

Phason dynamics in decagonal quasicrystals

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Abstract. In a spectacular experiment of the year 2000 Edagawa et al. observed white spots in HRTEM images of d-Al-Cu-Co, which formed the vertices of a tiling. On a time scale of seconds to minutes the spots changed positions corresponding to phason flips. To illuminate the origin of the spots, their jump mechanism and frequencies we employ a structure model of Zeger and Trebin of 1996. It consists of quasiperiodic double layers stacked periodically by 4.18 Å. Each double layer contains rings of ten atoms whose centers form the vertices of a Tübingen triangle tiling. Correlated jumps of two atoms in each sublayer cause a simpleton phason flip of the entire ten ring. The stacking of the double layers leads to columns of the ten rings which might be interrupted due to the flips. Columns which contain a critical minimum number of complete ten rings are considered visible as white spots. Simultaneous appearances of vertices and their flipped positions give rise to the pentagonal Penrose pattern as observed by Edagawa et al. and also in other experiments. Postulating microscopic flip rates for the correlated jumps of pairs of atoms in the sublayers we calculate the probabilities for the numbers of complete ten rings in a column and confirm the mesoscopic time scales for the jumps of the white spots.

1. Introduction

Phasons are elementary excitations peculiar to quasicrystals. The notion comprises alternate positions of vertices and their flips in quasicrystalline structures. If these vertices are occupied by atoms, they are separated by a few angströms, and the time between the flips is of the order of picoseconds. The first direct observation of phason flips in a quasicrystal was reported by Edagawa et al. in a widely noticed article of the year 2000 [1]. The authors detected white spots in HRTEM images of decagonal Al₆₅Cu₂₀Co₁₅, which formed the vertices of a pentagonal Penrose tiling and which performed phason flips. The spots themselves, however, had diameters and separations in the order of nanometers. The time between their flips ranged from seconds to minutes. In the present contribution we attempt to explain the spots and their jumps by taking recourse to a structural model for decagonal Al-Cu-Co established by Zeger and Trebin in 1996 [2]. It contains columns of rings with ten atoms whose projections form the vertices of a Tübingen triangle tiling. We interpret these columns as the positions of the white spots. By collective jumps of atoms a column or part thereof can perform a simpleton flip of the triangle tiling. If the part which has flipped is large enough, both the original white spot and the flipped position are visible. In this way the original Tübingen triangle tiling turns over into the pentagonal Penrose tiling, which Edagawa et al. [1] and others (for example Ref. [3]) claim to observe. By postulating microscopic flip rates for the jumps of individual atoms we calculate the probabilities for jumps of the white spots and confirm the mesoscopic time scales.

2. Model for the structure of d-Al-Cu-Co

2.1. Model of Zeger and Trebin

The structural model of Zeger and Trebin [2] which we apply here is a slight modification of a model, which Burkov proposed in 1993 [4] based on experimental data of Steurer of 1990 [5]. It consists of quasiperiodic double layers stacked periodically by 4.18 Å. The projection of each double layer is a complex decoration of the two golden triangles comprising the decagonal Tübingen triangle tiling (Fig. 1). There are 34 atoms in the large and 21 in the small triangle. The composition is $\text{Al}_{62}\text{Cu}_{19}\text{Co}_{19}$. Each vertex of the tiling is the center of a ring of ten atoms. These rings form a column along the stacking axis. We join the assumption in the literature that these columns are to be identified with the white spots. Zeger and Trebin [2] documented a self-similarity both for the structure and the dynamics of the model. The structure is equivalent to a three times deflated triangle tiling containing at most two atoms in a triangle. In the highest deflation step one finds closely neighbored oriented rhombs in each layer, consisting of two large and two small golden triangles (Fig. 1). There is an aluminum atom on the central vertex and one within one of the large triangles. Through correlated jumps of these two atoms, each by 0.87 Å, the inner vertex performs a simpleton flip and the rhomb reverses its orientation. If this flip is occurring in the rhomb of the lower and the upper layer simultaneously, then an entire ten-ring of atoms is jumping and performing a simpleton flip in the initial, undeflated tiling (Fig. 1).

