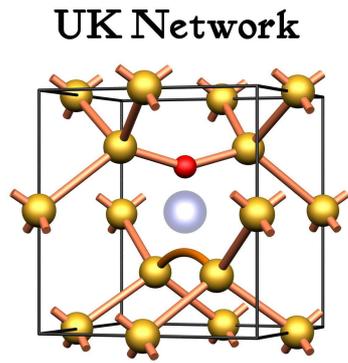


**UK Network on Diamond
& Diamond-like Carbon**

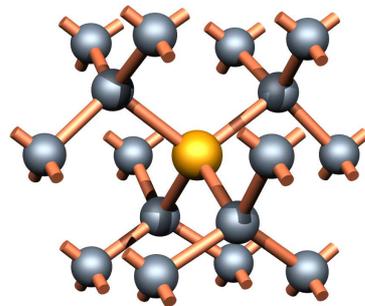
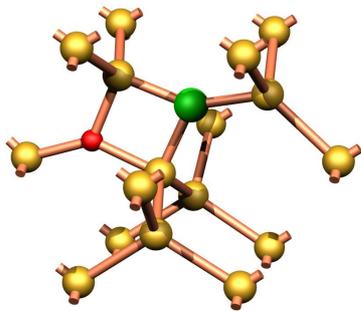


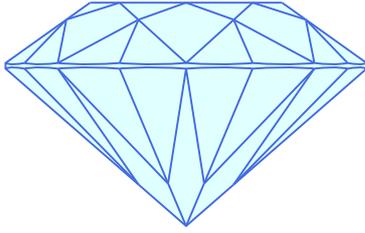
Defects in Si & SiGe

The Physics of Group-IV Semiconductors

7th - 10th April 2003

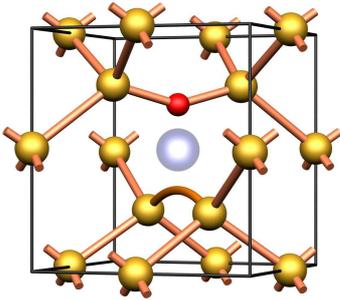
University of Exeter, U.K.



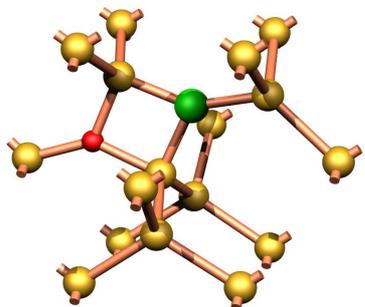
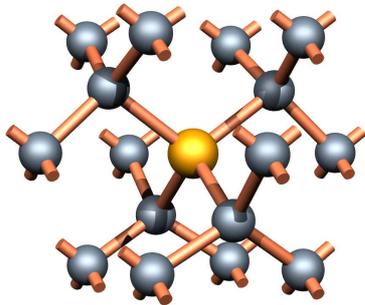


**UK Network on Diamond
& Diamond-like Carbon**

UK Network



Defects in Si & SiGe



The brilliant cut diamond

In 1919, the young Belgian mathematician and diamond cutter Marcel Tolkowsky published “Diamond Design” in which he systematically analysed the optics of a diamond, and calculated the best proportions for cutting round brilliant diamonds. With some minor changes, today’s standards for “ideal cut” diamonds are based on Tolkowsky’s work. Tolkowsky was a pioneer in the respect that he was the first to present a mathematical analysis of diamond cutting.

The vacancy-oxygen centre

The vacancy-oxygen (VO or *A* centre) is one of the most common defects produced by room-temperature electron irradiation of Si or Ge containing oxygen. It is believed to form by the trapping of mobile vacancies by interstitial oxygen atoms. The accepted structure is shown in this logo and involves a weak Si-Si reconstructed bond, seen in the lower half of the cell. In Si, the defect has an acceptor level at $E_c - 0.17$ eV, while the corresponding defect in Ge has a second acceptor level located at $E_c - 0.25$ eV.

Arsenic in diamond

Recent theoretical work has identified substitutional arsenic as a potential shallow donor in diamond. Preliminary calculations have resulted in a donor level located at $E_c - 0.31$ eV for this defect, compared to an experimental donor level at $E_c - 0.6$ eV for substitutional phosphorus. While there is concern over the inclusion of arsenic into diamond, the atom shares some physical properties with nickel, which is known to be present in some as-grown synthetic diamond samples.

$B_i O_i$ defect in silicon

The $B_i O_i$ defect, which has a single donor level at $E_c - 0.23$ eV, is formed when interstitial boron atoms (shown here in green) become mobile at ~ 230 K and are trapped by oxygen atoms (red). It was this defect that was used by Troxell and Watkins to monitor the annealing of the acceptor level of B_i in *p*-type silicon where the $E_v + 0.45$ eV level of B_i could not be observed directly.

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1 Introduction

1.1 Scope

The Physics of Group-IV Semiconductors Workshop 2003 is a collaboration between the *U.K. Network on Point Defects in Silicon and Silicon-Germanium* and the *U.K. Research Network on Diamond and Diamond-Like Carbon*.

1.2 Organisers

Programme chairs

Alison Mainwood is the chair of the EPSRC-funded *Research Network on Diamond and Diamond-Like Carbon*.

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Jan Evans-Freeman is the network co-ordinator of the *Network On Point Defects In Silicon And Silicon-Germanium*.

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1.3 Editorial committee

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2 Invited speakers

F. Danie Auret - University of Pretoria, Pretoria, South Africa

DLTS of defects introduced in Si (and SiGe) by low energy (< 5 keV) particles

Péter Deák - Institute of Physics, Technical University of Budapest H-1111 Budafoki ut. 8. Budapest, Hungary

Studies on defect complexes in Si and SiC

Bob Falster - MEMC SpA, Novara, Italy

The control and engineering of intrinsic point defects in silicon crystal growth and wafer processing

Tom Gregorkiewicz - Van der Waals–Zeeman Institute, University of Amsterdam, 65 Valckenierstraat, NL-1018 XE Amsterdam, The Netherlands

Using a free-electron laser for two-color spectroscopy of re-doped semiconductors

Dieter M. Gruen - Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, USA

Plasma processes of interest to the growth of ultrananocrystalline diamond and to etching of silicon semiconductors

Robert Hull - 116 Engineer's Way, P.O. Box 400745, Charlottesville, VA 22904-4745, USA

Interactions between misfit dislocations, surface morphology, and point defects during strain relaxation in semiconductor heteroepitaxy

Bob Jones - School of Physics, University of Exeter, Stocker Road, Exeter EX4 4QL, U.K.

Single hydrogen defects and hydrogen dimers in Si

Harris Kagan - Building 22, CERN, CH-1211 Geneve 23, Switzerland

Recent developments in diamond detectors

Erhard Kohn - Universität Ulm, Department of Electron Devices and Circuits, Albert-Einstein-Allee 45, 89081 Ulm, Germany

Diamond MEMS

Satoshi Koizumi - Advanced Materials Laboratory, NIMS, 1-1 Namiki, Tsukuba, Ibaraki, Japan

n-Type doping of diamond and the device applications

Brian Bech Nielsen - Institut for Fysik og Astronomi, Aarhus Universitet, Ny Munkegade, 8000 Århus C., Denmark

Properties of vacancy-hydrogen defects in group-IV semiconductors

Matthias Posselt - Forschungszentrum Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O. Box 510113 D-01314 Dresden, Germany

Ion implantation and ion-beam-induced defect formation in Si and SiC studied by atomistic computer simulations

Kimmo Saarinen - Laboratory of Physics, Helsinki University of Technology, P.O.Box 1100, FIN-02015 HUT, Finland

Vacancy-impurity complexes in highly n-type Si and SiGe: atomic structure, formation mechanisms, and electrical properties

Michael Seibt - IV. Physikalisches Institut der Georg-August-Universität Göttingen and Sonderforschungsbereich 602, Bunsenstr.13-15, D-37073 Göttingen, Germany

Quantitative high-resolution electron microscopy of defects and interfaces in silicon-based systems

Bengt G. Svensson - University of Oslo, Department of Physics, Physical Electronics, P.B. 1048 Blindern, N-0316 Oslo, Norway

Epitaxial 4H-silicon carbide and high-purity/low-doped silicon; irradiation-induced point defects

Alberto Tagliaferro - Dip. Fisica & Unità INFM, Politecnico di Torino, Torino, Italy
Optical properties of amorphous carbons and amorphous carbon nitrides

Dan Twitchen - Element Six, King's Park Ride, Ascot, Berks SL5 8BP, U.K.
Single crystal microwave plasma deposited CVD diamond

George D. Watkins - 16A Memorial Drive East, Sherman Fairchild Laboratory, room 209A, Lehigh University, Bethlehem, PA 18015, USA
Vacancies and interstitials in group-IV semiconductors: what has been learned from EPR studies

4 Programme

Unless stated all events take place in the Harrison building, rooms 101, 102 and 103.

