Computer simulation of HREELS from low dimensional semiconductor structures

Introduction

In today's society, technology that uses semiconductor devices is commonplace; hard discs, mobile phones and anything which uses an LED all rely on semiconductors in some way. For this reason, in depth knowledge of these devices' properties is an important thing and my project focuses on gaining a more detailed insight into the electronic structure of the semiconducting material Indium Antimonide (InSb). More specifically, my project focuses on modelling the electronic structure at the surface of this material.

Two semiconductors, one Indium Antimonide (left) and the other Indium Arsenide (right). [1]

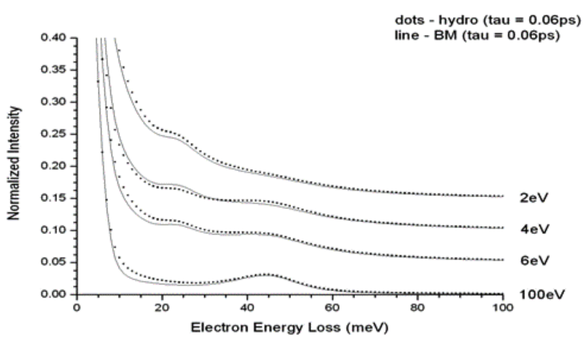
The Problem

High Resolution Electron Energy Loss Spectra (HREELS) can be obtained readily by experiment and show the energies at which lattice vibrations (phonons) and charge vibrations (plasmons) occur, from which charge distributions can be deduced. A Fortran code has been produced which the Physics Department have adapted to reproduce experimental data fairly accurately using the Botlzmann-Mermin dielectric function [2]:

$$\varepsilon_{BM}(q,\omega)=\varepsilon(\infty)\left(1+\frac{\tilde{\omega}\left[\varepsilon_0(q,\tilde{\omega})-1\right]}{\omega+i\gamma\left[\varepsilon_0(q,\tilde{\omega})-1\right]/\left[\varepsilon_0(q,0)-1\right]}\right)$$

. The problem is that this program approximates smooth input curves by a crude 'two-step' graph. A closer approximation would hopefully be obtained by splitting the graphs into 100 layers, and this was the goal of my project.

Initial Testing

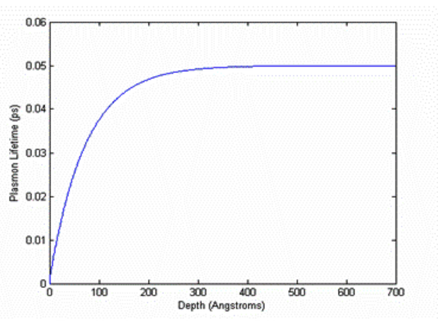


Model vs. model stack plot showing greater loss peak definition given by implementing the Boltzmann-Mermin Dielectric Function

The first step after editing the code was to compare results with a previous model known to provide reasonable results. This model uses a simpler dielectric function called the hydrodynamic function. As can be seen in the graph, the general trend is similar, while there is greater definition between the features in the new improved model compared to the simpler model. This is likely due to the fact that the simpler model does not take collisional damping effects into account.

Depth dependence of tau

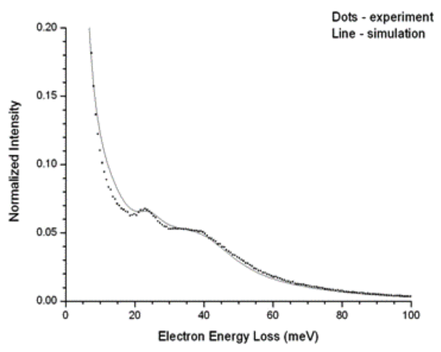
In previous models, the plasmon damping parameter tau had been set by hand, but with a 100 layer model a more efficient depth dependence was required. We settled on an exponential decay to the surface characterised by a decay depth z_0. The final smooth profile can be seen in the picture. This formulation allows the number of parameters in the problem to be reduced from over 100 to just 5, a great improvement. This also makes the problem of fitting the model to experimental data much simpler as there are less parameters to keep an eye on.



Depth dependence of the plasmon damping parameter.

Final results

At the end of the eight weeks I had obtained a fairly good fit at an incident energy of 8 electron volts (eV) as can be seen in the graph and was working at obtaining a suitable fit for an incident energy of 2eV. Once this is done, the parameters can be compared and a fit obtained for any incident energy using the same set of parameters; this will then constitute a fully working simulation and will hopefully be eligible for publication in a scientific journal.



My final fit for an incident energy of 8eV

My Experience

The URSS has provided me with an excellent experience, both in terms of giving me an interesting job to do and also as an introduction into the world of scientific research. The latter particularly has helped me towards deciding upon a career after University and will stand me in good stead when I do my Fourth Year Project and when I come to applying for a PhD or a job. I would recommend this scheme to any student considering a career in research, or even those just interested in gaining insight into a working environment.

References

[1] http://sales.hamamatsu.com/assets/img/products/SSD/Comp/InSB/InSb.jpg
[2] G. R. Bell, T. D. Veal, J. A. Frost and C. F. McConville, Phys. Rev. **73**, 153302 (2006)

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