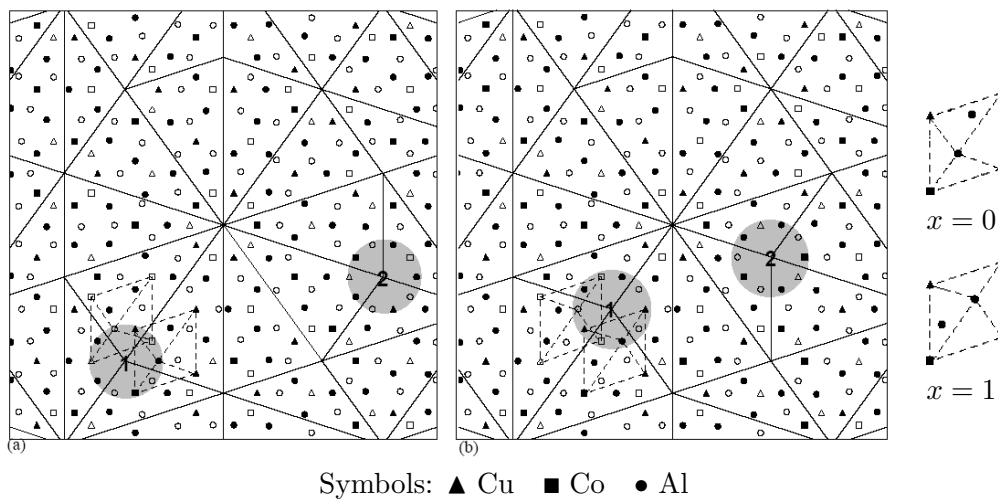


Figure 1. Double layer in the model structure for d-Al-Cu-Co. Empty and filled symbols denote atoms in the lower and upper layer, respectively. Each vertex is surrounded by a ring of ten atoms. The aluminum atoms of a ring belong to rhombs (dashed) of the deflated tilings (left figure). A rhomb can change from its original state ($x = 0$) to a reflected one ($x = 1$) by a simpleton flip. While doing so the Al atom inside the large triangle moves by 0.87 Å to the new vertex position; the previous vertex atom leaves by the same distance for the interior of the freshly formed large triangle. If both rhombs perform this flip (from state 00 to 11) an entire ten-ring is jumping in the original, undeflated tiling (right figure) [2].

2.2. Visibility criteria

Let us now consider a number N of (single) layers as in Fig. 2 and attach to each layer the state $x = 0$ or $x = 1$ of its small rhomb. Whenever we find successive states 00 or 11, a complete

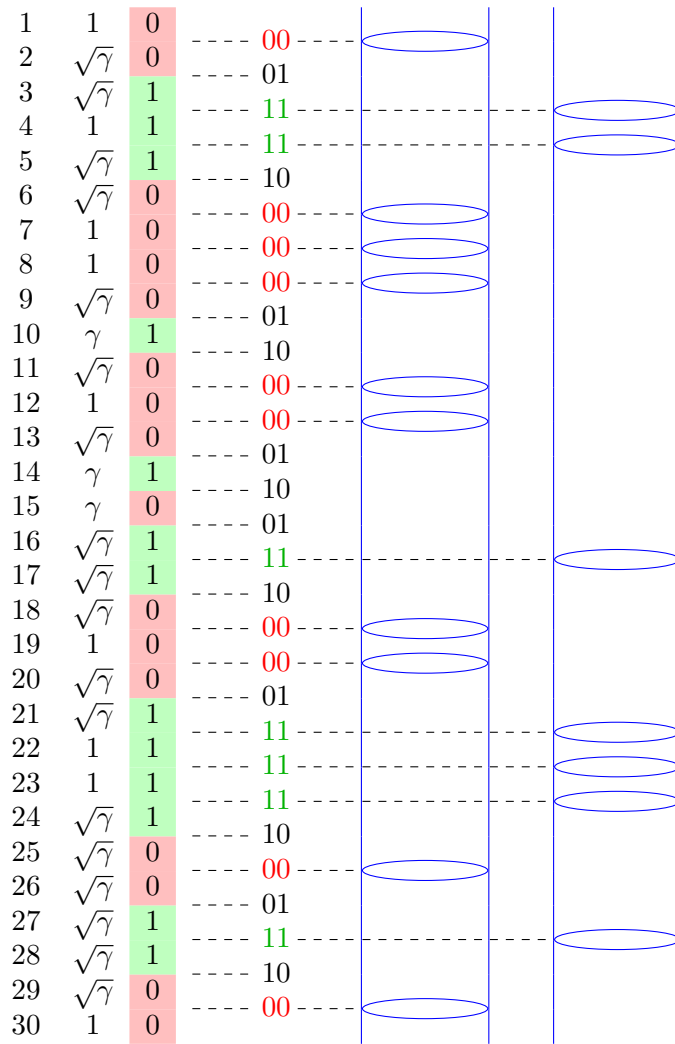


Figure 2. First column: numbering of the single layers. Second column: relative flipping probability of a single small rhomb. Third column: state of the small rhomb and cluster structure. Fourth column and adjacent rings: state of the double layer, forming a ten-ring to the left if of type 00, to the right if of type 11.