Silicon-related posters can be exhibited from Sunday onwards, but should be taken down before lunch on Tuesday. Diamond-related posters can be exhibited after lunch on Tuesday, but should be taken down before the close of the conference on Thursday.

Sunday April 6th

Participants arrive; a ferry service will run between Exeter St. David's Station and Mardon Hall.

17:00-20:00

Registration: Foyer of Mardon Hall

19:00-23:00

Wine Reception and Registration: Mardon Hall

20:00-21:00

Buffet Dinner: Mardon Hall

19:00-23:00

Bar facilities available in Mardon Hall

Monday April 7th

7:30-8:30 Breakfast: Mardon Hall

Session I: Chair J. Evans-Freeman

9:15-9:30 Introduction

9:30-10:15 *Properties of vacancy-hydrogen defects in group-IV semiconductors*, B. Bech Nielsen, Institut for Fysik og Astronomi, Aarhus Universitet, Ny Munkegade, 8000 Århus C., Denmark

10:15-10:30 Discussion

10:30-11:00 Coffee

Session II: Chair G. Davies

11:00-11:45 *Using a free-electron laser for two-color spectroscopy of re-doped semiconductors*, T. Gregorkiewicz, Van der Waals-Zeeman Institute, University of Amsterdam, 65 Valckenierstraat, NL-1018 XE Amsterdam, The Netherlands

11:45-12:00 Discussion

12:00-12:25 *The origin of the 0.78 eV luminescence band in strained layer SiGe/Si samples*, A. J. Kenyon, Department of Electronic & Electrical Engineering, University College London, Torrington Place, London WC1E 7JE, U.K.

12:25-12:30 Discussion

12:30-12:55 *Photoluminescence as a probe of defect evolution in ion-implanted silicon*, R. Harding, Department of Physics, King's College London, London WC2R 2LS, U.K.

12:55-13:00 Discussion

13:00-14:00 Buffet Lunch

Session III: Chair K. Saarinen

14:00-14:45 *Studies on defect complexes in Si and SiC*, P. Deák, Physical Institute of the Technical University of Budapest, Budapest, Hungary

14:45-15:00 Discussion

15:00-15:45 *Epitaxial 4H-silicon carbide and high-purity/low-doped silicon; irradiation-induced point defects*, B. Svensson, University of Oslo, Department of Physics, Physical Electronics, P.B. 1048 Blindern, N-0316 Oslo, Norway

15:45-16:00 Discussion

16:00-16:30 Tea

Session IV: Chair P. Deák

16:30-16:55 *Recent developments in Laplace deep-level transient spectroscopy*, A. R. Peaker, Centre for Electronic Materials Devices and Nanostructures, University of Manchester Institute of Science and Technology, Manchester M60 1QD, U.K.

16:55-17:00 Discussion

17:00-17:25 *Electronic structure of divacancy-hydrogen complexes in silicon*, J. Coutinho, Department of Physics, University of Aveiro, 3810 Aveiro, Portugal

17:25-17:30 Discussion

17:30-18:15 *The control and engineering of intrinsic point defects in silicon crystal growth and wafer processing*, R. Falster, MEMC SpA, Novara, Italy

18:15-18:30 Discussion

19:30-20:30 Dinner: Mardon Hall

20:30- Poster Session (silicon) and Bar: Mardon Hall common room

20:00-23:00 Bar in Mardon Hall

Tuesday April 8th

| | |
|--|---|
| 7:30-8:30 | Breakfast: Mardon Hall |
| Session V: Chair R. Falster | |
| 9:00-9:45 | <i>Interactions between misfit dislocations, surface morphology, and point defects during strain relaxation in semiconductor heteroepitaxy</i> , R. Hull, Department of Materials Science and Engineering, University of Virginia, 116 Engineer's Way, P.O. Box 400745, Charlottesville, VA 22904-4745, USA |
| 9:45-10:00 | Discussion |
| 10:00-10:45 | <i>Vacancy-impurity complexes in highly n-type Si and SiGe: atomic structure, formation mechanisms, and electrical properties</i> , K. Saarinen, Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 HUT, Finland |
| 10:45-11:00 | Discussion |
| 11:00-11:30 | Coffee |
| Session VI: Chair B. Bech Nielson | |
| 11:30-12:15 | <i>Ion implantation and ion-beam-induced defect formation in Si and SiC studied by atomistic computer simulations</i> , M. Posselt, Forschungszentrum Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O. Box 510113, D-01314 Dresden, Germany |
| 12:15-12:30 | Discussion |
| 12:30-14:00 | Buffet Lunch |
| Session VII: Chair R. Hull | |
| 14:00-14:45 | <i>Quantitative high-resolution electron microscopy of defects and interfaces in silicon-based systems</i> , M. Seibt, IV. Physikalisches Institut der Georg-August-Universität Göttingen and Sonderforschungsbereich 602, Bunsenstr. 13-15, D-37073 Göttingen, Germany |
| 14:45-15:00 | Discussion |
| 15:00-15:45 | <i>DLTS of defects introduced in Si (and SiGe) by low energy (< 5 keV) particles</i> , D. Auret, University of Pretoria, Pretoria, South Africa |
| 15:45-16:00 | Discussion |
| 16:00-16:30 | Tea |
| Session VIII: Chair M. Seibt | |
| 16:30-17:15 | <i>n-Type doping of diamond and the device applications</i> , S. Koizumi, Advanced Materials Laboratory, NIMS, 1-1 Namiki, Tsukuba, Ibaraki, Japan |
| 17:15-17:30 | Discussion |
| 17:30-17:55 | <i>Electrical behaviour of antimony implants in silicon at large tilt angle</i> , G. Claudio, School of Electronics and Physical Sciences, University of Surrey, Guildford GU2 7XH, U.K. |
| 17:55-18:00 | Discussion |
| 19:30-20:30 | Dinner: Mardon Hall |
| 20:30- | Poster Session (diamond) and Bar: Mardon Hall common room |
| 20:00-23:00 | Bar in Mardon Hall |

