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Short Communication

A model for a transition from a quasicrystalline to a microcrystalline state

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Résumé. — Nous proposons un modèle mono-atomique pour une transition quasicristal-microcristal du types de celles observées récemment dans des systèmes à symétrie icosaédrique [3] et décagonale [5]. Il est développé ici pour la symétrie décagonale et est inspiré par des résultats expérimentaux concernant l'alliage Al-Cu-Co-Si [5,6]. Le modèle va au-delà d'une description purement géométrique par un aspect physique important : la transition se fait *via* une seule distance de saut inter-atomique de telle sorte qu'un seul double-puits de potentiel doit être pris en compte ; conformément à la symétrie, il y a 10 directions de saut. Dans le cadre du modèle, la phase microcristalline est énergétiquement favorisée par rapport à une phase approximante monocristalline.

Abstract. — We propose a monoatomic model for a quasicrystal to microcrystal transition as observed recently in systems with icosahedral [3] and decagonal [5] symmetry. It is developed here for the case of decagonal symmetry and is inspired by the experimental results on the system Al-Cu-Co-Si [5,6]. The model goes beyond the purely geometrical description by an important physical aspect: the transition mediates through a single atomic jump distance such that only one unique double-well potential has to be invoked to describe it; in conformity with the symmetry there are 10 jump vectors. In the framework of the model, the microcrystalline state is energetically more favourable than a monocrystalline approximant phase.

1. Introduction.

Important progress is to be expected in our understanding of quasicrystals (QC) if one succeeded in determining an average periodic lattice from which a QC could be derived by a transformation involving only finite displacements. To be physically relevant such an average lattice ought to be

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in a 1-1 - correspondence with the quasilattice obtained from it, such that the number of points is preserved and one keeps track of the individual points in the transformation between the two lattices. However, nailing down an average lattice seems to be much more intricate a task for QC than for other, more classical, incommensurate structures. A theorem [1] reveals how the existence of such a lattice depends on some very restrictive conditions which may often be prohibitive. This can manifest itself by the unphysical circumstance that atoms appear or disappear at the transition [2]. We have taken the recent discovery of transitions between a QC high temperature (T) phase and a microcrystalline (MC) low T phase both in icosahedral [3,4] and decagonal [5,6] systems as a hint that the "average state" might be a MC state. This possibility could provide a loophole of escape from the consequences of the theorem in [1] which assumes an average lattice that corresponds to a single crystal.

A MC state consists of a coherent disposition of periodic domains having orientational relationships [4,6-8]; these restore the overall, forbidden crystallographic symmetry in the diffraction patterns; the coherence of the domains preserves the long range order even for small domain sizes. Various aspects of the QC to MC transition have been addressed recently but the real atomic displacements remain elusive [8,9].

In the present communication, we are able to describe for the first time a QC to MC transformation together with the associated atomic displacements, for an approximant type decoration of the domains, in agreement with [3-6]. Our model is monoatomic and applies to the case of one specific decagonal symmetry but there are probably generalisations to other cases and other QC symmetries.

2. The model.

2.1 STRUCTURE OF THE HIGH T AND LOW T PHASES. — The high T QC phase chosen is the pentagonal Penrose tiling [10] (Fig. 1a) in resemblance to many experimental results on decagonal

Fig. 1. — a) Part of a pentagonal Penrose tiling (atoms: o). b) A unit cell of the approximant periodic lattice (dashed lines). Solid lines indicate the partial decoration found in [5,6]. Atoms are represented by crosses, or stars for those inside the solid line rhombs, to which a 1/2-1/2 occupation probability is associated in order to obtain a centered rectangular unit cell like in [5,6].

QC [11]. The low T periodic lattice is displayed in figure 1b. It is inspired by the unit cell observed in Al-Cu-Co-Si [5,6]: we added one level of deflation τ^2 (where $\tau = (1 + \sqrt{5})/2$ is the golden mean) to its pentagons and rhombs such that figures 1a and 1b resemble very closely, in qualitative agreement with the probable approximant type decoration expected from X-ray diffraction data [6]. In fact this QC-crystal resemblance is not only qualitative but also quantitative: the respective densities are $\rho_c = 58/(\tau^8\sqrt{3-\tau}a^2)$ for the crystal and $\rho_p = 10\tau/(\sqrt{3-\tau}(2+\tau)^2a^2)$ for the QC, where a is the edge of the (small) pentagons of figures 1a and b. The difference $\Delta\rho/\rho$ is about 1/1000, which is physically negligible. This close agreement is the result of the deflation mechanism chosen for the elaboration of the low T unit cell such that one can anticipate a built-in mechanism to improve it even further.

2.2 ATOMIC JUMPS, DOUBLE-WELL POTENTIAL AND MC. — Figures 2a and b show the differences between the QC and the crystal if we try to make the two lattices coincide in a small area.

Fig. 2. — a) Superimposed Penrose quasi-lattice (o) and crystal lattice (+). b) Non coincidence sites between the QC (o) and crystalline (+) lattices. Initial and final points, in 1-1 correspondence, are joint. Note that the crystal points with 1/2 -1/2 probability are related by the jumps involved in the transition, hence the condition of centered unit cell can be realized. c) Geometrical illustration of a jump: it occurs over a constant distance $(a\sqrt{3-\tau})$ and in 10 directions.

Fig. 3. — a) Positions in the QC (o) and in one crystalline domain (+) which do not coincide, for a large area. All possible jumps (Fig. 2c type) are represented, allowing to visualise the jump densities. "Errors" in 1-1- correspondence disappear by taking into account properly the 50% probability sites. b) Same as a) for another domain (rotated over 36°).

The atomic jumps achieving the transformation are shown as well (Fig. 2c). Careful inspection reveals that on a local scale these occur always in identical environments. The jump vectors all have the same length (with 10 different directions) such that we can associate a unique double-well potential to all of them. Numerical verification shows that one can move out rather far keeping the same set of jump vectors (it has been checked in the area $r \leq 16a$). However, as figure 3a illustrates clearly, when one moves away from the starting point where the two lattices were made to match well (i.e. imply a few number of jumps; Fig. 2a), the number of jumps increases dramatically which in a double-well potential model becomes energetically costly.

Figure 3b illustrates how an appropriate rotation, here 36° , and translation of the unit cell from

which the periodic lattice is propagated, i.e. the selection of a different domain analogous so that observed for Al-Cu-Co-Si by HREM in [5,6] can heal the situation at any place. The microcrystal would thus be energetically favoured with respect to the single crystal. Figure 3 suggests that each domain could include only a relatively small number of periodic unit cells, but note that this would be in qualitative agreement with experimental results on Al-Cu-Co-Si [5,6]. Note also that figures 3a and b show remarkable loop-like patterns for the jumps in the "low energy" region, which could be a clue for future investigations on the precise interatomic forces responsible for the propagation of the crystalline order inside one domain.

3. Conclusion.

In the present communication we have presented our first results on a model for a transition from a QC to a MC. Although the precise interatomic forces responsible for the propagation of the crystalline order inside one domain still remain to be studied, it is the first time that a transition can be described by a single double-well potential, which is a point of physical relevance. We also point out that the transition from a QC to one single, infinite crystalline approximant phase could be energetically unfavourable in agreement with experimental results.

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