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(U) OXFORD UNIV (ENGLAND) DEPT OF THEORETICAL PHYSICS  
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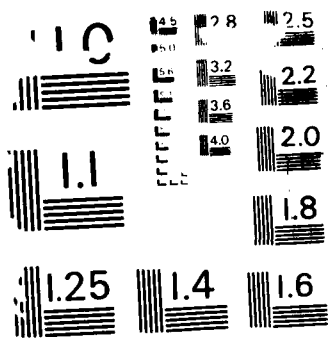
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DEFECTS AND DISORDER IN AMORPHOUS AND DAMAGED Si

Final Technical Report

by

Professor Sir Roger Elliott, FRS

December 1987

United States Army

EUROPEAN RESEARCH OFFICE OF THE U.S. ARMY

London England

CONTRACT NUMBER : DAJA 45-83-C-0056 R&D 4193PH

University of Oxford

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SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

Form Approved  
OMB No 0704-0188  
Exp Date Jun 30, 1986

1a REPORT SECURITY CLASSIFICATION Unclassified		1b RESTRICTIVE MARKINGS	
2a SECURITY CLASSIFICATION AUTHORITY		3 DISTRIBUTION / AVAILABILITY OF REPORT Approved for public release; distribution unlimited	
2b. DECLASSIFICATION / DOWNGRADING SCHEDULE			
4 PERFORMING ORGANIZATION REPORT NUMBER(S)		5. MONITORING ORGANIZATION REPORT NUMBER(S) R&D 4193-PH-01	
6a. NAME OF PERFORMING ORGANIZATION University of Oxford	6b. OFFICE SYMBOL (if applicable)	7a. NAME OF MONITORING ORGANIZATION USARDSG-UK	
6c. ADDRESS (City, State, and ZIP Code) Department of Theoretical Physics 1 Keble Road , Oxford, OX1 3NP		7b. ADDRESS (City, State, and ZIP Code) Box 65 FPO NY 09510-1500	
8a. NAME OF FUNDING / SPONSORING ORGANIZATION USARDSG-UK                      ARO-E	8b. OFFICE SYMBOL (if applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER DAJA45-83-C-0056	
8c. ADDRESS (City, State, and ZIP Code) Box 65 FPO NY 09510-1500		10. SOURCE OF FUNDING NUMBERS	
		PROGRAM ELEMENT NO. 61102A	PROJECT NO. 1L161102BH
		TASK NO. 7	WORK UNIT ACCESSION NO. 00
11. TITLE (Include Security Classification) Defects and Disorder in Amorphous and Damaged Silicon			
12. PERSONAL AUTHOR(S) Professor R.J. Elliott			
13a. TYPE OF REPORT Final	13b TIME COVERED FROM May 1984 TO June 87	14 DATE OF REPORT (Year, Month, Day) December 1987	15 PAGE COUNT 10
16. SUPPLEMENTARY NOTATION			
17. COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)	
FIELD	GROUP	SUB-GROUP	
20	12		
20	03		
19. ABSTRACT (Continue on reverse if necessary and identify by block number) This study of defects and disorder in Si has focussed on models of excitation near defects in the crystal, in structurally disordered amorphous material, and at interfaces between crystal and amorphous material. The first section deals with the vibrations of Si slabs with (111) faces subject to varying boundary conditions. In particular slabs with free boundaries, with dangling bonds saturated by hydrogen and slabs embedded in amorphous material were considered. The shift and broadening of the Raman peak was calculated and it was shown how this could be used to obtain estimates of crystallite size in disordered material. The main work related to a model of electron states at an interface between crystalline Si and amorphous SiO <sub>2</sub> . The latter material was modelled using a Bethe lattice. In the tight binding approximation the defect states associated with the dangling bonds of the P <sub>b</sub> centre were calculated and shown to depend on the crystallographic direction of the surface and in particular on the number of oxygen neighbours involved. The dependence of the peak position of the defect states in the energy gap was found to be sensitive to the local energy parameters and an attempt was made to calculate these self-consistently in the			
20 DISTRIBUTION / AVAILABILITY OF ABSTRACT <input checked="" type="checkbox"/> UNCLASSIFIED/UNLIMITED <input checked="" type="checkbox"/> SAME AS RPT. <input checked="" type="checkbox"/> DTIC USERS		21 ABSTRACT SECURITY CLASSIFICATION Unclassified	
22a NAME OF RESPONSIBLE INDIVIDUAL Dr. G.R. Andersen		22b TELEPHONE (include Area Code) 01-409 4423	22c OFFICE SYMBOL AMXSN-UK-RP