Wednesday April 9th

- 7:30-8:30 Breakfast: Mardon Hall
- Session IX: Chair A. Mainwood**
- 9:00-9:45 *Vacancies and interstitials in group-IV semiconductors: what has been learned from EPR studies*, G. D. Watkins, Sherman Fairchild Laboratory, Lehigh University, Bethlehem, USA
- 9:45-10:00 Discussion
- 10:00-10:45 *Single crystal microwave plasma deposited CVD diamond*, D. Twichen, Element Six, King's Park Ride, Ascot, Berks. SL5 8BP, U.K.
- 10:45-11:00 Discussion
- 11:00-11:30 Coffee
- Session X: Chair D. Twichen**
- 11:30-12:15 *Single hydrogen defects and hydrogen dimers in Si*, R. Jones, School of Physics, University of Exeter, Stocker Road, Exeter EX4 4QL, U.K.
- 12:15-12:30 Discussion
- 12:30-12:35 Conference photograph: Assemble outside Harrison building
- 12:35-14:00 Buffet Lunch
- Session XI: Chair W. I. Milne**
- 14:00-14:45 *Optical properties of amorphous carbons and amorphous carbon nitrides*, A. Tagliaferro, Dip. Fisica & Unità INFN, Politecnico di Torino, Torino, Italy
- 14:45-15:00 Discussion
- 15:00-15:25 *Multi-wavelength laser Raman and X-ray photoelectron spectroscopy of phosphorus-containing DLC films*, G. M. Fuge, School of Chemistry, University of Bristol, Bristol BS8 1TS, U.K.
- 15:25-15:30 Discussion
- 15:30-15:55 *The dissociation of dislocations in diamond*, A. T. Blumeneau, University of Paderborn, Theoretical Physics, Faculty of Science, D-33098 Paderborn, Germany
- 15:55-16:00 Discussion
- 16:00-16:30 Tea
- Session XII: Chair E. Kohn**
- 16:30-16:55 *The vacancy-nitrogen-hydrogen complex in diamond: a potential deep centre in CVD material*, J. P. Goss, School of Natural Sciences, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU, U.K.
- 16:55-17:00 Discussion
- 17:00-17:25 *Mapping the energy levels of the self-interstitial in diamond*, Hannah E. Smith, Physics Department, King's College London, Strand, London WC2R 2LS, U.K.
- 17:25-17:30 Discussion
- 17:30-18:15 *Plasma processes of interest to the growth of ultrananocrystalline diamond and to etching of silicon semiconductors*, D. Gruen, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, USA
- 18:15-18:30 Discussion
- 19:30-20:00 Banquet Reception: Reed Hall
- 20:00-00:00 Conference Banquet: Reed Hall

Thursday April 10th

| | |
|-------------|--|
| 7:30-8:30 | Breakfast: Mardon Hall |
| | Session XIII: Chair D. Gruen |
| 9:00-9:45 | <i>Diamond MEMS</i> , E. Kohn, Universität Ulm, Department of Electron Devices and Circuits, Albert-Einstein-Allee 45, 89081 Ulm, Germany |
| 9:45-10:00 | Discussion |
| 10:00-10:45 | <i>Recent developments in diamond detectors</i> , H. Kagan, Dept. of Physics, Ohio State University, 174 W. 18 th Ave, Columbus, OH 43210, USA |
| 10:45-11:00 | Discussion |
| 11:00-11:30 | Coffee |
| | Session XIV: Chair R. Jones |
| 11:30-11:55 | <i>Growth and characterisation of epitaxial and polycrystalline n-type CVD diamond films</i> , K. Haenen, Limburgs Universitair Centrum, Institute for Materials Research, Wetenschapspark 1, B-3590 Diepenbeek, Belgium |
| 11:55-12:00 | Discussion |
| 12:00 | Lunch and close of workshop |

5 Proceedings

Conference proceedings will be published by the Institute of Physics in the Journal of Physics: Condensed Matter. Workshop participants will be invited to contribute papers.

5.1 Manuscript submission

Participants who have agreed to provide an article for the proceedings should submit to the conference organisers three hard copies, a completed submission form (available online*) and a completed assignment of copyright form*.

Note that a camera-ready copy is not required, but an electronic version in Word or L^AT_EX format will be necessary after the referral process. The preferred formats for figures are Encapsulated PostScript (.eps) and TIFF (.tif). L^AT_EX users should download and use the IOP class file when writing their article. For more details please read the IOP instructions for authors available via <http://www.iop.org/>

Note that you should not submit the copyright form or the manuscript to the Journal of Physics: Condensed Matter, but directly to the workshop organisers. It is planned to involve participants at the workshop in the refereeing process, in order to guarantee an early publication date. The referee's report form is also available online*.

* Please see <http://groupiv-2003.ex.ac.uk/proceedings.html> for online access to these forms.

6 Talks

6.1 Monday

Talk 1.1 (Invited)

Properties of vacancy-hydrogen defects in group-IV semiconductors

B. Bech Nielsen

Department of Physics and Astronomy, University of Aarhus

In crystalline silicon and germanium, a vacancy defect V_m consisting of m vacancies may interact with n hydrogen atoms and form V_mH_n complexes, in which each hydrogen atom is bound to one of the host atoms neighbouring the vacancy defect by a strong covalent bond. Infrared absorption spectroscopy has previously been applied to identify the local vibrational modes of several of these complexes, and information about their electronic properties has been obtained from electron paramagnetic resonance (EPR) and deep level transient spectroscopy. Based on these investigations, it appears that the electronic states within the band gap essentially represent combinations of the “free” dangling-bond orbitals residing on the neighbouring host atoms that do not bind a hydrogen atom. Hence, a covalent bond between a hydrogen atom and a host atom appears to be electronically “inert”. In this talk, I will review some of our previous work and discuss the vibrational and electronic properties of V_mH_n complexes in simple terms. As an example, our findings for the VH_3 defect in silicon will be described in some detail. At low measuring temperatures this defect gives rise to an EPR signal displaying trigonal symmetry and hyperfine interactions from three equivalent hydrogen atoms. As the measuring temperature is increased the signal broadens and disappears and a new signal displaying cubic symmetry appears. From correlated EPR and infrared absorption studies two local modes at 2156 and 2186 cm^{-1} are identified as the E and A1 Si-H stretch modes of VH_3 , respectively. Uniaxial stress applied along the [110] or [111] direction during cooling of the sample induces optical dichroism of the E mode absorption. From the thermal decay of the dichroism, we have determined the activation energy for reorientation of VH_3 to be 0.50 eV. Thus, hydrogen atoms in VH_3 may well below room temperature jump from one site to another inside the vacancy. The implication of this finding will be discussed at the end of the talk.

Talk 2.1 (Invited)

Using a free-electron laser for two-colour spectroscopy of RE-doped semiconductors

T. Gregorkiewicz

Van der Waals–Zeeman Institute, University of Amsterdam, 65 Valckenierstraat, NL-1018 XE
Amsterdam, The Netherlands

Semiconductor matrices doped with Rare Earth (RE) ions feature an attractive combination of sharp atomic like emissions with relatively large cross section of band-to-band absorption. This makes these systems interesting for applications in solid-state light-emitting devices. The most investigated systems include InP:Yb, GaAs:Er and Si:Er. The latter one is currently recognised as a successful method for obtaining optical emission from silicon. Despite numerous studies, the knowledge of excitation and deactivation paths in these complex systems is mostly phenomenological. While the key role of the weakly bound states (excitons, shallow defect states) is generally accepted, details of their particular involvement remain not clear. For the best understood InP:Yb system a detailed energy transfer path has been proposed but urgently requires experimental confirmation. Here we present a spectroscopic approach to this problem by making use of a two-colour experimental set-up with a tunable free-electron laser (FEL). Photoluminescence (PL) of RE ions is achieved by primary band-to-band excitation (second harmonics of a Nd:YAG pulsed laser correlated with the FEL). Intense mid-infrared (MIR) radiation from the FEL is used to access directly individual steps of the energy transfer processes. Individual shallow levels available in the material are selectively addressed by appropriate tuning of the FEL energy. In the presentation I will discuss a variety of effects revealed in Er-doped silicon by two-colour optical spectroscopy with the FEL. These will include energy storage, manifested by luminescence “afterglow” and an optical memory effect, and optically-induced Auger process involving energy transfer from the RE ion core to free carriers in the bands. In addition, for the InP:Yb system, I will show the so-called energy “back transfer” effect of excitation reversal, selectively activated by the MIR beam.

Talk 2.2

The origin of the 0.78 eV luminescence band in strained layer SiGe/Si samples

A.J. Kenyon

Department of Electronic & Electrical Engineering, University College London, Torrington Place,
London WC1E 7JE, U.K.

E.A. Steinman

Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow District 142432,
Russia

The photoluminescence band around 0.78 eV that is sometimes seen in strained layer SiGe samples or deformed silicon containing a high density of dislocations has been attributed to the presence of oxygen complexes. In this study we have prepared a set of $\text{Si}_{0.9}\text{Ge}_{0.1}$ samples by MBE which have then been implanted with iron, erbium, or oxygen in order to study the effect of implanted impurities on photoluminescence in the technologically important region around 1.5 microns.

Following implantation with oxygen, two luminescence bands appear around 0.85 eV and 0.78 eV, respectively. However, these bands are not present in either the unimplanted sample or those subject to Er or Fe implantation. The correlation between oxygen doping and the appearance of these bands supports the conjecture that they are associated with oxygen complexes.

