



Session I - Monday, August 31 - morning

PL1

STRUCTURE AND STABILITY OF MG/QUASICRYSTAL INTERFACE IN Mg-Cd-Yb ALLOYS

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The icosahedral quasicrystal (iQc) is in equilibrium with either $(\text{Mg, Cd})_2\text{Yb}$ or an $\sim\text{Mg}$ phase over a wide composition range in the Cd-Mg-Yb system. High-angle annular dark field scanning transmission microscopic (HAADF-STEM) observation of the iQc verified the atomic positions of the Yb icosahedra and confirmed that the i-MgCdYb is isostructural to the i-CdYb. The formation of the eutectic structure is responsible for the high stability of the iQc/ $\sim\text{Mg}$ interfaces because of good lattice matching; that is coincident interplanar spacing over several planes for the

two phases. This coincidence in interplanar spacing was further confirmed in the real atomic structure, for which the two-fold planes of the iQc, and the [0002] and [2-1-10] planes of $\sim\text{Mg}$ are dominant factors in determining the stability of the interfaces. Replacement of Cd atomic sites in i-CdYb by Mg also contributed to the stability of the interfaces. The stability of interface between a periodic and a quasi-periodic structures will be discussed in terms of matching of lattice spacing.

S1-L1

SOME TRICLINIC APPROXIMANTS OF DECAGONAL QUASICRYSTALS

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Intermetallic phases are usually assumed to have structures with high rather than with low symmetry. This is actually not the case, however. For instance, there is not a single structure listed in the PCD [1], which has an occupied orbit

(leading to a cluster shell) with the highest point symmetry $m\bar{3}m$ and multiplicity 48. In contrast, at the low symmetry side, there are more than 30 triclinic structure types. It is remarkable that quite a few of them show structures with

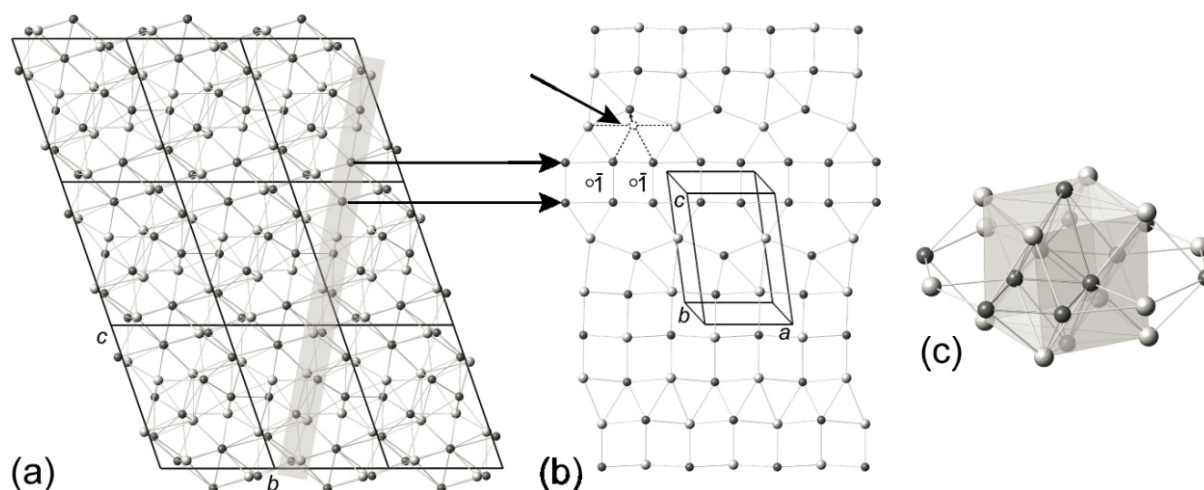


Figure 1. Some characteristic features of the structure of $aP20\text{-NdS}_3$ [1]. (a) Projection of the structure along [100] showing the topological layer structure. There is just a single type of layer with a period of $1 \times 2 \times 3$ unit cells. The layer shaded gray is depicted in (b). Copies of this layer are related by inversion centers located at the origin, edge centers, face centers and body center of the unit cell. The layers themselves show inversion centers in each square of the bands running through the decagons (marked in the first two squares of the decagon at left of (b)). The atomic displacement needed for the formation of these decagonal structure units is indicated by dotted lines. (c) Decagon centered by a pseudo-cubic unit cell resembling the $cP4\text{-AuCu}_3$ structure type.

similar features: the constituting atomic layers correspond to triangle/square tilings, which are periodically distorted forming decagonal structural units (Fig. 1). This has been overlooked so far, neither the topological layer structures nor the decagonal features have been discussed in litera-

ture. We will show several examples in different intermetallic systems.

