SERC GRANT GR/80240 FINAL REPORT
THEORY OF SOME ELECTRONIC PROCESSES IN SEMICONDUCTOR HETEROSTRUCTURES

Summary

The research carried out under this SERC Grant has been concerned with calculations of carrier transport and relaxation in GaAs/AlAs quantum well heterostructures with particular attention being paid to the properties of holes. The study of hole dynamics in quantum wells is interesting, both for fundamental and for commercial reasons. The quantum well laser is a device with commercial potential and the capture and thermalisation of injected holes is an integral part of its operation. There have also been proposals that the mobility of holes can be enhanced by band structure effects in some strained layer structures. In basic research there have been a number of experimental investigations of carrier thermalisation in quantum wells. There has been rather less theoretical work, and most of the calculations that have been made have been concerned with the behaviour of electrons and not holes.

The project has involved the development of two major computational calculations. Those have been calculations of (1) band structure for in-plane wavevector in the quantum well, and (2) transport and relaxation by Monte Carlo simulation. Since the information from the band structure calculations was to be used in the Monte Carlo simulations, it was necessary to seek methods that gave realistic subbands but were also economical on computer time. It was found that matching methods based on complex band structure were suitable in this regard. To study transient phenomena it was necessary to use ensemble Monte Carlo simulation. Both the band structure and Monte Carlo simulation calculations were developed from first principles and now constitute a valuable asset for the research group. It is believed that the calculations of hole dynamics in quantum wells are the first to include realistic band structure and scattering matrix elements.

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