Talk 2.3

Photoluminescence as a probe of defect evolution in ion-implanted silicon

Ruth Harding
King's College London

Gordon Davies¹, Paul Coleman² and Jennifer Wong-Leung³

1. Department of Physics, King's College London, London WC2R 2LS

2. Department of Physics, University of Bath, Bath BA2 7AY

3. Department of Electronic Materials Engineering, The Australian National University, Canberra, ACT 0200

Photoluminescence (PL) has recently become recognised as a powerful technique for probing the evolution of point defects in ion-implanted silicon [1]. PL has very high energy resolution, fast scan time, no sample preparation, no strict limit on the ion-implantation dose and energy, and *p*- or *n*-type silicon doped to any level can be used. The last is important since the annealing behaviour of intrinsic clusters of vacancies and interstitials can be measured independently of their strong interaction with dopants. However, it can be misleading to assume PL is intrinsically quantitative [2]. It is important to establish under what conditions we can convert the PL signal to a measure of concentration of the defects. Here we present PL studies of silicon implanted with MeV Si ions in the range 1×10^8 to 1×10^{15} cm⁻² and Positron Annihilation Spectroscopy (PAS) results for doses above 1×10^{12} cm⁻². We show that under controlled conditions, the PL intensity is proportional to the concentration of the defects, even at high doses, when normalised to constant excitation energy per defect. We use this result to derive the power laws of the production statistics for particular frequently observed defect aggregates (*e.g.* with zero-phonon lines at 997 and 1060 meV). The width of the PL lines indicate the mean strain the defects are experiencing and so is related to their spatial location in the implant profile. We show that a prerequisite of having a quantitative PL signal is to minimise the photoluminescence quenching, which occurs with a probability proportional to the separation of the vacancy clusters measured by PAS.

References:

- [1] Schmidt D.C. *et al.*, Journal Applied Physics **88**, 2309-2317 (2000)
- [2] Giri P. K. *et al.*, Applied Physics Letters **78**, 291-293 (2001)

Talk 3.1 (Invited)

Studies on defect complexes in Si and SiC

P. Deák, A. Gali & A. Solyom

Institute of Physics, Technical University of Budapest H-1111 Budafoki ut. 8. Budapest, Hungary

Defect engineering is a key part of microelectronic device processing. Tight control of the doping requires detailed knowledge about the incorporation and activation of the dopants as well as about the influence of intrinsic defects and impurities. One of the main concern in implantation doping and subsequent annealing is the formation of complexes. Dopant - dopant or dopant - defect complexes diminish the activation rate while defect-defect complexes may act as traps, again reducing the free carrier concentration. Identification of the most likely complexes might help designing successful annealing strategies to get rid of these effects. An effective way for this is the comparison of calculated spectroscopic properties of a variety of complexes with experimentally observed centres. Such a study is described here for boron interstitial clusters (BIC) in silicon and intrinsic defects in SiC. The large number of self-interstitials created during implantation mediate the fast transient diffusion of the implanted boron, leading to clustering. The BICs are either electrically inactive or the number of holes they can provide per number of boron atoms is significantly less than one. The standard approach for studying the deactivation of boron due to clustering is to try to elucidate defect properties from comparison of SIMS diffusion profiles and spreading resistance profiles. While the formation and dissolution energies of the possible clusters have been obtained earlier as fitting parameters of kinetic models, in recent years attempts have been made to determine these data a priori from theoretical calculations. However, energy calculations alone are not sufficient to establish the key players in the clustering process of boron. The present paper describes a systematic first principles quantum mechanical study of the characteristic vibration frequencies of a large number of possible configurational isomers of BICs containing up to 4 boron atoms. In binary semiconductors, such as SiC, the early stage of post-implantation annealing ought to lead to the “wrong type” of recombination between self-interstitials and vacancies, creating anti-site defects or their clusters. The carbon anti-site as well as the carbon self-interstitial are low energy mobile defects. As a result various various clusters are expected which might act as traps for free carriers. Electronic and vibrational properties of several such clusters will be presented based on first principles quantum mechanical calculations.

Talk 3.2 (Invited)

Epitaxial 4H-silicon carbide and high-purity/low-doped silicon irradiation-induced point defects

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Because of its intrinsic properties silicon carbide (SiC) is considered as a material of choice for devices operating at high powers, high frequencies and high temperatures. Moreover, SiC is usually associated with detectors for ionising radiation since the material is anticipated to be radiation hard. However, recent results have revealed that the generation of point defects in nitrogen-doped 4H-SiC epitaxial layers during particle irradiation as well as during device processing involving energetic ions (ion implantation and reactive ion etching) is about one order of magnitude higher than in *n*-type silicon at room temperature. Evidence is obtained for deactivation of the nitrogen donors and formation of electrically neutral complexes containing nitrogen.

For fabrication of particle detectors, high-purity and low-doped ($\sim 5 \times 10^{12} \text{ cm}^{-3}$) *n*-type float zone silicon (FZ-Si) is, however, still the material mainly used. In the late 1990's, it was reported that oxygenation of high-purity FZ-Si by diffusion at 1100 – 1200 C for an extended duration ($\sim 50 - 100 \text{ h}$) (DOFZ-Si) substantially increased the radiation hardness of the detectors. We have investigated DOFZ-Si samples after low-dose irradiation with MeV protons and electrons using ordinary deep level transient spectroscopy (DLTS) and Laplace-DLTS. In particular, annealing of the prominent divacancy (V_2) centre is found to give rise to a new double negative acceptor centre with levels close to those of V_2 , but readily resolved by Laplace-DLTS. A close proportionality holds between the loss of V_2 and the growth of the new centre, which is tentatively ascribed to a divacancy-oxygen complex. Further, the annealing kinetics of V_2 in Czochralski-grown, FZ and DOFZ *n*-type samples are compared and the efficiency of interstitial oxygen as trap for migrating V_2 centres is discussed.

Talk 4.1

Recent developments in Laplace deep-level transient spectroscopy

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The talk will focus on the use of LDLTS to probe the effect of the local environment on the binding energies of carriers to defects and impurities. We will present uni-axial stress studies undertaken on defects present in low concentrations often in a narrow near surface region of the semiconductor. This application of stress enables the symmetry of the defect to be determined and in relevant cases the motion of the atomic species under stress and the subsequent relaxation process, *i.e.* diffusion on an atomic scale. The cases of the A centre in silicon (VO) will be considered in this context.

In the case of alloys, Laplace DLTS has the energy resolution to determine the local composition in the immediate vicinity of the impurity. For example, in silicon germanium, whether 0, 1 or 2, *etc.*, germanium atoms exist in the nearest neighbour position. In favourable cases, it is also possible to probe the second nearest neighbour. We use the case of platinum in a silicon germanium alloy to illustrate this.

Recently, we have installed a Laplace DLTS system on a beam line at the University of Aarhus. This has enabled us to examine the defect evolution with annealing following a low temperature implant or irradiation damage. Results on hydrogen in silicon germanium will be presented.

The key advantage of Laplace DLTS over other techniques which have the capability to give structural information is its extremely high sensitivity and ability to examine defects in very thin regions of semiconductor. It is this attribute, combined with the type of result outlined above, which best illustrates the potential of LDLTS for the future. This will be discussed in relation to the possibility of observing transitions associated with individual quantum dots, the behaviour of atom clusters and the use of LDLTS to study the interface between silicon and dielectrics.

Talk 4.2

Electronic structure of divacancy-hydrogen complexes in silicon

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Divacancy-hydrogen complexes (V_2H and V_2H_2) in Si are studied by *ab-initio* modelling using large supercells. Here we pay special attention to their electronic structure, showing that these defects produce deep carrier traps. Calculated electrical gap levels indicate that V_2H_2 is an acceptor, whereas V_2H is amphoteric, with levels close to those of the well known divacancy. Finally our results are compared with the available data from DLTS and EPR experiments.

