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 cyto-chrome 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.

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.18-1   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 di-mensional 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 investiga-tion 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 hypoth-eses. Taken together this helps the initial map inter-pretation. This aspect of the implementation has simil-arities 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 build-ing 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 (crys-tallographic, NMR or structurally related proteins).
Our future developments are aimed at a networked environ-ment of work stations (of various capabilities) with cpu and data base servers. One of our goals is to

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 interpret 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.