conference abstracts

s1.m1.p9 **Structure of the octane+urea inclusion compound at 293 K** I. Peral, G. Madariaga , T. Breczewski, *Departamentos de Física de la Materia Condensada y Física Aplicada II, Facultad de Ciencias, Universidad del País Vasco, Apdo. 644, 48080 Bilbao, Spain.*
Keywords: urea inclusion compound, composite structures, superstructure refinement.

The urea inclusion compounds belong to the type of inclusion compounds in which guest molecules are spatially confined within a structure of linear and parallel tunnels formed by an extensively hydrogen-bonded arrangement of urea molecules[1] . The urea+alkane inclusion compounds show a particular rich variety of low dimensional order-disorder phenomena. One very important aspect is that there is no complete long-range order of the alkane molecules within one tunnel. This becomes particularly significant as the length of the guest molecules decreases[2]. The octane+urea inclusion compound is one of the smallest alkane chains for which the inclusion phenomenon is possible. The aim of this work is the study of the structure of the octane+urea system at room temperature. X-ray diffraction diagrams show a quasi-liquid distribution of octane molecules inside the urea tunnels. Nevertheless a structural model consistent with the experimental data can be achieved using the superspace formalism in which the inclusion compound is treated as a one-dimensional incommensurate composite.

s1.m1.p10 **Average Lattices of The Quasicrystalline Structures.** I.V. Lebedyuk. *Institute of Physics, Rostov State University 194 Stachki av., 344090 Rostov-on-Don, Russia.*
Keywords: average lattice, Fibonacci chain, quasicrystal.

Recently, the important role of average lattices for the description of crystal-to-quasicrystal phase transitions was pointed out[12]. In Ref. [2], it was shown for the polygonal quasicrystals that under certain linear continuous inhomogeneous strains the direct-space basis vectors a_i of an quasicrystalline lattice can become rationally commensurate. In this case, a quasilattice transforms into the appropriate defect periodic lattice which is an average lattice of quasicrystalline structure. There exist an average lattices related to the initial average periodic lattice both by the elements of the quasicrystal rotational symmetry and by the self-similarity transformation. For the Fibonacci chain (FC) and the three-dimensional Penrose tiling (3DPT), a way of enumeration of possible average lattices is proposed[3]. The requirement for basis vectors to be rationally commensurate results in the FC magnitude of the linear continuous inhomogeneous strain α defined by the ratio $(q - \tau p)/(p + \tau q)$. Here, p and q are the integers, and τ is the golden mean. Considering small α, one obtains an infinite set of periodic average lattices. Only for the FC case, there exists the one-to-one mapping between the quasilattice nodes and the average lattice ones[1]. The degree of imperfection of the average lattice is defined by the atomic surface and the values p and q.

The most symmetric average lattices possible for the 3DPT with the point groups of T_h, D_{3d} and D_{5d} symmetry are considered, where the first two lattices are periodic in 3D physical space, but the last lattice is periodic only in one direction - along the fivefold axis. Besides, the appearence of the linear continuous inhomogeneous strain in some classical cubic approximants of icosahedral quasicrystals Al-Mn-Si and Al-Cu-Li are analysed.

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