Non-redundant Graph Representation of Polyhedral Networks

Hans-Joachim Klein, *Inst. of Computer Science and Applied Mathematics, Univ. of Kiel, Germany*. E-mail: hjk@is.informatik.uni-kiel.de

Infinite homogeneous networks in crystal structures with a single kind of coordination polyhedron and a single kind of connection between polyhedra can be represented by so-called quotient graphs or direction-labeled graphs [1],[2]. These finite graphs may be obtained from periodic nets by graph folding based upon translational symmetries. Taking all given symmetries into account this folding can be generalized such that so-called symmetry-labeled graphs are obtained [3]. We show how to further reduce this representation form by checking whether edges exist which may be generated by applying symmetry operations to other edges. A similar proceeding can be applied to polyhedra graphs [4]. In these graphs nodes represent geometrical or topological views of polyhedra. Edges represent connections between polyhedra with vertices involved in the connections as labels. A suitable representation of faces in topological views allows to reflect the main characteristics of a given polyhedral network when polyhedra are assumed to be rigid bodies.

In both cases, the minimal graph forms are well-suited for enumeration processes since they allow to avoid the generation of isomorphic graphs in an early stage. A further application is the improvement of indexes supporting the efficient search for isomorphic substructures in large collections of crystal structures.

[1] Chung S.J., Hahn T., Klee W.E., *Acta Cryst*, 1984, **A40**,42-50. [2] Goetzke K., Klein H.-J., Kandzia P., Lect. *Notes Comp. Sc.*, 1988, **314**, 242-254. [3] Klein H.-J., *Math. Modelling and Scientific Comp.*, 1996, **6**, 325-330. [4] Klein H.-J., *Proc. 16th SSDBM*, 2004, 255-264.
Keywords: polyhedra, graph theory, enumeration