

Main Lectures

5

ML-08.01 INTERNAL SURFACES AS ORDER PRINCIPLES IN SOLIDS R. Nesper*,
Laboratory of Inorganic Chemistry, ETH Zürich, Switzerland

The existence of objects or particles which can be discriminated is a necessary condition for a structured world. Every assembly of particles thus must contain separators which are found in the intermediate space between them. The organisation of any such assembly, though a result of interaction types and energy optimization, is reflected in its most unique form by the symmetry.

As it is a general condition for structures that the particles are more stable than the whole arrangement the separators are found at the trajectories of weakest interactions. These are synonymous with surfaces in three dimensions. Surfaces, inner and outer ones, are essential parts of any structure and they do reflect the symmetry of the overall arrangement least disturbed by the actual nature of the particles.

Attention is focussed on the generation and classification of three periodic surfaces (PS) which may be minimal surfaces (PMS) or nodal surfaces (PNS). While PMS are very difficult to derive, PNS can simply be calculated by very short Fourier series whose symmetry properties are given by the choice of appropriate geometrical structure factors. The topology of PMS and PNS is in general very similar, and hence PNS are sufficient to discuss the general organisation or symmetry - topology - relations of structures, especially crystal structures.

Besides purely geometrical considerations on structural organisation, the relationships between structures, and the development of complexity, some attention is focussed on the implications of PMS/PNS on physical properties of crystalline chemical compounds. It is a fact that different chemical interactions in compounds are segregated into different spatial regions with the result of cluster, molecular and supramolecular arrangements. In this way covalent ionic and van der Waals forces are separated on different inner surfaces which, depending on actual particle numbers and volumes, are bubbles, planar or PNS-like curved in space.

References

- [1] L. Faeth, S. Andersson; *Z. Kristallogr.* **160** 313
- [2] S. Andersson, S.T. Hyde; *Angew. Chem. Int.Ed.Engl.* **22** (1983) 69
- [3] R.Nesper, H.G.v.Schnering; *Z.Kristallogr.* **170** (1985) 138
- [4] R.Nesper, H.G.v.Schnering; *Angew.Chem.* **98** (1986) 111; *Angew.Chem.Int.Ed.Engl.* **25** (1986) 110
- [5] A.-C.Eliasson, K.Larsson, S.Andersson, S.T.Hyde, R.Nesper, H.G.v.Schnering; *starch/stärke* **39** (1987) 147
- [6] M.Oehme, R.Nesper, H.G.v.Schnering; *Z.Kristallogr.* **182** (1988) 201
- [7] H.G.v.Schnering, R.Nesper; *Colloque de Physique C7* (1990) 383
- [8] H.G.v.Schnering, R.Nesper; *Z.Phys.B.* **83** (1991) 407

ML-09.01 COMPUTER SIMULATION OF INORGANIC STRUCTURES WITH FIRST-PRINCIPLE INTERATOMIC POTENTIALS, Shinji Tsuneyuki, Institute for Solid State Physics, University of Tokyo, Japan.

Realistic simulation of crystal structures of materials has long been a goal of scientists involved in condensed matter physics. Recent dramatic advances in available computer power have enabled us to construct *ab initio* models and to perform large-scale simulations including molecular dynamics and lattice dynamics. These can be used not only to understand experimental observations of minerals in terms of their microscopic structures but also to predict properties of materials with lesser experimental support.

We have developed an interatomic potential of silica with use of a first-principles total-energy calculation of a small cluster (Tsuneyuki, S., Tsukada, M., Aoki, H. & Matsui, Y. (1988), *Phys. Rev. Lett.* **61**, 869-872). Although the potential has a pairwise functional form suitable for any kind of computer simulation, it can reproduce structures and elastic properties of the polymorphs of silica with considerable accuracy, showing that the framework structures of silica are primarily subject to the local packing of large oxygen atoms. The potential has also been applied to simulations of dynamical properties of silica, such as phonons, structural phase transitions, pressure-induced amorphization, and so forth. In this talk, the principle, applications, extension to silicates and limitation of the method will be reviewed.

ML-10.01 FULLERENES By W I F David, ISIS Science Division, Rutherford Appleton Laboratory, Chilton, Didcot, OXON., OX11 0QX, U. K.

Carbon is a fascinatingly versatile element. It forms the basis of organic chemistry; its traditional allotropes, diamond and graphite, show distinctly different behaviour in almost all of their physical properties. Nevertheless, the discovery of carbon-cage structures, the fullerenes and their derivatives, the fullerides, has introduced numerous new possibilities. This talk will begin with an overview of fullerene crystallography, from C_{60} to the massive fullerene tubes. Attention will be focussed on crystal structures of the smaller fullerenes and fullerides, C_{60} , C_{70} and the superconductors A_3C_{60} ($A = Na, K, Rb$). The likely origin of superconductivity in A_3C_{60} will be discussed in conjunction with other cluster compounds. Particular attention will be given to the structure, dynamics and phase transition behaviour of solid C_{60} , the most symmetrical of all fullerenes.