QUASICRYSTALS AND STRUCTURAL HIERARCHY: MODEL STRUCTURES FOR PROBABLE METALLIC IMPACT MATERIALS. Sz. Bérczi[1] and S. Kabai[2], [1]Eötvös University, Faculty of Science, Dept. Materials Physics, Cosmic Materials Space Research Group, H-1117 Budapest, Pázmány Péter sétány 1/a. Hungary, (bercziszani@ludens.elte.hu), [2]UNICONSTANT, H-4150 Püspökladány, Honvéd u. 3. Hungary, (unico@t-online.hu).

Introduction: High pressure and rapid cooling at impacts are extarordinary conditions and new material microstructures, stable at large pressures, can be expected there. Quasicrystals are such unusual structures discovered in the last two decades and looking for their natural occurrences impact materials arose as candidates. Therefore we studied quasicrystals both for their geometric structure and for the possibility to recognize among impact metals.

Clusters of atoms forming icosahedral point group: The most important characteristic of quasicrystals is their fivefold symmetry of the Laue X-ray pattern. (However, theoretically, other quasicrystalline structures were also shown, like as that of Watanabe.)

Although quasicrystalline structure with five fold symmetry has been found first in Al alloys, till today many other metallic alloys were identified with this structure, mainly produced in very rapid cooling.

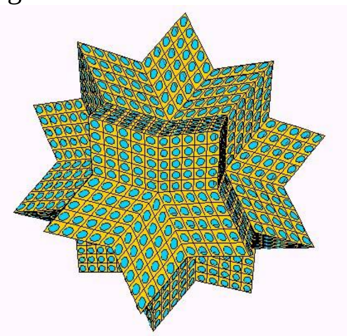

Fig. 1. Larger Al-alloy quasicrystalline structure found in 1987. Graphics from S. Kabai, 2000.

Theoretical background: There is an atomic arrangement, which is economical only for small number of atoms, forming in quenched metals. This is a cluster of identical balls taking the shape of an icosahedral "germ". Such local order with fivefold symmetry can exist only for a small number (2-3-4) of layers of identical atoms around one atom. In the first layer 12 atoms form a dodecahedron. The next layer can be arranged so, that atoms subside in the pits of the dodecahedral layer: these 20 atoms form an icosahedral second layer around the central atom. This second layer is compact enough to give a dense ball, but the atoms of the second layer touch three atoms of the first layer only, and they do not touch each other. The third layer is very loose, and this is the reason that the quasicrystalline fivefold symmetric point group structure can not grow larger: it becomes very loose and undetermined.

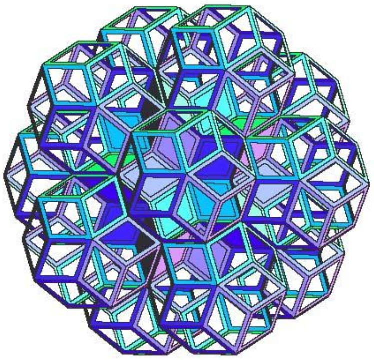

Fig. 2. This graphics show that the layers of the “balls” of fivefold symmetry can fit higher hierarchy levels layers, too. (graphics by S. Kabai, 2000.) These super clusters are also balls – a good approximation – and therefore they follow the structural hierarchy of the lower hierarchy units (which are the atomic icosahedral clusters).

Hierarchy: But a new principle may help. If the clusters with 2 layers rapidly form new super clusters then such a construction around the central cluster, and two layers of clusters may form super cluster also with fivefold symmetry. This hierarchy may result in frequent occurrence of original rapidly cooled clusters and also the super clusters which may grow up to micron sized scale to be observed in electronmicroscope.

Mathematica: In the last year we developed an interactive Mathematica in space materials studies and modeling. Focusing 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.