Talk 4.3 (Invited)

The control and engineering of intrinsic point defects in silicon crystal growth and wafer processing

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Silicon produced for the microelectronic industry is far and away the purest and most perfect crystalline material manufactured today. It is done so routinely and in very large volumes. Many of the advances in integrated circuit manufacturing achieved in recent years would not have been possible without parallel advances in silicon crystal quality and defect engineering. Of particular importance has been the control and engineering of micro-defects and oxygen precipitation. This paper reviews some of the recent advances in the control and engineering of the intrinsic point defects which are centrally important to both classes of defect. Advances in the engineering of intrinsic point defects in both crystal growth and wafer processing has been central to a recent revolution in silicon defect engineering for advanced integrated circuit applications. The installation of initial point defect concentration fields, their redistribution, relaxation, binding with impurities and subsequent reaction are covered. The production of very large micro-defect free “perfect” crystals is discussed along with the creation of controlled vacancy concentration “templates” in thin silicon wafers in order to imprint robust, reproducible and ideal oxygen precipitation profiles for internal gettering applications.

6.2 Tuesday

Talk 5.1 (Invited)

Interactions between misfit dislocations, surface morphology, and point defects during strain relaxation in semiconductor heteroepitaxy

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It is well established that relaxation of lattice-mismatch strain during heteroepitaxial growth can occur both by roughening of the epitaxial layer surface and by injection of misfit dislocations into the heteroepitaxial interface. While reasonably detailed mechanistic understanding has been developed for each of these processes, there has been relatively little quantitative treatment of the competitive or cooperative interactions between them. Further, the effects of point and planar defects upon these phenomena are not well understood.

In this presentation we describe experiments employing real time transmission electron microscope (TEM) observations during annealing and/or growth of metastably strained GeSi/Si heterostructures to elucidate and quantify the kinetic processes governing the evolution of the misfit dislocation array. Ion implantation is also used to study the effects of point defect concentrations upon misfit dislocation nucleation and propagation. Further, in-situ wafer curvature (WC) observations of stress relaxation during heteroepitaxial GeSi/Si growth are coupled with ex-situ atomic force microscopy and TEM measurements to explore and quantify the coupling between dislocation generation and the development of surface morphology. As well as providing significant practical information for design of high quality strained layer semiconductor growth, such cooperative processes can be used as a very sensitive probe for studying the fundamental properties of dislocations in semiconductors.

Our ultimate goal is to incorporate measurements of dislocation kinetics, surface morphology, point defect atmospheres and the resulting cooperative/competitive interactions between these processes into an existing simulator we have developed for predicting misfit dislocation densities generated during $\text{Ge}_x\text{S}_{1-x}/\text{Si}$ growth and annealing sequences. ("Relax", preliminary version available at [1]). This should provide an invaluable tool for predictive growth and processing of strained layer heterostructures, and for exploring fundamental mechanisms of dislocation kinetics.

This work has been funded by the National Science Foundation, and by IBM, and is performed in collaboration with Jennifer Gray, Chi-Chin Wu, and John Bean (University of Virginia); Jerry Floro (Sandia National Laboratories); Eric Stach (Lawrence Berkeley National Laboratories); and Frances Ross (IBM Yorktown Heights Research Laboratories).

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Talk 5.2 (Invited)

Vacancy-impurity complexes in highly n -type Si and SiGe: atomic structure, formation mechanisms, and electrical properties

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The detailed atomic structure of vacancy-impurity complexes in highly n -type Si or SiGe can be experimentally determined by combining positron lifetime and electron momentum density measurements [1]. The monovacancy surrounded by three As atoms is the dominant vacancy-impurity complex in Czochralski Si doped with As up to 10^{20} cm $^{-3}$ [1]. By studying the annealing of V-As pairs formed by electron irradiation, we can show that the V-As $_3$ complexes are formed as a result of the subsequent migrations of V-As and V-As $_2$ [2]. The V-As $_3$ complexes are dominant defects also in highly As-doped MBE grown Si, where they exist at concentrations relevant to the electrical deactivation of doping [3]. Larger complexes, identified as V $_2$ -As $_5$, are also present at high concentrations. The V-As $_3$ and as V $_2$ -As $_5$ defects are removed by annealing at 800 and 900 C, respectively. However, they are likely to reconstruct during the cooling down by migrations of V-As and V-As $_2$, as demonstrated in electron irradiated material [2]. The rapid thermal annealing is shown to lead to smallest concentrations of V-As $_3$ and as V $_2$ -As $_5$, most likely due to the limited time available for the migration processes.

In P-doped strained Si $_{0.96}$ Ge $_{0.04}$ layers grown on Si the vacancy-phosphorus pair is identified as the dominant vacancy defect after 2 MeV proton irradiation at room temperature. After annealing at 150 C the V-P pairs convert to V-P-Ge complexes consisting of a vacancy surrounded by P and Ge atoms. We conclude that the V-P-Ge complex is formed when a migrating V-P pair encounters a Ge atom. The V-P-Ge complex anneals at 200 C, corresponding to about 0.1 – 0.2 eV higher binding energy than that of the V-P pair. By *ab-initio* calculations we reproduce this value and conclude that the V-P pair in SiGe becomes more stable when neighbored by a Ge atom [4].

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Talk 6.1 (Invited)

Ion implantation and ion-beam-induced defect formation in Si and SiC studied by atomistic computer simulations

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Ion implantation is one of the major techniques to introduce dopants into Si and SiC in a controlled manner. However, ion irradiation produces defects which prevent their electrical activation. Therefore, subsequent annealing is necessary in order to restore the crystallinity and to obtain dopant activation. The precise knowledge of the spatial distribution of the implanted ions and the radiation damage as well as the understanding of the nature of ion-beam-induced defects are important prerequisites for further improvements in the technology of ion implantation doping. Besides experimental investigations, atomistic computer simulations play an important role to achieve progress in this field. Simulations based on the binary collision approximation (BCA) are employed to determine the depth profile of implanted ions and atomic displacements. The influence of various implantation parameters like energy, direction of ion incidence, dose, dose rate and temperature is considered. A phenomenological model is used to treat the dependence of channelling effects on damage buildup and dynamic annealing during ion bombardment. The implantation profiles determined by the simulations show a good agreement with available experimental data. On the other hand, BCA simulations are limited to the treatment of ballistic processes. They do not yield details of the (meta)stable defect structure formed in subsequent fast relaxation processes. In order to obtain such information, a combined simulation method is employed. Processes in the collision cascade with energy transfers above 100 eV are treated by BCA simulations. Classical molecular dynamics (MD) calculations are applied to consider processes in certain parts of the cascade which start with energy transfers less than 100 eV. Detailed investigations are performed to study the temporal evolution of the defect structure, and to determine the damage morphology obtained after the fast relaxation is finished. The influence of nuclear energy deposition and target temperature is discussed. The combination of BCA and MD methods allows the effective calculation of the total number and the depth distribution of different defect species (*e.g.* isolated vacancies and self-interstitials as well as more complex defects) formed on average per incident ion. The results obtained allow a microscopic interpretation of the phenomenological model employed in conventional BCA simulations to describe the enhanced dechannelling of implanted ions due to damage buildup during implantation. In particular the explicit dependence on the ion mass can be explained. Furthermore, the procedure yields more realistic initial conditions for the simulation of post-implantation annealing than hitherto used.

Talk 7.1 (Invited)

Quantitative high-resolution electron microscopy of defects and interfaces in silicon-based systems

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Extended defects in silicon as well as hetero-interfaces play an important role in modern silicon-based microelectronics and the rapidly growing field of solar cell production from crystalline silicon materials. Modern techniques of transmission electron microscopy allow studying the structure and chemistry of defects and interfaces on a quasi-atomic level and hence providing insight into the underlying physics of their formation and properties.

The first part of this contribution summarises electron microscopy studies on the formation of metal silicide precipitates in crystalline silicon materials containing extended defects (*e.g.* dislocations), or subjected to the in-diffusion of a high concentration of phosphorus. For defect-free silicon materials it is well known that nickel precipitates as thin platelets consisting of NiSi_2 that are bounded by a dislocation with a Burgers vector $b = \frac{a}{4}$. Such dislocations serve as a reaction channel which allows fast incorporation of nickel atoms during growth. In dislocated materials, however, polyhedral precipitates are observed which strongly modify the dislocation geometry. This indicates that the pre-existing dislocations are an integral part of precipitate growth rather than merely a nucleation site. In particular, a special NiSi_2 -related precipitate structure is obtained exclusively at dislocations.

