MODELLING PLANETARY MATERIAL'S STRUCTURES: FROM QUASICRYSTALLINE MICROSTRUCTURE TO CRYSTALLOGRAPHIC MATERIALS BY USE OF MATHEMATICA. ***Kabai, S.*** [1]***, Bérczi, Sz.*** [2] [1]UNICONSTANT, H-4150 Püspökladány, Honvéd u. 3. Hungary, [2]Eötvös University, Faculty of Science, Department of G. Physics, Cosmic Materials Space Research Group, H-1117 Budapest, Pázmány Péter s. 1/a. Hungary, (unico@mail.matav.hu, berczişzani@ludens.elte.hu)

Introduction: In the last year we developed our interactive Mathematica in space materials studies and modelling. We focused on the structural hierarchy of materials and quasicrystals because impact materials may produce such semiordered structures. We used our system both to the classical structures like Widmannstadten texture of iron meteorites and to cryptocrystalline materials and also some industrial materials too.

Classical structural hierarchy: Well known basis is for materials studies to construct the hierarchy levels of the material structures observed by one technology. From cell units through crystal lattice, block mosaic structure, crystallite structure up to the macroscopic texture and macroscopic materials till the structure of composite materials. However this line of hierarchy is different for various special materials. Here the opal and the meteoritic iron`s **Widmannstadten structure** is mentioned only. (Fig. 1.)

Nonclassical structures (metallic glasses): Studies of mineralogy of the not well ordered materials were triggered by production **of metallic glasses** with **cluster type** structural units. Icosahedral morphology of viruses, of the large carbon-network molecules, (fullerene), also focused interest to structures built from basic units with fivefold in some planar sections (and dodecahedral-fold in space) symmetry. Both tiling of Penrose type and ball arrangements of cluster type ones seems good approach to quasicrystalline structure from the geometrical point of view. **The X-ray pattern** of the quasicrystal materials gave clear evidence of **the local fivefold symmetry** in some metals (alloys) and even crystal forms proved that polyhedral shapes of quasicrystals grow larger then the local atomic layers (clusters) with icosahedral symmetry. Here we take the following steps in construction **of quasicrystal modelling**. First we show the basic elements of quasicrystal construction with golden rhombohedral unit cell. From this unit we construct various higher hierarchy level forms and replacing the original unit by these higher units give a series of unit-cells. Hierarchy of these unit polyhedra and their super cluster constructions allow the building up a rich set of hierarchically embedded structures.

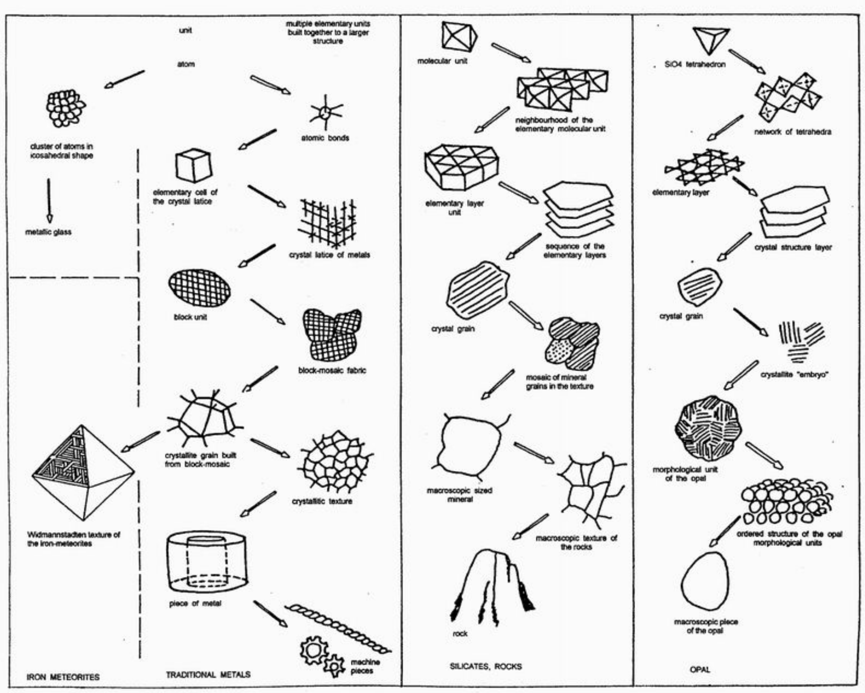

Fig. 1. Structural hierarchy table of various solid crystalline materials (Bérczi, 1991).

