through the membrane; however, only one of them is used for electron transfer. The folding of the subunits L and M is very similar with five membrane-spanning helices per subunit as the outstanding feature. The aminoterminal segment of the subunit H is folded into a membrane-spanning helix; the remainder of the subunit forms a globular domain which is bound to the cytoplasmic side of the L-M complex. The cytochrome subunit is attached to the L-M complex at the periplasmic side of the membrane and contains the four heme groups in a linear arrangement. This atomic model provides insight into the architecture of membrane proteins, and can serve as a basis for the explanation of functional properties of the RC.

ML.18-1 COMPUTER GRAPHICS IN STRUCTURE ANALYSIS. By T.A. Jones, Dept. of Molecular Biology, BMC, Box 590, S751-24 Uppsala Sweden.

Computer graphics allows one to present complex three dimensional data such that it can be more easily absorbed by the viewer. This data is often merely illustrative, or is constructed with the aim of allowing the viewer to make some kind of decision. The term "computer graphics" covers a multitude of equipment whose power varies by 5 orders of magnitude and of applications ranging from illustrating the results of a crystallographic investigation to designing a protein mutagenesis experiment.
My primary interest has been concerned with the protein crystallographers' problems first to construct a model then to improve it during refinement (Jones, 1978, J. Appl. Cryst. 11, 268-272). Our recent work (Jones and Thirup, 1986, 5, 812-822) was made possible by hardware developments resulting in affordable 32 bit computers and high performance colour displays. This work makes use of a skeletal representation of electron density (Greer, 1974, J. Mol. Biol. 82, 279-302) to present a much larger volume and colour to represent possible folding hypotheses. Taken together this helps the initial map interpretation. This aspect of the implementation has similarities to the Grinch system developed at the University of North Carolina. However, our skeleton can then be used as a framework to locate the best matching fragments from a data base of well refined proteins. Alternatively the fragments may be chosen from 170 five residue building blocks which are the result of a cluster analysis study (Jones and Levitt, in preparation). This technique Proleg, (PROtein LEGo) has affected our general attitude to molecular modelling which then becomes a problem of picking the best fragment to fit our observations (crystallographic, NMR or structurally related proteins).
Our future developments are aimed at a networked environment of work stations (of various capabilities) with cpu and data base servers. One of our goals is to produce a real space fitted protein model (Diamond, 1971, Acta Cryst. A27 436-452; Jones and Liljas, 1984, Acta Cryst. A40, 50-57) without manual intervention and to locate and correct the majority of conformational errors during refinement.

ML.18-2 X-RAY CHARACTERISATION OF SUPERLATTICES AND EPITAXIAL LAYERS. By M. Sauvage-Simkin, Laboratoire de Minéralogie-Cristallographie, F-75252, Paris-Cedex 05, and LURE, Bât. 209D, UPS, F-91405 Orsay.

Since about ten years, multilayer stacking of semiconducting materials has become a fundamental step in optoelectronic and hyperfrequency device elaboration. Molecular Beam epitaxy and Metal Organic Vapor Phase Epitaxy, both allow the preparation of tailored ultra-thin layer heterostructures. However, a perfect control and reproducibility of the individual layer thickness and composition, in the case of semiconductor alloys, cannot be guaranteed. Post-growth assessment of the actual heterostructure parameters is then still needed to predict or interprete the multilayer system optical and transport properties.

It is now well recognized that X-ray imaging and diffractometric methods are mostly suitable for this purpose, being non-destructive and accurate enough to provide the searched information. A review of the experimental and theoretical work performed in the various laboratories involved in the field will be presented and it is worth mentioning that among these, several are industrial research centers.

In order to fully characterise a heterostructure, the two approaches mentionned above should be combined :
X-RAY IMAGING : standard Lang topography in the transmission or reflexion geometries, Synchrotron Radiation (SR) White Beam or Plane-Wave topography are used to detect extended interface defects such as misfit dislocations and to qualify the lateral homogeneity of the sample. For example, SR topography on high order satellite reflexions enable to reveal lateral gradients in both the composition and period for superlattices.

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.

ML.19-1 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.

ML.19-2 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 Go.

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 $\beta$-$K_2SO_4$, $Na_2SO_4$ III, glaserite and $CsLiSO_4$ types are treated as the differently ordered states of $\alpha$-$K_2SO_4$ aristotype. The ordering of tetrahedra in $\beta$-$K_2SO_4$ type and derivatives of $\beta$-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 ($G_o = O_h^5$). Among them there exist the crystals undergoing successive structural PT's. Group-theoretical and crystallographic analysis of $G_o$ 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 $G_o$-lattice connected with the mutual tilts of octahedral groups.

3. Structural changes arising in perovskite-like crystals of $TlAlF_4$ ($G_o = D_{4h}^1$) and of $K_2MgF_4$ ($G_o = D_{4h}^{17}$) types due to tilts in octahedral layers were analysed.