and Audier, 1985) in which big $m\bar{3}5$ -atomic clusters were observed. On the other hand, it is known that a crystal can be a “good” approximant when its lattice parameters are relatively important.

We have at first given a formal definition of an approximant crystal and then tried to reformulate the question of propagating icosahedral order in crystals in as general terms as possible. Does there exist any specific feature to a space group to give rise to approximant crystals? Intuitively, we need atoms per unit cell and Wyckoff positions in sufficient number. The number ($=N$) of atoms per unit cell of the Bravais lattice can reach several hundreds, while the number of different “occupied” Wyckoff positions ($=w$) is limited by the order of the point group and N . The question can be reformulated like this: taking a space group, what are the minimal values of the couple (w, N) and what are the corresponding position parameters for which the crystal can be considered as an approximant crystal? When it is the case, how many orientational families of icosahedra do we recover in the crystal and what are the spatial extents of the respective icosahedral clusters? For instance, the approximant crystal c-Ti₂Ni ($Fd\bar{3}m$) exhibits 8 families of non equivalently oriented icosahedral clusters for $N = 96$ and $w = 3$.

Assuming that the position parameters are rational numbers, the basic tool for studying this problem appears to be the function $r_3(n)$ (Bateman, 1951) which counts the total number of solutions (x_1, x_2, x_3) in integers of the Diophantine equation $x_1^2 + x_2^2 + x_3^2 = n$ (with n an integer). Indeed, we need sites of exact coordination 12 for which the 12 vertices form a perfect icosahedron and are located on a sphere (whose radius is $\sqrt{n}$). Centers of icosahedral clusters are not any atomic site and we

discuss this viewpoint. In this approach, the usual constraints for packings of spheres have to be satisfied, namely not too short interatomic minimal distances and no hole.

The second part is essentially dealing with the observation of such icosahedral clusters of atoms in $m\bar{3}5$ -approximant crystals and how they interpenetrate. It is observed that incomplete icosahedral polyhedra exist sometimes as layers in icosahedral clusters. This is the case in the μ -AlMnSi phase (Tamura and Verger-Gaugry, 1991) where icosahedral local order resembles that which can be found in the α -AlMnSi and β -AlMnSi approximant crystals.

From a more theoretical viewpoint, we have developed a theory of diffraction of matter, when matter is constituted by the long-range interpenetration of icosahedral atomic clusters, positioned periodically as in the case of $m\bar{3}5$ -approximant crystals, or aperiodically, as in the case of icosahedral quasicrystals. For crystals, the structure factor is developed as a perturbation over icosahedral symmetry and site multiplicities. For quasicrystals, some additional convergence conditions have to be fulfilled. We illustrate these notions (Verger-Gaugry, 1991). This formalism provides a "continuous link" between classical crystallography and "quasicrystallography".

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