accepted courses, which teach how to obtain structural information and to describe crystal structures. In the presentation we demonstrate several examples from lectures and practicals.

[1] E.V. Boldyreva, *J. Appl. Cryst.* **2010**, *43*, 1172-1180.

Keywords: crystallographic teaching

MS.84.1

Measures of complexity

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The term *complex* is frequently attributed to crystal structures with giant unit cells containing hundreds or thousands of atoms. It is commonly used in a non-defined, fuzzy way. It would be advantageous, however, to have a quantitative measure of structural complexity, to be able to compare periodic and quasiperiodic structures, for instance. Why could this be of interest? Some physical properties, which strongly depend on medium- and long-range order, could be related to complexity and used as knowledge basis for their prediction. Another interesting question is the time evolution of a structure (crystal growth) as function of its complexity. For instance, it is obvious that a crystal with a simple cubic close packed structure such as copper will have a much simpler growth mechanism than a ternary quasicrystal.

Recently, it was suggested in different context to apply the concept of *algorithmic complexity* to crystal structures, periodic and quasiperiodic ones [1]. This way of quantifying the complexity of a system is related to the minimum size of an algorithm needed for its full description. If we apply this concept to the Fibonacci sequence (FS) in the nD description, for instance, then we obtain the same algorithmic complexity for the quasiperiodic FS and all its periodic approximants, from the smalls to the largest one. This is somehow counterintuitive.

If we use the concept of *symbolic complexity,* we arrive at drastically different results for periodic and quasiperiodic structures. Symbolic complexity is related to the number of different structure motifs (AET) as a function of system size, which is a function of the repeat period in case of the approximants and of the system size in case of the FS. For another example, let's start from a simple periodic structure and apply a sinusoidal incommensurate modulation. This immediately increases the period of the incommensurately modulated structure (IMS) to infinity. However, the algorithmic complexity of the IMS is only slightly higher than that of the small-unit-cell periodic structure. In case of a commensurate modulation, we can continuously increase the number of atoms per supercell without changing the algorithmic complexity of the structure, while the symbolic complexity would grow with the system size to infinity.

Another kind of complexity measure is the *combinatorial complexity,* which can best account for high symmetries of structural subunits (clusters). The less probable (symmetic) a configuration is the higher is its complexity. For instance, in case of equally sized hard spheres, close sphere packings such as the $cF4$-Cu structure are more probable from different point of views than the $cP1$-Po structure. Consequently, the latter has the higher combinatorial, but lower algorithmic complexity, and both have equal symbolic complexities.

In conclusion, no single complexity concept alone is able to reflect all facets of structural complexity, to quantify what we intuitively grasp.

[1] E. Estevez-Rams, R. Gonzaléz-Férez, *Z. Kristallogr.* **2009**, *224*, 179-184.

Keywords: complexity, quasicrystal, structure

MS.84.2

Frustrated Order

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Frustration occurs whenever a local order (atomic configuration) cannot be extended perfectly throughout the space. A paradigmatic example is that of polytetrahedral order encountered in dense packing models. In that case, a direct connection with icosahedral order is present, which makes the frustration concept useful in different contexts, like clusters, glassy materials or quasicrystals. Similar situations can be found with covalent materials and soft matter systems; in most cases, the real structure shows intricate relations between ordered regions and topological defects[1].

We shall first recall how frustration and order interfere in the general case. Then, some new results will be presented, related to dense frustrated order in confined (cylindrical) geometry, a topic which might prove interesting in the nanophysics context. Indeed, a rich phase diagram is found, with many different types of different order occurring while increasing the cylindrical radius, showing a nice competition between chiral, icosahedral, crystalline and disclinated icosahedral order.

[1] J-F-Sadoc et R. Mosseri, " *Geometrical Frustration* ", Cambridge University Press, **1999.**

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MS.84.3

Local Rules and Global Order

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An appropriate concept for describing an arbitrary discrete atomic structure is the *Delone set* (or an (*r,R*)-*system*). Structures with long-range order such as crystals involves a concept of the space group as well.

A mathematical model of an *ideal monocrystalline matter* is defined now as a Delone set which is invariant with respect to some space group. One should emphasize that under this definition the well-known periodicity of crystal in all 3 dimensions is not an additional requirement. By the celebrated Schoenflies-Bieberbach theorem, *any space group contains a translational subgroup with a finite index*.

Thus, a mathematical model of an ideal crystal uses two concepts: a Delone set (which is *of local character*) and a space group (which is *of global character*).

Since the crystallization is a process which results from mutual interaction of just nearby atoms, it is believed (L. Pauling, R. Feynmann et al) that the long-range order of atomic structures of crystals (and quasi-crystals too) comes out local rules restricting the arrangement of nearby atoms.

However, before 1970's there were no whatever rigorous results until Delone and his students initiated developing the *local theory of crystals.* The main aim of this theory was (and is) *rigorous derivation* of space group symmetry of a crystalline structure from the pair-wise identity of local arrangements around each atoms. To some extent, it is analogous to that as, in due time, it was rigorously proved that space group symmetry implies a translational symmetry.

In the talk it is supposed to expose some results on local rules for