19. ABSTRACT (cont.):

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## Final Technical Report

Abstract:

This study of defects and disorder in Si has focussed on models of excitation near defects in the crystal, in structurally disordered amorphous material, and at interfaces between crystal and amorphous material. The first section deals with the vibrations of Si slabs with (111) faces subject to varying boundary conditions. In particular slabs with free boundaries, with dangling bonds saturated by hydrogen, and slabs embedded in amorphous material were considered. The shift and broadening of the Raman peak was calculated and it was shown how this could be used to obtain estimates of crystallite size in disordered material.

The main work related to a model of electron states at an interface between crystalline Si and amorphous  $\text{SiO}_2$ . The latter material was modelled using a Bethe lattice. In the tight binding approximation the defect states associated with the dangling bonds of the  $\text{P}_b$  centre were calculated and shown to depend on the crystallographic direction of the surface and in particular on the number of oxygen neighbours involved. The dependence of the peak position of the defect states in the energy gap was found to be sensitive to the local energy parameters and an attempt was made to calculate these self-consistently in the Hartree-Fock approximation. The effects of local polarization on the electron correlation was also studied using an extension of the Haldane-Anderson model.

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## 1. INTRODUCTION

The original proposal to study defects and disorder in Si focussed on models of the excitations near defects in the crystal, in structurally disordered amorphous material, and at interfaces between crystal and amorphous material. The earliest work studied vibrational problems but following discussion with Dr. E. Poindexter at the Fort Monmouth Laboratories it was decided to concentrate on the electronic properties and in particular on the defect states which occur at the interface of crystalline Si and amorphous or glassy  $\text{SiO}_2$ . The electronic states in this region have a profound effect on the desirable properties of Si devices. At a later stage some time was devoted to the study of excitations in thin layers of semi-conductor material which have come to be known as quantum wells which are also of interest to the group at the Fort Monmouth Laboratories. The electronic states near the band gap in these materials again controls the electrical and optical properties and their properties can be used for characterising devices. It was intended to continue this work to study defects and interface states but this was not possible before the end of the contract.

This report is therefore divided into three sections. The first deals with the vibrations of Si slabs with varying boundary conditions which approximate to slabs with free surfaces, embedded in amorphous material, and with surfaces saturated by hydrogen. The second part, which contains the bulk of the work, deals with the electronic states near the interface of crystalline Si and amorphous  $\text{SiO}_2$ . In particular the  $P_b$  centres which correspond to isolated dangling electronic bonds have been studied in detail on interfaces of different crystallographic orientations. In an attempt to justify the parameters of the tight binding model which is employed, self-consistent calculations of electron energies are attempted and the effects of local polarisability also estimated. The third part reports calculations on the electron hole and exciton states in various quantum well structures.

Details of all this work deriving from the grant are given in the 10 published papers listed.

## 2. VIBRATIONS OF CRYSTALLINE SLABS AND INTERFACES

The vibrational modes of a Si crystal with the diamond structure can be reasonably represented by the Born Hamiltonian using non-central forces between the displacements of neighbouring atoms. This takes the form

$$\begin{aligned}
 V(\ell, \ell') &= \frac{1}{2}(\alpha - \beta) \left| [\underline{u}(\ell) - \underline{u}(\ell')] \cdot \hat{n}_{\ell\ell'} \right|^2 + \frac{1}{2}\beta \left| \underline{u}(\ell) - \underline{u}(\ell') \right|^2 \\
 &= \sum_{i,j} H_{ij}(\ell, \ell') u_i(\ell) u_j(\ell')
 \end{aligned}
 \tag{1}$$

In the infinite crystal the normal modes can be enumerated using the perfect periodic symmetry to specify modes with characteristic wave vector  $k$ . In the presence of interfaces it is convenient to exploit the planar geometry. The periodic symmetry within the planes allows a  $k$  value to be defined and then an effective one dimensional model with effective interaction between planes must be evaluated to determine the full properties. We have found it convenient to carry out this calculation for finite slabs using the transfer matrix method.

