SERC GRANT GR/D67033 **FINAL REPORT**

CALCULATIONS OF AUGER RECOMBINATION IN SEMICONDUCTORS

Summary

Band-to-band Auger recombination and impact ionization play a significant role in many semiconductor devices and it is important to have realistic theoretical descriptions of the processes. Grant GR/D67033 was awarded for research in the theory of Auger recombination in bulk semiconductors of device relevance. As well as developing a method to provide what are believed to be the best available calculations of Auger recombination rates in narrow gap semiconductors, we have also been able to carry out calculations of impact ionization rates which have yielded interesting results.

The accurate evaluation of Auger recombination rates involves the use of a large computer program to deal with the multidimensional integration of the transition probability over all initial and final states. It is important that such a numerical scheme uses realistic band structure and accurate overlap integrals for the Bloch periodic parts of the wavefunctions for the states involved in the transitions. These overlap integrals occur in the transition matrix element, and may be obtained straightforwardly from band structure calculations. However, the magnitude of the total computation makes it impossible to incorporate a large band structure calculation directly into a transition rate program, so that it is necessary to devise an algorithm to give values of sufficient accuracy without recourse to large scale calculations.

Dr Beattie at Cardiff and Drs Abram and Brand at Durham were able to come together to collaborate as a result of this grant. Dr Beattie had already developed a large numerical scheme for calculating Auger transition rates, albeit with an insufficiently accurate model of the band structure; and the Durham group had expertise in accurate band structure calculations. As a result of work under the grant, computer programs now exist for the calculation (with realistic band structure) of

a) Auger recombination rates

b) Impact ionization threshold energy surfaces

c) Impact ionization rates as a function of energy for a specified direction in **k**-space of the ionizing carrier, and also as a function of energy averaged over all directions in **k**-space.

Auger recombination rates have been calculated as a function of temperature and carrier concentration for InSb and InGaAsP. For the same materials, interesting new result on the softness of the impact ionization threshold have also been obtained. Similar calculations for other narrow gap materials can now be carried out in a relatively straightforward way, and there is considerable scope for further work, particularly in the area of impact ionization.

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