ten-ring is found in the original or flipped state, respectively. We denote their numbers by n_{00} and n_{11} and introduce a visibility parameter α between 0 and 1. A white spot is assumed visible, whenever $n_{00} > \alpha N$ or $n_{11} > \alpha N$. When α is smaller than $\frac{1}{2}$ it might occur that both unflipped and flipped positions are visible. In the insert of Fig. 3 we display the original HRTEM image of Edagawa et al. (Fig. 2 of Ref. [1]) where we have imposed a part of the model of Zeger and Trebin [2] (black). The white lines denote the rhomb, pentagon and hexagon by which Edagawa et al. depicted a section of the pentagonal Penrose tiling before and after the flip (Fig. 3 of Ref. [1]). To the right of this insert the corresponding section of a Tübingen triangle tiling is drawn. The blue vertices are positions of the basic tiling, the green ones positions of simpleton flips, comprising a first deflation stage. The colored lines connect vertices corresponding to those of the HRTEM image. Further flips can proliferate the vertices and give rise to the pentagonal Penrose tiling.

3. Visibility probabilities and dynamics

For analyzing visibility probabilities of the white spots and from there the mesoscopic flipping times, the notion of clusters is very useful. A cluster is a consecutive series of identical states of the small rhombs in the single layers, see colored sections in the third column of Fig. 2.

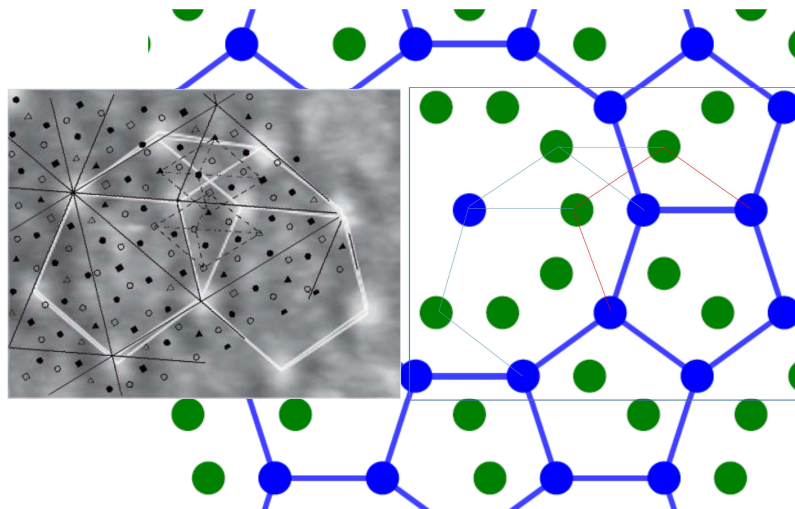


Figure 3. Left: HRTEM image of Edagawa et al. [1] with imposed tiles of the pentagonal Penrose pattern before and after the flip (white) and model of Zeger and Trebin [2] (black). Right: Corresponding section of a Tübingen triangle tiling (blue) and singleton flipped positions (green).

If the number S_c of clusters is small, then the number of complete ten-rings is large, which becomes clear by the very simple relation $n_v := n_{00} + n_{11} = N - S_c$. To determine the probability for S_c clusters to occur we have associated relative jump rates to the small rhomb in a single layer. The highest rate $\gamma > 1$ is assigned, if the adjacent layers are in the same state, but different from the considered layer. If the rhombs in a layer and its neighbors are pointing to the same direction, the lowest jump rate $\gamma = 1$ is postulated. An intermediate rate $\sqrt{\gamma}$ is assumed, if the neighbors differ in their state. Thus we favor the formation of clusters.

By enumerating all flip processes which change the number of clusters in combination with kinetic Monte Carlo simulations we found that the numbers of clusters S_c are binominally distributed, as consequently are also n_v , n_{00} and n_{11} . The probabilities were calculated for one spot to appear, for two spots and for none. Finally the mesoscopic flip rates were derived. There are ranges of the jump rate γ and the visibility parameter α where these probabilities and the mesoscopic flip rates agree with the data of the video clips of Edagawa et al. [1]. Details are found in the thesis of Hansjörg Lipp [6].

References

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