It is now more convenient to work with the displacement-displacement Greens function which is directly related to the response functions for the material. The transfer equations of motion for  $G$  take the following form

$$G_k(n,m) [ E\delta(n,n) - H_k(n,n) ] - \delta(n,m) 1 + G_k(n,m+1)H_n(m+1,m) + G_k(n,m-1)H_k(m-1,m) \quad (2)$$

Here  $n$  numbers the planes, and there is an equation of this type for each  $k$  within the two planar dimensions. Each component of  $G$  is a  $3 \times 3$  matrix. The transfer matrices relate the  $G$  on different layers

$$G_k(n,m,E) = t_k(n) G_k(n-1,m,E) = G_k(n,m-1)t_k(m) \quad (3)$$

The amorphous phase is modelled by Bethe lattices which are relatively simple to handle analytically but which do not have long range order. The density of states for a single Bethe lattice of coordination 4, using the Hamiltonian in (1), give a reasonable representation of the vibrational spectrum. This is especially true at high frequencies though the representation of the lower end of the spectrum is unsatisfactory because of the inadequate representation of the longer range density of material. In fact the continuous branching of the Bethe lattice leads to increasing atomic density and this must be corrected by an appropriate weighting factor if any realistic results are to be provided.

Detailed calculations were made on Si slabs with (111) surfaces of varying thickness which were terminated in three ways.

- (i) The two slab surfaces were free but not reconstructed;
- (ii) The dangling surface bonds were terminated by H atoms;
- (iii) The bonds at the surfaces were attached to Si Bethe lattices.

All these three cases maintain the translational symmetry within the plane. The transfer matrix method can be used between planes and in case (iii) the set of equation is extended for the semi-infinite set of layers in the Bethe lattice.

In addition to the density of states close to the interface, the Raman response was calculated by an appropriate sum over layers

$$R = \text{Im} \sum_j \sum_{\ell \ell'} c_j(\ell) c_j(\ell') G_{jj}(\ell, \ell', E). \quad (4)$$

The layers of the Bethe lattice are weighted to give the same density in each layer. The results show a two peak response. There is a relatively broad peak around  $480 \text{ cm}^{-1}$  associated with the amorphous material and a sharp peak near  $520 \text{ cm}^{-1}$  for the crystal, with appropriate weights. The former effectively mimics the density of states of the amorphous material since construct interference is no longer a significant effect in the absence of translational symmetry. The sharp crystalline peak is dominated by response near  $k=0$  which is the allowed response in a perfect lattice. This sharp peaks shifts to lower frequencies and broadens slightly for thin slabs but the effect is only significant from slabs of less than about 10 layers. The shift is greatest when (ii) where the attached H atoms follow the Si on the surface and give it effectively larger mass, hence lowering the frequency. It is least for case (iii) as might be expected on physical grounds since the bonding pattern of the surface atoms is maintained in this situation.

The results are in qualitative agreement with experiments on samples containing micro-crystallites made from salve or by laser anneal of irradiated Si. This agreement is improved if a correction is applied to allow for the difference in surface to volume ratio between the slabs of the model and the more spherical crystallites expected in real systems. This suggests that the quantitative shift in the Raman peak can be used reliably to estimate crystallite size in such materials. If so this should prove a simpler and more reliable experiment than the estimates of crystallite size obtained from careful X-ray diffraction measurements.

This work has been written up and published in reference 1.

### 3. MODEL OF ELECTRON STATES AT THE Si-SiO<sub>2</sub> INTERFACE

The methods developed for the vibrational problem in section 1 were then extended to study the electronic properties close to an interface between crystalline Si and an amorphous SiO<sub>2</sub>. The tight binding model with four sp<sup>3</sup> orbitals on each Si was used, with appropriate sp orbitals on the oxygen atoms. This required extensions in two directions.