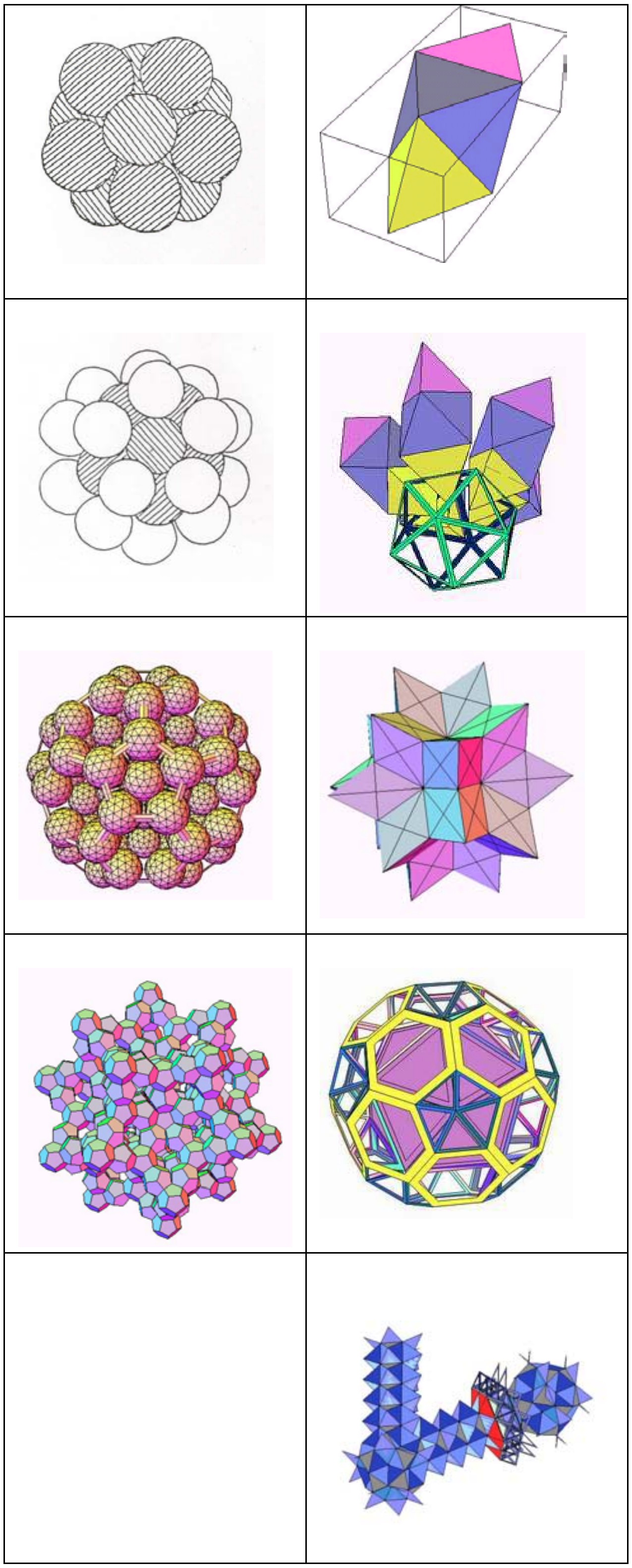

Fig. 2. From clusters of atoms forming the metallic glassy structure to the goldenrhombohedral architectures (S. Kabai).

We can show one place for quasicrystal structures in this system. This is the cluster structure of the metallic glass, for example. (Left column in this table.) Its bond structure may be represented by the polyhedral units. First we begin that modelling by seeing that atomic cluster units have fivefold symmetry because the arrangement of one layer of equal spheres around the central sphere has pentagon-dodecahedral shape. (Fig. 2. top) If the the congruent spheres are placed in the pits of the previous layer then the **second layer of balls** (the central initial one was considered to be the zero-th one) we have an icosahedral stellated structure (Fig. 2.) The corresponding polyhedral construction can be seen in the second column with golden rhombohedral units. The superimposed next layer is shown first by spherical (3) then by golden-rhombohedral (GR) units built from pentagon dodecahedra (4). In the right column from the stellated rhombic triacontahedron (3) we can see higher architectures of (5,6,6) fullerene like (4) and finally a crystalline-quasicrystalline joint construction.

Golden rhombohedral unit: Now we focus on the hierarchical structure of the quasicrystalline system built up from metal cluster units. In the construction we use golden rhombohedral units, because fivefold symmetry of the initial cluster determines the higher hierarchy levels of the arrangement. This construction results a kind of "spongy" structure for materials. (Our unit is remarkable: it is faced by 6 golden rhombi; such rhombus has diagonals which have ratio of tau, the famous number of golden section). 20 golden rhombohedron units meeting at their piramidal vertex, form the stellated rhombic triacontahedron. This unit is parallelepipedon, bordered with two parallel faces in 3 main directions in the space therefore this unit is capable to tile the space congruently, (in a classical way of the symmetry of translation and the connected rotations) and at the same time it can be used to tile the space in a noncrystallographical way (no translational symmetry) exhibiting a local fivefold symmetry.

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