

New Tool based on the Superspace Concept to discover Structure Relations

Ivan Orlov, Gervais Chapuis, Ecole *Polytechnique Fédérale de Lausanne*, CH-1015, Switzerland E-mail: Ivan.Orlov@epfl.ch

Relations between crystal structures imply relations between their space groups, which can be expressed by group-subgroup relations. Recently, the superspace formalism has been extensively used for the unified description of sets of commensurate structures [1, 2]. The method consists of finding possible structures by identifying their space group symmetry from rational cuts in superspace. For practical purpose, the inverse problem is more useful but requires a large amount of compilation.

We constructed a complete tree linking (3+1)- and the corresponding 3-dimensional space groups derived by rational cuts. The aim is to discover possible (and impossible) space group chains for structural relations and phase transitions. The corresponding tree for (3+2)-dimensional groups will soon be completed.

A database providing the subgroup-supergroup relations is available at <http://lcr.epfl.ch/page55041.html>

This tool is particularly helpful in finding common superspace denominators for various series of modular ('composition-flexible') structures. We shall illustrate the use of the database with a few examples drawn from various fields of crystal chemistry.

[1] Perez-Mato J. M., Zakhour-Nakhl M., et al., *Journal of Materials Chemistry*, 1999, **9(11)**, 2795-2808. [2] Zakhour-Nakhl M., Darriet J., et al., *International Journal of Inorganic Materials*, 2000, **2(6)**, 503-512.

Keywords: superspace symmetry, composition-flexible structures, modular structures