Modular Aspects of Inorganic and Mineral Structures

Emil Makovicky, *Geological Institute, University of Copenhagen*. E-mail: emilm@geol.ku.dk

With the increasing complexity of known inorganic and mineral structures, the importance of *moduli*, composed of a number of coordination polyhedra, became obvious for the understanding of these structures. The moduli are fragments of simpler structure types, so called *archetypes*, which have been recombined into a recombination structure according to a set of new structural principles, unit cell (chemical) twinning, crystallographic shear, non-commensurate interfaces, and coherent intergrowths. Structures built on the same principles, but with an incrementally increasing fragment size, form *accretional homologous series*/*polysomatic series*. The homologous approach allows distinction into *extensive* and *combinatorial* categories. *Variable-fit structures* have two (sub)lattices present in one structure. Combination of the accretional and variable-fit principle leads to new complex structures, including 'sliding series' and 'box-work structures'. *Configurational homology* reaches beyond the limits of the usual 'isoelemental' concept. Introduction of small but substantial changes into distinct homologous structures leads to *plesiotypes*. Structures in which one set of layers/slabs is identical (or homologous) for the entire family whereas the alternating set differs from a member to a member are *merotypes*. Besides 'proper' (*OD*- and *non-OD polytypes*), with structurally unmodified layers, '*improper' polytypes* can be recognized, with modifications of component layers, as well as *pseudopolytypes* between which pronounced changes in bonding patterns occur, and *endopolytypes* in which only, e.g., the cation component is subject to polytypy whereas the anionic framework remains (in principle) unchanged. *Non-commensurability* and *semicommensurability* can lead to polytypism.

Keywords: modular crystallography, structural series, polytypes