For the crystalline Si the tight binding equations are similar to those given in eqn. (2)-(4) for the vibrational case except that 4 × 4 matrices are required instead of 3 × 3. The parameters were chosen to give the best fit for the valence bands, the energy gap and the bottom of the conduction band. It is well known that this tight binding model does not give a good representation of the higher conduction bands where further orbitals are needed. Since, however, our attention was focussed on states in and near the gap it is believed that this has little effect on the results, and that the model is adequate for our purposes.

The amorphous SiO<sub>2</sub> was modelled by Bethe lattices in which each bond connecting the tetrahedral Si sites was dressed with an intermediate oxygen. Again the tight binding Hamiltonian was used and the effect of the oxygens was transformed away so that an effective interaction between the silicons remained. This effective interaction is energy dependent and hides much of the extra structure found in the bands of this material. Nevertheless it allows the treatment of the Bethe lattices to go through exactly as before. The model used attached these Bethe lattices to each of the surface Si atoms. It therefore preserved the planar translational symmetry and again allowed the surface to be treated as a problem of interacting planes using the transfer matrix method for each value of k within the plane.

The first case treated was that of a semi-infinite Si crystal with no reconstruction and dangling bonds on all the surface atoms. A significant difference of behaviour was observed for different crystallographic directions. A (111) surface has a single dangling bond perpendicular to the plane which has an energy state, when isolated, in the gap above the valence band edge. For a full surface the interaction between these bonds spreads this state into a surface band which overlaps the top of the valence band.

For the (110) surface there is again a single dangling bond at each surface site although the symmetry is such that two types of surface atom exist. This leads to two surface sub-bands one of which lies within the gap and the other of which is depressed into the valence band.

The (100) surface on the other hand has two dangling bonds per site and hence an appreciable interaction between the electron states associated with them. This leads to a significant splitting of the surface bands, one of which lies well up in the gap

and the other well down below the valence band edge.

Of course such surface bands are not observed in clean Si surfaces because reconstruction takes place to saturate the dangling bonds. However it is believed that this surface structure is stabilised if oxygens are attached to the dangling bonds. The bond strength in  $\text{SiO}_2$  is much greater than that in Si itself, so that the gap between conduction and valence bands is much larger and spans the smaller Si gap. Thus any surface states are driven away from the gap region. These effects are reproduced by the model.

Attention was then focussed on the  $P_b$  centres which are regarded as single dangling bonds at the interface. It is believed that because of the larger size of the oxygen atoms, it is stoichiometrically difficult to saturate all the surface sites and therefore isolated dangling bonds occur in significant concentrations on all of these interfaces. The problem is treated as a single defect incorporated into the interface problem by cutting one of the bonds between a surface Si and its attached Bethe lattice. It is straightforward, using Greens functions, to determine the energy states of such isolated defects. In this case the local electron state is largely confined to the dangling bond with some electron density on the bonds leading back into the crystal. Its position is therefore largely determined by the parameters chosen for the electron tight binding Hamiltonian on this site. These in turn depend critically on the number of oxygen neighbours for the silicon. For (111) and (110) surfaces the  $P_b$  centre is on an atom which has only Si neighbours. The localised state is found to be very similar in both these cases and to occur just above the valence band edge. For the (100) surface the  $P_b$  centre has a single oxygen neighbour and this changes in a dramatic way the energy of the localised state. If the parameters are taken as the average it is found that the state is removed to such a high energy that it is lost in the conduction band. This is a significant result since it predicts that  $P_b$  centres will have different properties on (100) interfaces. While this is true to some extent experimentally, well defined local states are still found within the gap for this orientation. In our theory the position of this level depends critically on the parameters chosen for the tight binding Hamiltonian. In particular it would appear that the crucial question is that of the number of oxygen neighbours attached to the site of the  $P_b$  centre. One explanation, which is still being pursued, is that the centres which are observed for this crystallographic direction, called  $P_b'$ , arise from other sites deeper in the Si which have no oxygen neighbours.