Phosphorus-diffusion gettering (PDG) is widely used in solar cell fabrication for the formation of *pn*-junctions and the simultaneous cleaning of the wafers by the redistribution of metal impurities into the highly P-doped region. Besides the increased solubility of substitutional metal impurities due to electronic effects and pairing with P atoms, silicide formation may play an important role for the gettering process. For Pt in silicon it will be shown that a substantial part of gettered Pt atoms (measured by *e.g.* secondary ion mass spectroscopy) are due to PtSi precipitates which form during P diffusion either near SiP precipitates or at the interface between silicon and a phosphorus silica glass.

In the second part, high-resolution electron microscopy is used to determine the structure of interfaces between crystalline and amorphous materials. A recently developed technique is used to extract the two-dimensional density of atoms in amorphous solids near crystalline substrates from focal series either by quantitative image matching or by exit wave function restoration. As an example, amorphous germanium is deposited by room-temperature molecular beam epitaxy on hydrogen-passivated unreconstructed (111) silicon surfaces. The resulting interface is characterised by (i) a width of about 1.2 nm; (ii) a bond angle distribution slightly smaller than for bulk amorphous germanium; and (iii) atomic positions compatible with tetragonally distorted germanium on silicon.

Talk 7.2 (Invited)

DLTS of defects introduced in Si (and SiGe) by low energy (< 5 keV) particles

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Ion implantation and plasma processing techniques are routinely used for the fabrication of semiconductor devices. In particular, these techniques employ low-energy ions, which modify the electrical and optical properties of the semiconductor material, and, consequently, of the devices that are fabricated thereon, by creating defects in the semiconductor lattice. It is, therefore, of both technological and scientific interests to investigate the optical and electrical properties of defects created in low-energy ion bombarded semiconductors. In this paper, we review our investigations of the electrical characterisation of defects created in Si by low-energy noble gas ions (He, Ne, and Ar) and hydrogen ions using deep level transient spectroscopy (DLTS). Noble gas ions are of great interests since they are used in plasma processes, and of their ability to form a class of noble-gas-ion-related defects by interacting with the intrinsic I1 defect in Si. On the other hand, hydrogen possesses the peculiar ability to passivate electrically active defects and dopants. The properties of defects introduced in $\text{Si}_{1-x}\text{Ge}_x$ during ion etching and electron-beam evaporation of metal contacts are also reviewed.

Talk 8.1 (Invited)

n-Type doping of diamond and the device applications

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n-Type diamond thin films were successfully formed by optimising the growth condition of chemical vapour deposited diamond under phosphorus doping to obtain better crystalline perfection. Phosphorus atoms can be incorporated in 111 oriented surfaces during the growth and the concentration can be controlled within the range of 10^{17} to $\sim 5 \times 10^{19} \text{ cm}^{-3}$. Phosphorus forms a donor level at 0.6 eV below the conduction band minimum that is confirmed by Hall measurements, photocurrent and infrared absorption (FTIR). The maximum electron mobility is $400 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ at room temperature obtained from lightly doped samples ($3 \times 10^{17} \text{ cm}^{-3}$). Cathodoluminescence of phosphorus doped films show strong bound exciton luminescence at 5.19 eV at low temperatures and free exciton luminescence (5.27 eV) can be observed even at room temperature. As a next step, we have studied *pn*-junction of diamond by stacking boron doped *p*-type layers and phosphorus doped *n*-type layers. The *pn*-junction has shown good rectification characteristics with the ratio of 10^{10} at ± 10 V. The diode characteristics and the behaviour of *pn*-junction interface have been characterised by temperature dependent IV and CV measurements. By forward bias operation, the diode shows ultraviolet light emission at 235 nm that attributes free exciton luminescence. The diode also shows photoelectric response against ultraviolet light with the wavelength shorter than 225 nm that corresponds the band-gap of diamond. It is expected these characteristics of diamond *pn*-junction will be applied in the next generation of opto-electrical devices.

Talk 8.2

Electrical behaviour of antimony implants in silicon at large tilt angle

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A dose of 5.0×10^{14} Sb⁺ was implanted with energy of 70 keV at different tilt angle (0, 15, 30, 45, 60 degrees) in crystalline Si <100> fixing the twist angle at zero degrees. Secondary Ion Mass Spectroscopy (SIMS) was performed to determine the retain dose before and after annealing. After implantation the samples were annealed in the range 700°C for 30 seconds in flowing nitrogen. Van der Pauw measurements and Hall effect were made to obtain values of the sheet resistance (RS), Hall mobility (mH) and sheet carrier concentration (NS) as a function of the tilt angle. Differential Hall Measurements were done to evaluate the electrical profile of Sb at 0 and 60 degrees. Rutherford backscattering was performed to study the damage as a function of the tilt angle.

The results show that the sheet resistance, the sheet carrier concentration and the damage are a function of the tilt angle. High electrical activation combined with a shallow junction depth was also found.

6.3 Wednesday

Talk 9.1 (Invited)

Vacancies and interstitials in group-IV semiconductors: what has been learned from EPR studies

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Our understanding of the intrinsic defects - vacancies and interstitials - and their interactions with other defects in the group-IV elemental semiconductor silicon has advanced greatly since 1959, when successful EPR identifications were first reported. The major part of this talk will be to review this progress and to summarise what we think we currently know. Recently there have also been remarkable advances in our understanding of the corresponding defects in diamond, spearheaded again from EPR studies. There are strong similarities with what has been learned in silicon, but there are important differences as well. These will also be briefly discussed.

Talk 9.2 (Invited)

Single crystal microwave plasma deposited CVD diamond

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The desire for electronic devices with higher power throughput, wider frequency bandwidth and higher operational temperatures is driving research and development of new semiconductors. One such area is wide band gap materials. Diamond is extreme in this group of materials that includes SiC, ZnO and GaN, having a direct band gap of 7.5 eV, an indirect gap of 5.5 eV and a room temperature thermal conductivity in excess of $2000 \text{ Wm}^{-1}\text{K}^{-1}$. Diamond electronic devices, such as power diodes and high-frequency field effect transistors, are expected to deliver outstanding performance due to the material's excellent intrinsic properties such as high carrier mobilities and high breakdown field. However, the development of diamond electronics has been hampered by several problems including a lack of shallow dopants, heteroepitaxy as a route to large area single crystal growth, low crystal quality and poor consistency of synthetic material.

We will report recent results on the fabrication and characterisation of device quality single crystal CVD diamond [1]. These results show, not only that material can be fabricated with performance that matches the very best natural diamond, but also that key properties such as the mobility and lifetime of the carriers, far exceed expectations. It has been lack of material quality that has limited diamond's progress in the past, making it a minority player against SiC and GaN. However, the figures of merit now demonstrated for diamond are so extreme that the material should be re-examined as an ideal material for the most demanding power electronics and switching applications.

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Talk 10.1 (Invited)

Single hydrogen defects and hydrogen dimers in Si

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The behaviour of hydrogen in many semiconductors is still unexplored but is best understood in Si. DLTS measurements show that isolated H can be a donor which diffuses rapidly at low temperatures and is subsequently trapped by other defects. Several defects consisting of a single hydrogen atom and another impurity are known such as complexes with carbon or oxygen. These impurities have been thought to simply perturb the electronic structure of H. However, recent combined Laplace DLTS and theoretical studies, to be described, have shown that in the case of carbon this is not the case and we find that the electrical properties of carbon-hydrogen pairs are surprisingly different from those of isolated H [1].

One possible product of the anneal of H is a hydrogen dimer which as a molecule has been found theoretically to be exceptionally stable although evidence for its existence has been hard to come by. The recent observations by infra-red absorption of modes attributed to hydrogen molecules has led to a considerable debate. Here we discuss the origin for this activity and investigate in detail the possible IR-transitions.

