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Frustration and defects in non-periodic solids

Frustration et défauts dans les solides non périodiques

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A B S T R A C T

Geometrical frustration arises whenever a local preferred configuration (lower energy for atomic systems, or best packing for hard spheres) cannot be propagated throughout space without defects. A general approach, using unfrustrated templates defined in curved space, have been previously applied to analyse a large number of cases like complex crystals, amorphous materials, liquid crystals, foams, and even biological organizations, with scales ranging from the atomic level up to macroscopic scales. In this paper, we discuss the close sphere packing problem, which has some relevance to the structural problem in amorphous metals, quasicrystals and some periodic complex metallic structures. The role of sets of disclination line defects is addressed, in particular with comparison with the major skeleton occurring in complex large-cell metals (Frank–Kasper phases). An interesting example of 12-fold symmetric quasiperiodic Frank–Kasper phase, and its disclination network, is also described.

R É S U M É

La frustration géométrique apparaît lorsqu'une configuration préférentielle (par exemple de plus basse énergie pour des systèmes atomiques ou de compacité maximale dans les modèles sphères dures) ne peut se propager dans l'espace sans engendrer de défauts. Une approche générale a été proposée dès les années 1980, basée sur des modèles non frustrés définis dans des espaces courbes et qui permet d'analyser de nombreux cas, comme les intermétalliques complexes, les matériaux amorphes, les cristaux liquides, les mousses et même certains édifices biologiques dans une vision multi-échelle allant du niveau atomique au niveau macroscopique. Nous discutons dans cet article le problème de l'empilement de sphères en connexion avec le problème structural des amorphes métalliques, quasicristaux et intermétalliques complexes. On s'intéressera ensuite au rôle des ensembles de disinclinaisons, dont ceux rencontrés dans les grandes mailles des composés métalliques complexes comme les phases de Frank–Kasper. On décrira enfin un exemple intéressant d'une phase de symétrie locale dodécagonale quasipériodique de type Frank–Kasper, avec son réseau de disinclinaisons.

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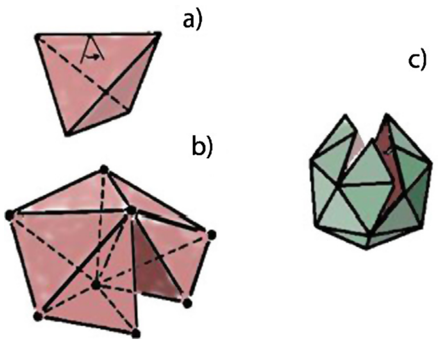

Fig. 1. Geometrical frustration for close tetrahedral packing in R^3. (Colour online.)

1. Introduction

Geometrical frustration appears in different contexts like complex crystals, amorphous materials, liquid crystals, foams and even biological organizations, with scales ranging from the atomic level up to macroscopic scales. It is generically encountered whenever a local configuration, which minimizes energy, cannot be freely propagated throughout space, leading to complex organizations. In this paper, we first recall the curved space approach, whose first step consists in curving the underlying space (here going to the three-dimensional sphere S^3) to release frustration. The real Euclidean structure is then analyzed, along the decurving procedure to R^3, in terms of ordered regions (close to that occurring in S^3), interrupted by topological defects, whose presence and density is directly related to the change of curvature from the curved to the flat space.

We shall focus here on the sphere dense packing problem in three dimensions, in relation with polytetrahedral and icosahedral order. An ideal, unfrustrated, template, the polytope $\{3, 3, 5\}$, is described in Section 2, in particular with the help of the so-called Hopf fibration. Section 3 relates decurving modes of this curved space template in terms of topological defects called disclination lines. These lines can be sequentially entered in the polytope using the Hopf fibration, leading to a first set of slightly decurved polytopes. A method to fully map the polytope into flat space, the iterative flattening method, is recalled, leading to hierarchical structures, with interlaced disclination defects. Such lines are also identified in known large-cell metallic alloy phases called Frank–Kasper phases. A related 12-fold quasicrystalline Frank–Kasper phase is described, and its disclination network displayed. This paper ends by an analysis of coordination number and disclination lengths in polytetrahedral close packings.

2. Hard sphere packing, frustration and curved space template

2.1. Dense sphere packing and icosahedral order

Consider the a priori simple but eventually very different geometrical hard sphere and hard disks packing problem. In two dimensions, three disks densely pack in the form an equilateral triangle, a configuration easily extended throughout the plane in the form of a periodic triangular packing; local and global order are compatible; this is an unfrustrated case. In three dimensions, the local densest packing of four spheres is achieved by placing their centers at regular tetrahedron vertices. The geometric frustration reveals immediately that the three-dimensional Euclidean space cannot be filled completely by regular tetrahedra. Indeed, the tetrahedron dihedral angle is $\theta = \cos^{-1}(1/3)$, slightly less than $2\pi/5$, which leads to the conclusion that five tetrahedra can be arranged around a common edge, with some remaining extra room. The latter accumulates when trying to propagate such a polytetrahedral dense packing, leading to pseudo-icosahedral arrangements at medium range and eventually a disordered sphere packing (Fig. 1).

The misfit angle around one edge can be made vanishing by changing the curvature of the underlying space. In the present case, upon embedding in a 3-dimensional positively curved space, the hypersphere S^3, the tetrahedron dihedral angle increases, and eventually reaches the value $2\pi/5$, which allows a perfect propagation of polytetrahedral order on a hypershere S^3 of appropriate radius (here the tetrahedral edge times the golden ratio $\tau = (1 + \sqrt{5})/2$). One gets a regular structure, a polytope, called the “600-cell” or the $\{3, 3, 5\}$ polytope [1], providing a very dense sphere packing (filling factor $\sim$0.78, therefore surpassing the Euclidean case), which has been intensively studied as an ideal template in the context of amorphous and complex crystalline metals [2–11].

Let us recall Coxeter notation for regular polytopes. A regular polyhedron $\{p, q\}$ has q p-gonal faces around each vertex: $\{4, 3\}$ is a cube, $\{3, 3\}$ is a tetrahedron. A polytope $\{p, q, r\}$ has r $\{p, q\}$ polyhedra around each edge. The $\{3, 3, 5\}$ is a finite structure on S^3, comprising 120 vertices, 600 tetrahedral cells. Each edge shares five tetrahedral cells, and each site is surrounded by a perfect icosahedral first shell. This polytope has a very large symmetry group, of order 14 400, the square of the double icosahedral group Y in $SU(2)$.