A summary of this work was published in reference 2.

Because of the sensitivity to the values of the local parameters it was thought to be useful to investigate the way in which these parameters varied in a self-consistent calculation. To date it has proved too complex to do the whole problem self-consistently and initially it has been investigated for a simpler model. In this, both the Si and the  $\text{SiO}_2$  are taken to be Bethe lattices joined by a single bond. The result is then effectively a one dimensional problem between the successive layers of the Bethe lattice. The Hamiltonian now includes electron-electron interaction assuming a short range screened interaction so that the tight binding parameters depend on the local density. The density itself is calculated self-consistently from the Greens function and the whole is iterated. These self-consistent variations change with distance from the interface between the two lattices. The tight binding Hamiltonian is given by

$$H = \sum \Delta_{ij} |\ell, i \times \ell, j| + \sum V_{ij} |\ell, i \times j, \ell'| + \frac{1}{2} U P_{ii}(\ell, \ell) |\ell, i \times \ell, i| + K \sum P_{ii}(\ell, \ell') |\ell, i \times i, \ell'|. \quad (5)$$

where the effective densities  $P$  are given by

$$P_{ij}(\ell, \ell') = -\frac{2}{\pi} \text{Im} \int_{-\infty}^{E_F} \langle \ell, i | G | \ell', j \rangle dE \quad (6)$$

The integral is over occupied states up to the Fermi energy.

The  $P_b$  centre is then modelled by breaking the lattices apart, essentially leaving a single Si Bethe lattice with a dangling end. There are now two dangling bond states depending on electron occupancy. The single electron state again lies just above the valence band and the state for double occupancy lies some 0.7eV above that in the gap. This is in good agreement with measurements of spin resonance and optical properties.

A full account of this work is given in reference 3.

Subsequently attempts have been made to extend this work in two directions. Since we are interested in the effects of oxygen neighbours we extended the self-consistent calculations to the situation where the Si atom at the interface is surrounded by one, two or three oxygen atoms. Thus the Si atom considered has a single dangling bond and three Bethe lattices of varying types. The charge density on the orbitals was found to vary with the number of oxygens in a non-linear way. A single attached oxygen introduces a polarisation by attracting a charge of approximately 0.4e from the adjacent silicon. In the normal  $\text{SiO}_2$  lattice some 50% of the valence charge on the silicon is transferred to the oxygen. We have found it difficult to explain the values needed to give the correct results using only the effects of electron-electron correlation. Although this work has been partly written up for publication it has been decided to check the results again carefully before it is submitted.

In this theory the effects of correlations are studied for a well defined Hamiltonian but the input parameters for that Hamiltonian must still be chosen. The electron-electron Coulomb interaction  $U$  in the Hubbard Hamiltonian is found to be smaller than that expected from the atomic values. This effect has been partially explained in band systems using the model of Haldane and Anderson which includes the hybridisation of the local states with the band states and hence increases the volume occupied by the defect electrons. Fowler has pointed out that a similar reduction occurs in insulators due to the polarisation of the host crystal when the defect is charged. We have been able to show that this effect can be included in the Haldane-Anderson Hamiltonian by reducing the defect Coulomb interaction to  $U-2K$  where  $-K$  is a polarisation energy. At the same time the electron core energy  $E_d$  is shifted to  $E_d+K(2n_0-1)$  where  $n_0$  is the number of valence electrons at the neutral defect. Estimates have been made for these parameters in the dangling bond of Si and for the  $P_b$  centre which give results in reasonable agreement with those used in earlier calculations. The two effects of hybridisation and polarisation can lead to a very small effective  $U$ , and indeed in some defects the possibility of a negative  $U$

exists. Using such an effective value alters the level positions and the net defect charge in the dangling bond and this and other examples are considered in reference 4.

