

X-RAY DIFFRACTOMETRY : X-ray rocking curves recorded with the proper resolution provide information on the depth dependence of the lattice parameter and unit cell composition from the sample top surface to a few micrometers below. A fitting procedure between the experimental curve and a computed profile is applied. Depending on the type of heterostructure under investigation several computing approaches have been developed.

i) For slightly mismatched non periodic epilayer stackings, a numerical scheme based on the integration of Takagi-Taupin differential equations for X-ray propagation is adequate. A purely analytical treatment can be derived when the heterostructure may be considered as built up with perfect thin slices. Satisfactory results have also been obtained with a kinematical description of the thin epilayers and proper boundary conditions at the interface with the substrate where the dynamical theory is applied. The sensitivity of the method in terms of strain evaluation and profiling will be discussed in some typical structures.

ii) In the case of periodic superlattices, satellite reflexions are present whose location and relative intensities carry the searched information on the super unit cell : individual layer thickness, composition and state of strain, average misfit with respect to the substrate and period of the structure. Departure from true periodicity and interface roughness can also be detected by this method with a monolayer sensitivity in the case of very short period superlattices.

A brief comparison with some other non-destructive characterisation techniques such as Rutherford Back Scattering will be presented.

ML19-1 STRUCTURAL CORRELATIONS IN THREE-DIMENSIONAL NETWORK SOLIDS. By F.C. Hawthorne, Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba, Canada, R3T 2N2.

Inorganic crystal structures may be usefully represented as translationally symmetric networks or graphs. Vertices may represent atoms or larger structural groups, and edges represent the linkage (bonds) between the vertex elements. Although this is a graphical (often called topological) description, it contains significant chemical information. When the vertices represent atoms in a finite molecule, the eigenvectors of the adjacency matrix are identical with the molecular orbitals in the Hückel approximation; in a translationally symmetric solid, the successive numbers of circuits of gradually increasing length can be used via the method of moments to generate the density of states of the eigenvalue spectrum. In both cases, it is the graphical (topological) characteristics of the network from which the electronic spectra are derived. Thus, a graphical approach to hierarchical structure relationships may be a much more 'fundamental approach' than was originally conceived, as the graphical aspects on which such schemes are based seem to play a dominant role in the energetics of the structures.

Some approaches associate an atom with a vertex and a chemical bond with an edge; others associate a coordination polyhedron with a vertex, and interpolyhedral linkage with an edge. The latter method has the virtue of visual simplicity and graph theoretic convenience whereby *a priori* chemical constraints can be used in combinatorial applications. This may be combined with bond valence theory to produce simple arguments that may easily be applied to very complex structures. Associating cation coordination polyhedra with the network vertices, a structure may be considered as an array of complex anions that polymerize in order to satisfy their

(simple) anion bond-valence requirements. This suggests that structures may be profitably described and ordered according to the polymerization of those coordination polyhedra of higher bond-valences.

Structures may be ordered into classes according to the dimensionality of these strong linkages; essentially, that is ordering them in terms of the anisodesmic nature of the bonding, a feature that is common to most hierarchical schemes developed.

There seem to be firm energetic reasons for a graphical basis to correlation and hierarchical ordering of network structures, and the next step should be to optimize the physical/chemical content of this approach with a view to explaining structure-chemistry and structure-property relations in these materials. Bond-valence theory has a significant role to play in this regard, and some recent developments along these lines will be discussed.

ML19-2 ATOMIC MECHANISMS OF STRUCTURAL PHASE TRANSITIONS. By K.S. Aleksandrov, Institute of Physics, 660036 Krasnoyarsk, USSR.

The lecture is devoted to the relations between minor variations of structure, the mechanisms of phase transitions (PT's) and the physical properties of crystals belonging to several broad families originated from the few aristotypes G_0 .

1. The families of A_2BX_4 and $AA'BX_4$ crystals (A, A', B - cations, $X = O, S, F, Cl, Br, I$) containing tetrahedral groups BX_4 are considered. The structures of β - K_2SO_4 , Na_2SO_4 , III, glaserite and $CsLiSO_4$ types are treated as the differently ordered states of α - K_2SO_4 aristotype. The ordering of tetrahedra in β - K_2SO_4 type and derivatives of β -tridimite type crystals testifies to competing interactions between the nearest, next-nearest and third neighbour groups. PT's to ferroelectric, ferroelastic and incommensurate phases are well known in these families of crystals and many new examples have been found recently and others are likely to be discovered. The results of theoretical description and experimental studies of PT's are given.

2. A variety of new ferroelastics was found in halide crystals $A_2BB'X_6$ with the elpasolite type structure ($G_0 = O_h^f$). Among them there exist the crystals undergoing successive structural PT's. Group-theoretical and crystallographic analysis of G_0 was carried out. The structure changes and some physical properties of crystals at successive PT's were studied. It was proved that PT's in elpasolites like the corresponding PT's in perovskite type crystals are determined by two soft modes of G_0 -lattice connected with the mutual tilts of octahedral groups.

3. Structural changes arising in perovskite-like crystals of $TlAlF_4$ ($G_0 = D_{4h}^1$) and of K_2MgF_4 ($G_0 = D_{4h}^2$) types due to tilts in octahedral layers were analysed.

There exist new possibilities of distortions in these layered structures. Due to the relative weakness of forces bonding the layers, the distortions in nearby layers, the tilts, for example, may differ in tilt angle values, in tilt axes etc. This peculiarity of layered structure distortions was referred to as distortional polytypism, or polydistortion (Aleksandrov et al., Successive PT's in layered perovskite-like crystals, Pt's I and II / Inst. of Physics, Krasnoyarsk, Preprints No. 333 - June 1985 and No. 381 - April 1986). The available experimental data and existing contradictions in the PT-mechanism explanation are discussed.