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Talk 11.1 (Invited)

Optical properties of amorphous carbons and amorphous carbon nitrides

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In this presentation, we will review the current assessment about the density of electronic states (DOS) in amorphous carbons, either hydrogenated (a-C:H) or not (a-C) and discuss its role in determining the optical constants (refractive indexes $n(E)$, extinction coefficients $k(E)$, real and imaginary parts of the complex dielectric constant, $\epsilon_1(E) + i \cdot \epsilon_2(E)$) in the visible-near UV photon energy range ($E = 1 - 5$ eV). a-C(:H) films differ from amorphous silicon (a-Si(:H)) ones as they involve a significant contribution of π -electrons, arising from the sp^2 (and, possibly, sp^1) hybridised carbon sites.

We will discuss how the density of π -states is affected by the organisation of the sp^2 carbon sites in nano-clusters with different electronic structure and gap states, and by the statistical distribution of nano-clusters of different shape and size and the indirect effect of the sp^3 (diamond-like) backbone in determining the rigidity and the amount of disorder. In a-C(:H) parameters such as the Tauc optical gap and the Urbach energy bear only a conventional meaning, since they are not only controlled by tail properties (such as in a-Si:H) or by the shape and size of a typical, isolated, sp^2 cluster (such as in an hypothetical 'cluster model' of a-C:H). The optical properties of a-C:H can be better understood in terms of mutual interdependency relationships between causally related optical constants (*e.g.* $n(E)$ and $k(E)$, or $\epsilon_1(E)$ and $\epsilon_2(E)$) of different films, occurring at each given photon energy E [1].

Nitrogen addition in amorphous carbons not only leads to larger amounts of π -electrons, but it is often accompanied by strongly localised lone-pair (LP) electrons. LP states are stabilised in energy by the local structure of amorphous materials. Thus nitrogen not only affects the density and the nature of the states determining the optical properties but also their spatial extension and it may introduce strong changes in the DOS [2]. We will address the very important role of lone-pairs and LP- π mixing in determining the DOS and the interdependency relationships between the optical constants in amorphous carbon nitrides, to be compared with the corresponding relationships between $\epsilon_1(E)$ and $\epsilon_2(E)$ and existing in non-nitrogenated amorphous carbons. A picture of the DOS of amorphous carbon nitrides in the visible-near UV energy range will be given.

Finally we will discuss some applications of the above mentioned concepts to the study of the polarisability of the electronic states and the photoluminescence of amorphous carbons, either nitrogenated or not.

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Talk 11.2

Multi-wavelength laser Raman and x-ray photoelectron spectroscopy of phosphorus-containing DLC films

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DLC films deposited on Si and quartz were produced by pulsed laser ablation of graphite/phosphorus targets made with varying phosphorus percentages. Deposition was carried out in vacuum ($\sim 1 \times 10^{-5}$ Torr) and at a range of substrate temperatures ($T_{\text{sub}} = 25 - 400$ °C). Laser Raman spectroscopy was performed on the as-deposited films using 325, 514.5 and 785 nm laser wavelengths, and the intensity of the D and G peaks ($I(\text{D})$ and $I(\text{G})$, respectively) was measured as a function of temperature. Nanocrystalline graphitisation was seen to occur at higher T_{sub} , which is consistent with results seen previously for undoped DLC and CN_x films. In the case of P-containing DLC films deposited at lower T_{sub} , the $I(\text{D})/I(\text{G})$ ratio is higher than for carbon films deposited in vacuum. An initial estimation of the sp^3 content can be made from the G-peak position combined with the $I(\text{D})/I(\text{G})$ value which agrees with the deconvolution of the C 1s peak from XPS analysis. XPS results show a decrease in P incorporation in the DLC films with increasing substrate temperature ($\sim 6\%$ at $T_{\text{sub}} = 25$ °C, $\sim 1\%$ at $T_{\text{sub}} = 400$ °C). P-containing DLC films deposited on undoped Si were tested for room temperature conductivity.

Keywords: DLC, amorphous carbon, laser ablation, phosphorus

Talk 11.3

The dissociation of dislocations in diamond

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The dissociation of 60 degree and screw dislocations in diamond is modelled in an approach combining isotropic elasticity theory with *ab-initio*-based tight-binding total energy calculations.

Both dislocations are found to dissociate with a substantial lowering of their line energies. For the 60 degree dislocation, however, an energy barrier to dissociation is found. These results agree well with recent high resolution electron microscopy investigations.

Further, the glide motion of Shockley partials is discussed, in terms of a process involving the thermal formation and subsequent migration of kinks along the dislocation line.

Talk 12.1

The vacancy-nitrogen-hydrogen complex in diamond: a potential deep centre in CVD material

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It is known that complexes of nitrogen and lattice vacancies are grown into CVD diamond despite the theoretically high formation energy. This defect is a potential trap for hydrogen which is present in the growth gas mixture. A V–N–H complex might give rise to infrared, optical, magnetic and electrical signatures, with some similarities being drawn with the hydrogen-free defect. We present the results of local density functional calculations regarding the structure and properties of V–N and V–N–H defects.

Talk 12.2

Mapping the energy levels of the self-interstitial in diamond

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Keywords: diamond, self-interstitial, optical absorption, uniaxial stress

Diamond is the only group-IV semiconductor in which the self-interstitial has been identified [1]. Electron paramagnetic resonance studies show that it has a $\langle 001 \rangle$ split-interstitial structure, but those studies can only probe the electronic structure and determine the position of one excited state of the centre. The molecular structure in the ground state is controversial: distortions are predicted theoretically by total-energy calculations [2], whereas optical data have been fitted using a vibronic-coupling model which superficially produces a similar adiabatic potential surface but from a quite different origin [3].

Here we combine uniaxial stress perturbations, isotope effects and optical measurements to map, definitively, the lower energy states involved in the optical transitions. We report the presence of two new excited states, 1697 and 1865 meV above the ground state, which do not fit into existing energy-level schemes for the centre. Consequently we have five low-lying electronic states at the centre, in contrast to the four predicted theoretically [2]. The centre is very unusual in having almost zero first-order response to uniaxial stress perturbations almost all the perturbation comes from the coupling of states. These interactions allow us to define the symmetry of all the states. The strengths of the interactions are consistent with a structure in which the neighbouring carbon atoms distort dynamically from the ideal sites through their vibronic coupling, with the ideal D_{2d} symmetry observed as a time average.

References:

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Talk 12.3 (Invited)

Plasma processes of interest to the growth of ultrananocrystalline diamond and to etching of silicon semiconductors

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Plasma processes and plasma chemistries determine the fact that argon microwave discharges containing small amounts of CH_4 lead to the growth of ultrananocrystalline diamond (UNCD) films, but if the carbon containing molecule is CF_4 , etching of silicon semiconductors occurs instead. For UNCD synthesis, the growth species is carbon dimer, C_2 , while etching occurs largely as a result of reactions of fluorine atoms, F , with silicon to form SiF_4 . The details of the production processes of these reactive species are still being elucidated. It is clearly important to achieve a sound fundamental understanding of mechanisms so as to be able to optimise growth rates of diamond on the one hand and etch rates of silicon, on the other.

It turns out that important initial processes for the creation of both C_2 and F are charge-transfer (CT) and Penning ionisation of Ar^+ and Ar^* respectively with hydrocarbons in the case of diamond and with halocarbons in the case of silicon etching. Thermal energy CT and Penning ionisation reactions of noble gas ions with simple molecules of interest will be discussed. A scheme will be proposed for the efficient production of C_2 both from C_{60} and from CH_4 making use of dissociative electron recombination reactions.

Characterisation, properties and applications of UNCD films will be briefly reviewed.

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6.4 Thursday

Talk 13.1 (Invited)

Diamond MEMS

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Diamond is a multi-functional material with extraordinary properties for extreme applications. It can combine the properties of ceramics, refractory metals (when heavily doped) and semiconductors and has indeed been investigated for a variety of basic sensor and actuator devices. However it is a difficult material to produce in semiconductor quality and in sizes suitable for microelectronic manufacturing. In addition, a surface micromachining technology for three dimensional structures is needed. Essential elements here are a sacrificial layer technology, mechanical stress control, doping and increasingly also surface preparation.