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S1-L2

CLUSTER-BASED SOLIDIFICATION AND GROWTH ALGORITHM FOR DECAGONAL QUASICRYSTALS

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There are still two fundamental questions open in our understanding of quasicrystals (QCs). One is how QCs grow, and the other refers to their main stabilization mechanism. The discussion about 'energy vs. entropy stabilization' has been ongoing ever since their discovery. *Energy-stabilized* QCs would have a quasiperiodic ground state, while *entropy-stabilized* QCs would be quasiperiodic on average only, at sufficiently high temperatures (T), and transform into periodic approximant structures at low T . It has been demonstrated both theoretically [1] and by MC simulations [2, 3] that finite quasiperiodic long-range order (LRO) cannot be achieved in 2D systems with local interactions only (matching or overlap rules). The 2D local-interactions-based systems are therefore in a so-called *unlocked* (random tiling) state at any finite temperature T . For 3D layer models of DQCs based on local interactions, an unlocking phase transition is observed at finite T [4, 5]. The locked phase exhibits true quasiperiodic LRO. An interesting result for 2D systems was obtained by molecular dynamics (MD) simulations with a two-minima radially symmetric Lennard-Jones-Gauss potential [6], which results in an entropy-stabilized DQC transforming into an approximant at low T . We use a completely different approach, which is based on some fundamental experimental observations: (i) DQCs show distinct cluster structures, with the atomic decoration of these clusters breaking the tenfold symmetry [7]; (ii) even rapidly solidified quasicrystals exhibit a good LRO, therefore it is reasonable to assume that cluster-like arrangements of atoms exist already in the melt close to the solidification temperature; (iii) the atoms in DQCs are arranged on quasiperiodically spaced flat atomic layers parallel to the tenfold axis [8]; (iv) DQCs are not (!) layer structures in the crystal-chemical meaning. Therefore, their structures should be described in terms of systematically partially overlapping 3D columnar clusters instead of a stacking of quasiperiodic layers [9].

Consequently, our coarse-grained model system is based on decagonal clusters. We propose the evolution of LRO in DQCs based interactions provided by the energetically favourable formation of flat atomic layers parallel to the tenfold axis ('quasilattice planes', QLPs). Furthermore, we assume that the fundamental clusters forming the DQC have a decaprismatic shape but their atomic arrangement exhibits only mirror symmetry. This makes the interactions radially asymmetric, which is fundamentally different from the approach in ref. [6], where the interaction potential is radially symmetric. It is worth noting that while the interpretation of DQC stability in ref. [6] might be applicable to *monoatomic* colloidal DQCs, it is probably not appropriate for explaining the behaviour of intermetallic DQCs, where the cluster interactions are all but radially symmetric. In our Monte Carlo (MC) simulations, this leads to a long-range ordered quasiperiodic ground state. Indications of two finite-temperature unlocking phase transitions are observed related to the two fundamental length scales that are characteristic for the system.

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S1-L3

ATOMIC STRUCTURE OF R-Cd (R = Gd, Dy and Tm) ICOSAHEDRAL QUASICRYSTALS

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Recently, new binary icosahedral quasicrystals have been discovered in the R-Cd (R=Y and Gd - Tm) system [1]. They are believed to be isostructural to the i-YbCd_{5,7} quasicrystal. One fascinating point is that these new phases contain trivalent rare-earth elements, whereas in the case of i-YbCd_{5,7}, Yb is divalent and the Yb atom has no magnetic moment. On the other hand, the chemical compositions, e.g. i-GdCd_{7,88}, are slightly but significantly different from i-YbCd_{5,7}, which indicates a different chemical arrangement in the 3D quasiperiodic structure. The knowledge of details of the atomic structure of these new phases, especially position of the rare earth atom, are important to understand the nature of magnetic interaction in these systems [1].

