

OPEN COMMISSION MEETINGS

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

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OD Approach in Natural and Synthetic Inorganic Compounds: a useful Tool in Structure Solving and Structure Modeling

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The numerous researches carried on OD structures have clearly shown how that theory favours a deep insight into the various related phenomena of one-dimensional disorder, twinning (generally polysynthetic twinning), polytypism, and how it presents a comprehensive interpretation of the diverse anomalous features frequently displayed by diffraction patterns: diffraction enhancement of symmetry, diffuse spots, continuous streaking. However it is still far from constituting a 'normal' professional tool for mineralogists, inorganic chemists, material scientists. That is probably due to the erroneous assumption that the OD structures are relatively few in number and that their arrangements may be solved and described by 'normal' procedures. I shall try to clearly demonstrate its practical value and to show the various aspects in which OD approach may be extraordinarily and uniquely helpful, in particular:

- a) The capability of OD approach to suggest the possible existence of new phases (new minerals in the case of natural phases) polytypically related to already known compounds, with exact indication of their crystallography and structure and its aid in overcoming serious problems during the refinement process.
- b) The possibility to solve important problems where structural disorder had so far prevented the understanding of the 'real' structures. Interesting examples are presented by the C-S-H phases well known to the cement chemists, namely tobermorite, clinotobermorite, and their hydration and dehydration products.

Keywords: OD structures, polytypes, tobermorite

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Graph Theory, Symmetry and Inorganic Solids

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The Principle of Maximum Symmetry states that a structure adopts the highest symmetry consistent with the constraints acting on it.

Chemical constraints are determined by the properties of the bond graph, which for molecular compounds is the same as the bond diagram. Inorganic solids have infinite bond graphs, but a finite graph that retains all the essential nearest neighbour properties can be created by extracting one formula unit from the infinite graph. The lengths of the bonds can be predicted from this graph using the bond valence model and the principle of maximum symmetry. They necessarily have the symmetry of the graph.

Steric constraints are introduced when the bond graph is mapped into three dimensional space. The ideal space group adopted by the crystal must be a subgroup of the symmetry group of the graph, but the steric constraints may further lower the symmetry by distorting the structure along one or more of its normal coordinates.

Examples will illustrate this approach.

Keywords: bond graphs, symmetry, bond lengths

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News about the Inorganic Crystal Structure Database ICSD

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With the 2nd update 2004 82,876 entries are included in ICSD, including about 11,000 mineral structures. For about 22,000 structures a cross-reference to the Powder Diffraction File PDF is given. Inorganic structures don't contain C-H bonds together with C-C bonds in any residue. So some overlapping with organic structures is possible (e.g. with oxalate anions or tetramethylammonium cations). In addition organic residues are allowed in zeolites and in minerals.

For the introduction of **Structure types** the Pearson-symbols were unified as to get only one symbol per Bravais-type. The single-side centred cells were united under the letter "S". The remaining 14 symbols are: aP, mP, mS, oP, oS, ol, oF, tP, tl, hP, hR, cP, cl, cf. The number of atoms in the Pearson-symbol always refers to the standard setting, which for the rhombohedral structures is that of the rhombohedral primitive cell. The remarks of the prototype entries (one per structure type) will contain further information about the structure type in question, e.g. the "atomic environment types" of Daams & Villars [1]. The first about 100 structure types are ready to be incorporated into the first update of 2005.

Authors can easily help to complete the database ICSD! Just check your publication list against the entries in ICSD. Structures only published in a doctoral thesis or presented as a poster can be included into ICSD too.

[1] a) *J. Alloys Comp.*, 1992-97, **182**, 1-33; b) *J. Alloys Comp.*, 1992-97, **197**, 243-269; c) *J. Alloys Comp.*, 1992-97, **215**, 1-34; d) *J. Alloys Comp.*, 1992-97, **252**, 110-142

Keywords: inorganic structures, database, structure type

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Pressure Calibration Standard at high Temperature and high Pressure

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In high temperature and high pressure experiments, it is crucial to have a reliable pressure calibration standard over wide temperature and pressure ranges. At room temperature, the ruby-fluorescence pressure scale is found to accurate to within 1 % up to 55 GPa(Zha et al., 2000). However, severe discrepancies are reported between proposed pressure scales at high temperatures.

We showed previously (Matsui et al., 2000) that by combining the molecular dynamics(MD) method with quantum correction, it is possible to simulate very accurately the structural and physical properties of crystals over wide temperature and pressure ranges. Since the MD method derives thermal properties directly without any constraint on the atomic displacements, it is particularly useful and powerful for the simulation at high temperatures where anharmonic effects are important. In order to take into account the many-body forces in crystals, the breathing shell model(BSM) developed by Matsui(1998) is used for the MD simulation.

We have applied the MD method to the four cubic crystals, MgO, NaCl, Ar, and γ -Mg₂SiO₄. We show the MD simulation with BSM reproduces very accurately the observed properties of these crystals, including the volume compression data at room temperature, the volume thermal expansion data at 0 GPa, and the elastic constants and their temperature and pressure dependences. We then simulate and crosscheck the T - P - V equations of state of these crystals to provide them as reliable internal pressure calibration standards at high temperatures and high pressures.

Keywords: MD simulation, pressure standard, high temperature