

Cd₆R (R: rare earth elements) crystals are regarded as 1/1 approximants to the Cd_{5,7}Yb icosahedral quasicrystal [1]. At 300K, they are *bcc* phases which are made of so-called Tsai-type clusters. A Tsai-type cluster is composed of four successive atomic shells of, from the center, Cd₂₀ dodecahedron, R₁₂ icosahedron, Cd₃₀ icosidodecahedron and Cd₆₀ rhombic triacontahedron. At the center of the cluster, there exists a disordered Cd₄ tetrahedron.

An occurrence of a structural phase transition has been observed in a number of the Cd₆R crystals, which is attributed to orientational ordering of the central Cd₄ tetrahedra, resulting in various types of superstructures below *T_c*. First, we will describe and classify the superstructures of Cd₆R and then discuss key factors which strongly influence the transitions based on the observations.

The Cd₆R crystals are also of interest in view of the magnetism since recently they are found to exhibit magnetic transitions below *T_c* in a striking contrast with the cases of other 1/1 approximants. For instance, three successive magnetic transitions have been reported for R=Tb [2] and Sm [3] with different magnetic orders at the lowest temperature, i.e., antiferro- and ferrimagnetic orders at 2K, respectively. We will present magnetic properties of Cd₆R (R=Nd, Sm, Gd, Tb, Dy) having the same C2/c-type superstructure below *T_c* and comparison of the magnetic orders in the isostructural compounds will be made.

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Keywords: quasicrystal

MS.63.2

Acta Cryst. (2011) **A67**, C144

A dense quasicrystalline phase of hard tetrahedra

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Quasicrystals have traditionally been discovered in many binary and ternary metallic alloys. It has now become evident that aperiodic order can also be found on larger length scales in soft matter with micelles, colloids and macromolecules [1]. The experimental findings that nanoparticles can self-assemble into highly complex, ordered structures are also backed up theoretically by computer simulations [2] which, due to the larger size of the particles involved and resulting simpler particle interactions, are well suited to reproduce and study the crystallization process.

As it is now possible to synthesize nanoparticles of various shapes and interactions with high yield and high structural perfection, these particles can be seen as building blocks for assembling novel materials from bottom up with the goal of improved or unusual electrical, mechanical or other physical properties. In my presentation I focus particularly on the behavior of hard regular tetrahedra. The tetrahedral shape is highly anisotropic and therefore in its behavior distinctly different from what is known from atoms and spherical colloids.

The question of how densely tetrahedra pack has attracted much interest over the last years. In a first study, we have reported the spontaneous formation of a dodecagonal quasicrystal in Monte Carlo computer simulations [3]. A crystalline approximant of the quasicrystal with an 82-particle unit cell was compressed to a then-record packing fraction of 85.03% [3]. Very shortly after, a family of dimers packings were proposed, which were subsequently optimized to a packing fraction of 85.63% [4], the currently densest known packing of tetrahedra.

Due to its higher packing density, the dimer crystal is thermodynamically favored in the limit of infinite pressure. However, which structure is stable at finite pressures is an open question. I will discuss how we use thermodynamic integration and free energy calculations to explore the relative stability of these very different ordered phases as a function of packing density [5].

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Keywords: quasicrystal, nanoparticles, simulation

MS.63.3

Acta Cryst. (2011) **A67**, C144

Prediction of low-temperature phase transition in Al₁₁Ir₄ compound

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The average structure of the Al₁₁Ir₄ phase [1] exhibits mean occupancy of 0.5, providing 60 sites for 30 atoms in a cubic cell with 7.7Å long side. To resolve the occupancy correlations, we employ ab-initio methods and empirical pair potentials fitted to ab-initio data. Our first result is that the part of the structure plagued by many nearby low-occupancy sites is an irregular IrAl₁₀ cluster. Due to mismatch between high (icosahedral) symmetry of the cage surrounding the low-symmetric IrAl₁₀ “core”, the structure possesses configurational degrees of freedom down to low temperature. By simulated annealing in 4x4x4 supercell, we find phase transition at the temperature as low as 500 K. While the high-temperature phase has simple cubic symmetry (space group P23) in accordance with the experimentally refined structure, we predict the low-temperature phase is 2x1x1 supercell, with Pma2 space group. According to our ab-initio total energy calculations at T=0K, the low-temperature structure is stable against decomposition into competing crystalline phases.

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Keywords: phase transition, molecular dynamics simulation, atomic structure

MS.63.4

Acta Cryst. (2011) **A67**, C144-C145

The structure of Al-Cu-Me (Me = Co, Rh, Ir) quasicrystals

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We present a real space structure refinement of three decagonal phases: Al-Cu-Co, Al-Cu-Rh, Al-Cu-Ir. The structure factor, which