The single-grained crystals of i-R-Cd (Gd, Dy and Tm) were prepared with self-flux technique. The single-crystal X-ray diffraction has been carried out on the CRISTAL beamline at the synchrotron SOLEIL and 5237 common unique reflections have been measured at 120 K (CCD detector, 24.2244keV). Data reduction including integration and absorption correction has been performed using a computer package CrysAlisPRO and the structure analysis has been performed using QUASI07 [4].

After phasing the structure factors by low-density elimination method, we calculated the 6-dimensional (6-D) electron density distribution by Fourier synthesis which

confirmed that i-R-Cd is isostructural to i-YbCd_{5,7} [2, 3]. We then carried out the structure refinements based on the 6-D structure model of i-YbCd_{5,7} considering three main building blocks: a multi-shell large triacontahedron (located on the 12-fold vertices of a 3D Penrose tiling), an oblate rhombohedron, and a double Friauf polyhedron (DFP, filling the gaps). The refined structure, with a good R-factor (e.g. $R_w = 0.0724$, $R = 0.0376$ for i-Gd-Cd) shows a mixed R/Cd occupancy inside the DFP where one Yb site is pure R and the other is a Cd/R mixture. We also find that the icosahedron site is a R/Cd mixture with a ratio of about 0.8:0.2. The refined chemical compositions are GdCd_{7,881}, DyCd_{7,503} and TmCd_{7,283}, in very good agreement with the experimental ones GdCd_{7,88}, DyCd_{7,50} and TmCd_{7,28} [1]. The details of the resulting structure will be presented.

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S1-L4

DEFECTS IN TWO- AND THREE-DIMENSIONAL COLLOIDAL QUASICRYSTALS

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Due to the additional degrees of freedom in quasicrystals there are properties and phenomena that for quasicrystalline structures significantly differ from their counterpart in periodic crystals. For example, there are growth modes in quasicrystals that cannot occur in the growth process of a periodic crystal [1]. Furthermore, dislocations in quasicrystals are characterized by Burgers vectors that in addition to their phononic components possess additional phasonic components. Another consequence of the additional degrees of freedom is that the theories of defect mediated melting (e.g. the KTHNY theory) have to be modified [2]. Here, we first follow and describe dislocation lines in three dimensional colloidal quasicrystals. Secondly, we explore defects during the melting of a two-dimensional colloidal quasicrystal.

By using Monte-Carlo simulations of a monodisperse colloidal model system, we study defects of three-dimen-

quasicrystal. We find dislocation lines that bend, defects that fork into two defect lines, two defect lines that merge into a single one, or two defects with inverse Burgers vectors that annihilate when they meet.

Furthermore, we study how thermally excited excitations or defects develop in two-dimensional colloidal quasicrystals close to the melting transition. According to an extension of KTHNY theory [2], the formation and dissociation of pairs of dislocation and disclinations is expected to cause the melting of the quasicrystal and melting should occur via an intermediate phase termed pentahedric phase [2]. We determine positional and orientational correlation functions and analyse the formation and distribution of defects during melting. We compare the structure that includes thermally excited defects to structures obtained by the random tiling-like growth of a quasicrystal [1].

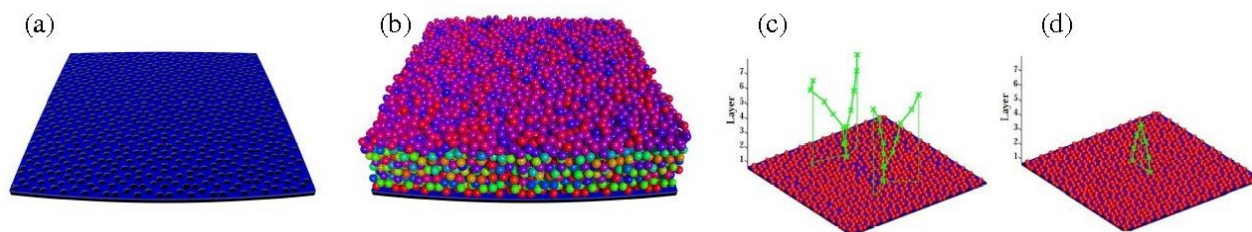


Figure 1. (a) Substrate with quasicrystalline symmetry. (b) Grown colloidal quasicrystal. (c) Forking dislocation lines. (d) Annihilation of dislocation lines. All figures are published in [3].

