Crystal meshes and symmetry relationships: An approach based on cellular hypergraphs

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Abstract

Like three-dimensional cellular automata, crystals are based on regular grids, too. Consequently, if we discuss questions about the symmetry of cellular automata, we can profit from results obtained in the field of crystallography. In this contribution it will be described how the elementary cells of a crystal can be formulated using three-dimensional cellular hypergraphs. These graphs allow us to model the geometrical properties of the elementary cells (e.g. distances and angles) on a high level of abstraction. Furthermore, the symmetry elements (e.g. mirror planes, symmetry axes, ...) can be expressed in terms of constraints on some cellular hypergraph. Finally, if there is given the graph of the elementary cell and a set of symmetry constraints, it is possible to construct the complete crystal mesh from this data. This allows us to build cellular automata models of crystals with arbitrary symmetry properties.

Keywords: Structure of cellular automata, cellular automata as models for real phenomena

Extended abstract

The results presented in this contribution were initiated by a discussion which I had several years ago with a colleague of mine: He was working at the classification of cellular automata models, and consequently it was necessary to clarify which repetitive regular (e.g. symmetric) structures can be built in three-dimensional space.

It is clear that we can profit from the results obtained in *crystallography* when discussing this question, because this discipline provides us with a catalogue of all conceivable symmetric repetitive meshes (see e.g. the textbooks [1, 5]). On the other hand, crystallography can profit from cellular automata models, too, when physical processes which take place in a crystal need to be simulated. But this requires that we are equipped with a description language for cellular systems (e.g. *CDL*, for an introduction see [4]) which allows us to deal with any imaginable symmetry relationships (for actual research from the point of view of crystallography, see e.g. [6]).

So I resumed the research mentioned above because of the finding that *cellular hypergraphs* are well suited for describing the elementary cells of a crystal as well as how the elementary cells are composed to form the complete crystal mesh. Initially cellular hypergraphs have been developed with respect to inhomogeneous and dynamically changing structures [2]. But they can be used as well for describing structures having some local inhomogeneity in combination with an overall regular character. And furthermore, the *relative addressing mechanisms* defined for cellular hypergraphs (see [3]) allow us to formulate the constraints on any symmetry elements of a given crystal.

The talk will consist of three major sections: The first section will give an overview about the essentials of crystallography. Based on the different types of *symmetry axes*, the terms *crystal system*, *point group* and *space group* will be illustrated. In the second section the fundamentals about cellular hypergraphs and about relative addressing within these graphs will be recalled. In the final section it will be demonstrated how the elementary cell of a sample crystal can be described using a cellular hypergraph. And it will be shown how the description of the elementary cell can be combined with additional symmetry constraints, such that a complete crystal mesh can be constructed.

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