EPSRC GRANT GR/L05570 FINAL REPORT
ELECTRONIC STRUCTURE AND LASER CHARACTERISTICS OF NITROGEN-BASED III-V SEMICONDUCTORS

Summary

This EPSRC research grant was awarded to Professor R A Abram and Dr S Brand of the Department of Physics, University of Durham. The project was part of a collaboration with Professor Blood's group in Cardiff to carry out calculations of the electronic structure and optical properties of the nitrides and their heterostuctures, and to model simple device structures. The intention was to generate data of direct relevance to the development of wide band gap nitride-based optical sources. The Durham group was responsible for the more fundamental electronic structure aspects of the work. The research grant provided funds for software, consumables, maintenance and technical support for two Unix workstations, and one postdoctoral research assistant for two years. The research was carried out between January 1997 and December 1998.

The work in Durham involved three different but inter-related types of electronic structure calculations to produce information required for the device related research in Cardiff. The three electronic structure methods employed were (i) first-principles total energy, (ii) semi-empirical pseudopotential, and (iii) **k**.**p**. We have successfully studied bulk GaN, AlN, InN and also GaAlN and GaInN alloys, in both zinc-blende and wurtzite forms, using the three different theoretical approaches. The first-principles calculations have been used to obtain accurate lattice parameters and band structure information. The eigenvalues from our own first-principles calculations and those of others have been used to provide energy eigenvalues to which the semi-empirical pseudopotentials have been fitted. A notable achievement has been the production of smooth form factor curves for the three compounds in the wurtzite structure, which have then been applied in the theory of strain and alloying effects.

The semi-empirical calculations have the advantage of providing reliable information on the conduction band as well as the valence. Effective masses and **k**.**p** parameters have also been derived from the semi-empirical pseudopotential results. In particular we have used our pseudopotential eigenfunctions and eigenvalues to carry out direct calculations of **k**.**p** parameters using the perturbation formulae of **k**.**p** theory; an approach which has the advantage over simple band structure fitting of producing a unique set of parameters for a given target band structure. We have also calculated the frequency-dependent dielectric functions (and refractive indices) of the nitride compounds. Finally, pseudopotentials representing GaAlN and GaInN alloys have been derived, and used to calculate alloy band gap and **k**.**p** parameters as a function of composition.

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