sional quasicrystal that grow on a substrate [3]. We consider special phononic and phasonic displacement fields in order to achieve purpose-made substrates that contain phasonic flips or well-defined point defects like dislocations. While local phasonic flips do not disturb the growth of the quasicrystals significantly, dislocations cause defect lines that reach through the whole three-dimensional

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S1-L5

ICOSAHEDRAL QUASICRYSTALS PRECIPITATED FROM AN ALUMINIUM MATRIX

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Aluminium quasicrystalline alloys represent a novel class of high-strength alloys. They possess a great potential for practical applications in many fields, thus they are the object of intensive investigations [1, 2]. Normally, they are produced by rapid solidification. However, recent studies have shown that they can be produced by casting into copper mode. It has been found that melt-spun Al-Mn-Be-Cu can be substantially strengthened by heat treatment at different temperatures, while the effect was not so pronounced by the alloy cast into copper mould [3, 4]. In order to reveal the reasons for such behaviour, a detailed analytical transmission electron microscopy study have been carried out using different imaging modes (TEM, STEM, HR-STEM), and several nanoanalytical techniques (EELS, EDS, EFTEM). Samples have been prepared by ion-beam thinning (PIPS), as well as by focussed ion beam (FIB). It was revealed that the main reason for high-strength of rapidly solidified ribbons was precipitation of a very large

number of quasicrystalline precipitates within the Al-rich matrix, having coherent interfaces and specific crystallographic orientation relationship with Al-matrix. This is clearly shown in Figure 1. When the alloy was cast into the mould, IQC-precipitates also formed. Since of their smaller number density, the strengthening effect was not so strong. Additionally, at higher temperatures IQC-precipitates were replaced by less effective Al₂₀Mn₃Cu₂ precipitates.

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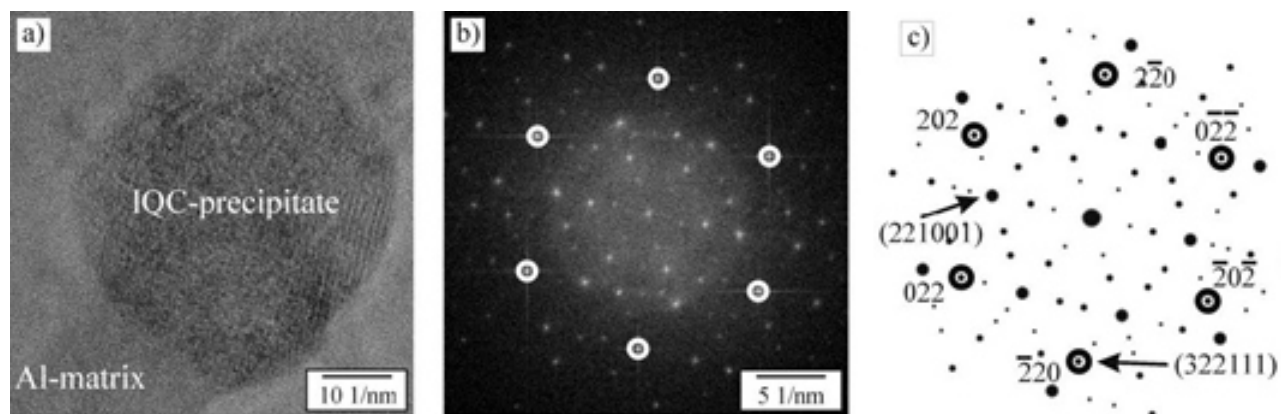


Figure 1. An icosahedral quasicrystalline precipitate (IQC) within an Al-rich solid solution. a) A high-resolution TEM-micrograph, b) A Fast-Fourier Transform showing non-periodic pattern of the IQC with six-aluminium spots belonging to a [111]-zone axis, c) a schematic presentation of the mutual orientation relationship between IQC and Al-matrix.