Canonical-cell geometry: a practical framework for describing the packing of icosahedral clusters

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The canonical-cell tiling (CCT) [1] is a geometrical framework for describing the packing of icosahedral clusters as tilings of four basic polyhedra called the canonical cells. To date, this framework has been applied to increasingly many approximants to icosahedral quasicrystals, successfully describing networks of clusters in the complex intermetallic alloys [2,3]. In quasicrystals research, however, the CCT has been much less referred to than the more standard rhombohedral Ammann tiling, also known as a three-dimensional analogue to the rhombic Penrose tiling. Reasons for the less-popularity might be as follows: i) the cells have less-aesthetical (or less-symmetric) shapes, ii) the geometrical constraints of the cells penetrate through the structure in more intricate manners, iii) diverse possibilities in the arrangement of cells may seem intractable and iv) in the 6-dimensional cut-and-project scheme, a potential quasiperiodic CCT is likely to have an atomic surface with fractal boundary, hence the construction of such a tiling may seem formidable. This contribution is aimed at providing a renewed account of the canonical-cell geometry, particularly focusing on its capability to represent a variety of cluster arrangements in approximant crystals and their defects. In so doing, we introduce a simplified atomic decoration rule of the canonical cells to construct an idealized atomic arrangement of Al-Pd-M type (M=transition metal) from a CCT. We also demonstrate that a range of stacking faults that respect the local constraints of cells can be introduced into periodic CCT's. Such planer defects can be the source of merohedral twin boundaries observed in approximants in Al-based alloy systems [4]. The recent discovery of an inflation-deflation rule to construct a quasiperiodic CCT [5] suggests that the applicability of the framework may extend to the atomistic description of icosahedral quasicrystals.

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