#### 4. ELECTRONIC ENERGY LEVELS IN QUANTUM WELLS

The electronic states in two dimensional semi-conductor systems such as quantum wells or hetero junctions has become increasingly important in recent years. The research assistant employed on the contract, Dr. U. Ekenberg, is an expert in this field and we believe it is of growing importance to the research group at Fort Monmouth Laboratories. An active programme of the work has addressed the question of the nature of the hole states due to the degenerate valence bands, the non-parabolicity of the conduction bands, and the effect of the pseudo two dimensional character of the system on the exciton binding energies.

A considerable time was spent on calculations of binding energies of excitons in quantum wells. Several simple exciton calculations, where the hole has been considered as a scalar-mass particle, have been performed in recent years. The main purpose of the work has been to go beyond this approximation and include the effect of coupling between the heavy- and light-hole bands, which earlier has been show to influence the sub-band dispersion strongly.

The holes have been described by a  $4 \times 4$  matrix, the so-called Luttinger-Kohn Hamiltonian. We have used a perturbation approach where the diagonal elements of this matrix have been included in the zeroth order Hamiltonian and the off-diagonal elements have been included in perturbation theory up to second order. The exciton binding energies have been calculated for several transitions between electron levels and hole levels. The matrix elements have been evaluated analytically, a straightforward but tedious procedure, and the numerical work has been reduced to evaluating some sums over bound states and integrals over continuum states and solving some simple transcendental equations. The continuum states of the two-dimensional exciton are found to give a dominant contribution and the continuum states of the quantum well are found to be important for higher-energy transitions. The inclusion of the off-diagonal matrix elements is usually found to increase the exciton binding energies by 1-2 meV, but for transitions involving some hole sub-levels the binding energies are found to decrease.

We have also considered the effect of conduction band non-parabolicity on the exciton binding energies. This effect has been ignored by most previous authors while some authors have used the same non-parabolicity expression for the confinement effects and the motion parallel to the layers. We point out that the non-parabolicity effects are much stronger for the parallel motion and find that the exciton binding energy can be enhanced by about 1 meV for a well width of 50 Å rather than <0.5 meV if the directional dependence of the non-parabolicity effects is ignored. Our results are in good agreement with recent experimental results obtained at the Clarendon Laboratory in Oxford. If we compare with the recent variational calculations in which the hole coupling has been taken into account we find good agreement with the calculations of Bauer and Ando and by K.S. Chan. The calculation by Sanders and Chang and by Broido and Sham give even more enhanced exciton binding energies.

The exciton calculations have recently been published in reference 5; a shorter version was presented at the Second International Conference on Superlattices,

Microstructures and Microdevices in Gothenburg, Sweden (reference 6).

The effects of conduction band non-parabolicity have also been investigated in more detail. The shift of the confinement energies in a quantum well have been investigated by several authors, often with the use of energy-dependent effective masses, but the dispersion of the electron sub-bands parallel to the layers has received less attention. Starting from an accurate expression for the bulk conduction band dispersion including fourth-order terms in  $k$ , analytical expressions are derived for the perpendicular mass, which determines the shift of the confinement energies, and the parallel mass, which gives the curvature at the bottom of a sub-band. The main result, which apparently has not been recognised earlier, is that the parallel mass is enhanced over the bulk mass roughly three times more than the perpendicular mass. Part of this enhancement is due to the anisotropy of the bulk conduction band dispersion which often has been ignored but turns out to be more important in quantum wells than in the bulk. This work has been accepted for publication (reference 7).

In order to compare directly with cyclotron resonance experiments the Landau levels when a magnetic field is applied perpendicular to the layers have been calculated and this shows that the measured cyclotron mass is equal to the parallel mass in the limit when the magnetic field goes to zero. Some recent experiments are well explained by the theory. These results were presented at the Third International Conferences on Modulated Semiconductor Structures (MSS-III), Montpellier, France and accepted for publication in *Journal de Physique* (reference 8).