The classical structural hierarchy forms a well known basis for materials studies. This hierarchy system embraces the material structures 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 in the technology level. However this line of hierarchy is different for various special materials. Here the opal and the meteoritic iron`s Widmannstadten structure is mentioned. (Fig. 3.)

Nonclassical structures of the not well ordered materials (i.e. metallic glasses with cluster type structural units, with icosahedral morphology, like viruses) can also be involved in this system. Both tiling of Penrose type and ball arrangements of cluster type ones seem 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 show the structural hierarchy construction from original elementary cell unit by a series of higher level units. Hierarchy of polyhedra builds up the set of the hierarchically embedded structures.

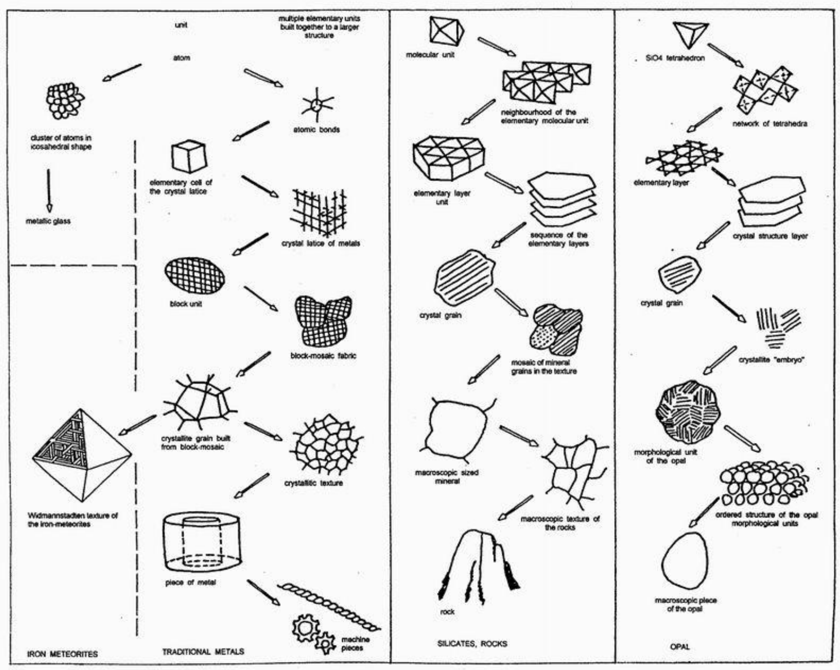

Fig. 3. Structural hierarchy table of various solid crystalline materials (Bérczi, 1991).

References: [1] Bérczi Sz. (1990): *Szimmetria és Struktúraépítés*. (*Symmetry and Structure Building*) (In Hungarian) Lect. Note Series, pp. 260. [2] Kabai S. (2002). Mathematical Graphics I. pp. 278. (English, Hungarian) UNICONSTANT, Püspökladány; [3] Bérczi Sz., Kabai S. (2002): *Kis Atlasz a Naprendszerről (5): Űrkutatás és geometria.* (Atlas of the Solar System (5): Space Research and Geometry.) In Hung. ELTE KAVÜCS UNICONSTANT, Budapest-Püspökladány; [4] Szilassi L., Karsai J., Pataki T., Kabai S., Bérczi Sz. (2001): How interactive graphical modeling helps space science and geometry education in Hungary. In *32nd LPSC*, #1184, LPI, Houston (CD-ROM); [5] Kabai, S., Miyazaki, K., Bérczi Sz. (2002): Space Science Education with Mathematica: Interactive Design of Modular Space Station Structures with Computer Algebra: Principles, Functional Units, Motions, Examples. In *33rd LPSC*, #1041, LPI, Houston, (CD-ROM); [6] Kabai, S.; Bérczi, Sz. (2004): Modelling Planetary Material's Structures: From Quasicrystalline Microstructure to Crystallographic Materials by Use of Mathematica. *35th LPSC*, #1081. LPI, Houston; (CD-ROM).