SERC/MOD GRANT XG10503 FINAL REPORT
ELECTRONIC STRUCTURE AND TRANSPORT IN STRAINED-LAYER SEMICONDUCTOR SUPERLATTICES AND HETEROSTRUCTURES

Summary

In the grant application, the stated aim of this project was for groups at Durham and Newcastle to mount a concerted effort to study the electronic structure and transport properties of strained-layer low-dimensional structures. The main function of the Newcastle work (to have been directed by Professor M. Jaros) was to have been a detailed study of the electronic structure of low dimensional structures with particular emphasis on Si/Ge based systems. This was to have been completed by the development of associated transport calculations, together with a rather more modest electronic structure programme at Durham. In practice, funding was received only for the Durham component of the application and thus the overall scope and ambitions of the project we necessarily substantially reduced.

The research carried out under the grant has been concerned with the calculation of the electronic structure of lattice-matched (GaAs/AlGaAs) and strained (Si/SiGe) heterostructures and the development of Monte Carlo simulations of carrier transport in these structures. The emphasis has been on those problems where certain band structure features have a significant influence on the carrier transport properties and where those features cannot readily be described by the simple one-band effective mass models that are commonly employed in transport calculations. Because of the failure to obtain funding for the complete project as described above, rather more work was done on GaAs/AlGaAs and rather less on Si/SiGe than originally proposed. In particular, we have carried out band structure pseudopotential calculations on GaAs/AlGaAs and Si/SiGe systems and **k**.**p** calculations on GaAs/AlAs quantum wells. We have studied hole tunnelling in GaAs/AlGaAs single-barrier structures and developed Monte Carlo simulations of holes in GaAs/AlAs and InGaAs/GaAs quantum wells, and electrons in GaAs/AlAs superlattices. Substantial progress has also been made in producing a simulation of electron transport in Si/Ge superlattices.

The completed work has been published and disseminated extensively. The Monte Carlo simulations of carrier transport using realistic band structure are amongst the first of their kind, and have attracted considerable interest from theoreticians and experimentalists working on transport studies.

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