Self-consistent sub-band structure calculations have been carried out for electrons and holes at the modulation-doped interface between lattice-matched  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  and  $\text{InP}$ . This system is under current interest for optical communication applications. The small effective electron mass contributes to the possibility the second and the third electron sub-band can be partly filled. Another important factor is that unintentionally doped  $\text{InGaAs}$  tends to be n-type and we thus have an accumulation layer of electrons. The sub-band separations and the electron density at which higher sub-bands start to fill are shown to be clearly different in an inversion layer with p-type  $\text{InGaAs}$ . The band bending in an accumulation layer has been analysed in detail and it is demonstrated that a proper treatment of this factor is much more important for an accumulation layer than for an inversion layer, which is simpler to treat theoretically (in particular from a numerical point of view). The intriguing experimental situation where the number of filled sub-bands has been different in different experiments even if the electron density and other sample parameters have been similar can not be fully explained by the difference in background doping in the  $\text{InGaAs}$ . The possibility of trapping of holes in the semi-insulating substrate by a persistent photoconductivity effect seems to be another important factor, as suggested by Kane, Anderson, Taylor and Bass.

If the  $\text{InP}$  is p-doped a two-dimensional hole gas is formed at the interface. One interesting feature of this system is that for typical input parameters the second and third sub-bands turn out to be very close to each other when  $k_{\parallel}$  (the wave vector parallel to the interface) is zero. This leads to a very strong interaction between these sub-bands for small but finite values of  $k_{\parallel}$  and for an inversion layer the second sub-band bends up (i.e. has an electron-like mass) as much as 5 meV before it bends down near  $k_{\parallel} \approx 2.10^6 \text{ cm}^{-1}$ . In this region it interacts strongly with the first sub-band, which here has an almost flat dispersion. For accumulation layers the excited hole sub-bands are very close to each other, which leads to very peculiar

anti-crossing effects. An article about both electron and hole sub-bands at the InGaAs-InP interface is ready for submission to Semiconductor Science and Technology (reference 9).

Towards the end of the grant some work pertaining to strained-layer superlattices was begun in collaboration with Eoin O'Reilly and his co-workers at the University of Surrey. We have calculated the valence band structure of  $\text{Si}_{0.5}\text{Ge}_{0.5}$ -Si superlattices. The lattice constant differs between these two materials by 2%. We have for the first time taken the combined effect of strain and the split-off band into account in a sub-band calculation. The holes reside in the SiGe layers, which are under biaxial compression. In unstrained materials (like GaAs-AlGaAs) the interaction between heavy-hole and light-hole sub-bands leads to strongly non-parabolic dispersion parallel to the layers, which is often not good for technological applications. By deliberately introducing a suitable amount of strain the first light-hole sub-band is pushed down in energy relative to the highest heavy-hole sub-band which achieves an almost parabolic dispersion over an energy range of the order 100 meV with a quite small parallel hole mass in the region 0.15-0.2. This is actually smaller than the relevant parallel electron mass in these systems, where the electrons usually reside in the Si layers. We have also investigated how the results are influenced by the composition of the buffer layer, which determines the lattice constant parallel to the layers. The lattice mismatch and layer widths are chosen to be small enough that dislocations can be avoided. By optimizing the well width and the strain configuration even lower effective hole masses and higher hole mobilities are expected to be achievable which makes strained-layer SiGe superlattices interesting candidates for transistors. Here one can combine the advantages of two-dimensionality with the well-established silicon technology. This work was also presented at MSS-III and accepted for publication in Journal de Physique (reference 10).

We also use this computer program for calculation of hole sub-bands in strained-layer superlattices made from  $\text{In}_x\text{Ga}_{1-x}\text{As}$  of two different compositions grown on InP substrates. The resulting hole sub-bands structure together with conduction non-parabolicity effects can be used as input for calculations of gain, threshold current, temperature dependence etc. for lasers. Preliminary results indicated that the threshold current can be reduced considerably compared to conventional heterostructure lasers. This is not only because the low effective hole mass makes it easier to achieve population inversion but above all because loss mechanisms like inter-valence-band absorption and Auger recombination are virtually eliminated.

The study of valence sub-bands is thus not only interesting from a fundamental point of view but also technologically useful since they can be manipulated in a controllable way by inclusion of strain. The corresponding possibilities of "band structure engineering" of the conduction band are much more limited than those of the valence band.

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The following papers have been prepared which derive from the work financed by this grant.

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INVENTIONS

There are no inventions or patents deriving from this work.

END

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