We found that the extreme properties are especially suited for heavy duty actuators applying the thermal and electrostatic actuation principle. Discussed will be (1) the diamond inkjet and aquajet using a diamond spot heater as active element, (2) the all-diamond micro switch realised using electrostatic actuation and the thermal bi-metal effect. The later allows bi-stable switching. This principle has then been used (3) to drive an all-diamond membrane pump. The sensor application discussed is (4) that of an electrochemical probe. Diamond is a largely electrochemically inactive material, which still can be surface conductive. Here some key issues concerning its surface activity depending on termination are still in debate. Thus, here diamond is still a material for electro-chemistry and bio-chemistry with its full potential not yet accessed.

Diamond MEMS structures are usually realised on polycrystalline material mostly deposited on Si. As a consequence the ideal materials parameters are still compromised. Recently first single crystal quasi-substrates have become available and have been used for electronic (FET) devices. Their size make these substrates already interesting as MEMS substrate, promising further improved performance as well as integration with electronics.

Talk 13.2 (Invited)

Recent developments in diamond detectors

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Chemical Vapour Deposition (CVD) diamond has been discussed extensively as an alternate sensor material for use very close to the interaction region of the LHC and other machines where extreme radiation conditions exist. During the last seven years diamond detectors have been manufactured and tested with LHC electronics toward the end of creating a device usable by experiments. Recently, a new form of CVD diamond has been developed: single crystal CVD (scCVD) diamond which resolves many if not all of the issues associated with polycrystalline CVD (pCVD) material. A historical approach of this work will be presented including the most recent status and results.

Talk 14.1

Growth and characterisation of epitaxial and polycrystalline *n*-type CVD diamond films

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As is generally known, the intrinsic properties of diamond surpass those of all classical semiconductors like Si and Ge. However, the use of diamond in all kinds of semiconductor applications has always been hindered by the lack of suitable *n*-type material. Although the realisation of phosphorus-doped *n*-type CVD diamond was a great breakthrough in diamond research, the limitation in size and availability of suitable substrates have slowed down the evolution of diamond devices.

With the recent progress in high quality *n*-type diamond films the reduction of the P concentration is possible while keeping the active dopant character and thus achieving high mobilities. These layers are very suitable for a study of the electronic fine structure in P-doped diamond, which was not completely resolvable before. In this work we have studied diamond samples with a P-concentration as low as 10^{17} cm^{-3} , using FTPS spectroscopy. The resulting fine structure in these layers confirms our first tentative results.

Finally, due to a recent breakthrough at IMO, large area diamond devices have come a step closer. By using undoped CVD diamond films as substrates, we were able to grow the first polycrystalline phosphorus-doped *n*-type films. The *n*-type conductivity was confirmed by Hall-measurements and CL-experiments showed the presence of strong P-bonded excitons. Photocurrent measurements on these layers also confirmed the successful incorporation of P as the PC-spectra showed a similar oscillatory photoconductivity and PTIS maxima as in the homoepitaxial single crystal films.

To demonstrate the potential of polycrystalline layers in the use for devices, a 2 μm -thin P-doped film was grown on a 100 μm -thick B-doped CVD diamond substrate, leading to the first polycrystalline diamond *pn*-junction. The best junctions showed a rectification over 7 decades in magnitude and a diode factor of 2.9 at RT.

7 Posters

7.1 Silicon-related (Monday)

Poster M-1

Laplace deep level transient spectroscopy of hydrogen interactions with ion implantation-induced defects in silicon

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We have investigated the difference between proton or electron irradiated silicon, and ion-implanted silicon using high resolution Laplace Deep Level Transient Spectroscopy (LDLTS). CZ silicon was either irradiated with high energy protons or electrons, to ensure that the irradiating particles passed through the samples, or implanted with very low doses of ions. The ions used in the study were silicon, germanium and erbium. Doses were in the region of 10^{10} cm⁻² to minimise deep state assisted carrier removal, and the implantation depths were of the order of 1 – 2 microns. Hydrogen was introduced into the samples by either wet chemical etching or by inserting the samples into a hydrogen plasma.

When hydrogen is introduced into the proton or electron irradiated silicon, the vacancy-oxygen centre (VO) concentration reduces, and a level due to VOH appears, as expected. When H is introduced into the ion implanted samples, the appearance of VOH depends upon the implanted ion mass. As the mass increases the concentration of VOH reduces until it is not apparent when very heavy ions are implanted. We show how the use of LDLTS has enabled us to establish whether or not VOH is present, and elucidate the differences in the deep level population when silicon is irradiated with heavy particles.

Poster M-2

Oxygen-related vacancy-type defects in ion-implanted silicon

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Defects in Czochralski silicon samples implanted to a dose of $5 \times 10^{15} \text{ cm}^{-2}$ with 0.5 MeV O and to a dose of 10^{16} cm^{-2} with 1 MeV Si have been studied by beam-based positron annihilation spectroscopy. Information on vacancy-type defects has been gained by Doppler broadening spectroscopy and by a novel full-spectrum fitting procedure, the latter being particularly sensitive to buried vacancy clusters. It is found that divacancies (V_2) are the dominant vacancy-type defects in both as-implanted samples. The evolution of V_2 to vacancy-oxygen complexes loses out to the recombination of vacancies with interstitials at 400 °C in the Si-implanted sample. The same is not seen until 500 °C in the O-implanted sample, because the higher oxygen concentration makes the formation of oxygen-related vacancy-type defects compete better against recombination. The annealing of vacancies starts from the region beyond the ion-projected range (R_p) resulting from the injection of interstitials from the end of range (EOR). Vacancy-dominated vacancy-oxygen complexes, V_mO_n ($m > n$), are formed in the shallow region the most effectively at 700 °C in both kinds of implantation. Oxygen-dominant vacancy-oxygen complexes, V_xO_y ($x < y$), are produced in the annealing near $-R_p$, although the formation mechanisms are different in the two kinds of implantation. The diffusion of implanted Si reduces m and that of implanted O increases n in V_mO_n at 800 °C. It is believed that all oxygen-related vacancy-type defects begin to dissociate at 950 °C. The dissociation of V_xO_y can facilitate the formation of oxygen clusters. It is supposed that oxygen precipitates are formed just before R_p in O-implanted silicon after annealing at 1100 °C.

Poster M-3

Recombination-generation states at silicon oxide and oxynitride interfaces after hydrogen and deuterium incorporation

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The effect of hydrogen/deuterium incorporation in Si/SiO₂ and Si/SiO_xN_y on interface defects states has been studied. Incorporation of hydrogen/deuterium took place by remote plasma exposure and high temperature in-diffusion. We report a significant improvement of the Si/SiO_xN_y interface state density after plasma treatments. In the case of the Si/SiO₂ interface the plasma treatments proved to be benign in relation to the fixed charge density but, in contrast to our Si/SiO_xN_y case, rather detrimental regarding interface state density. On the other hand high temperature in-diffusion of hydrogen in the Si/SiO₂ interface was found to have no effect on fixed charge density but in contrast to plasma treatments proved to be a very effective method for reducing interface state densities.

Poster M-4

Alloy dependence of photoluminescence bands in SiGe alloys

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We report high-resolution photoluminescence (PL) spectra of dilute Czochralski (CZ) SiGe (< 5.5 at. % Ge) samples that have been irradiated at room temperature with 4 MeV electrons. The prominent radiation damage centres in CZ Si, C_i-C_s and C_i-O_i , commonly referred to as the G- and C- centres respectively, are also produced in dilute SiGe after room temperature electron irradiation. The energy of the zero-phonon C-line moves linearly to increasing energy with increasing Ge concentration, with a shift rate $dE/dx = +330$ meV (for $0 < x < 0.055$), while the energy of the G-line is essentially independent of the Ge content. These findings demonstrate that the defect levels are not pinned to the band edges, as also reported for the C_i and C_i-C_s centres [1]. The PL transition for the C line occurs from a state trapped near the conduction band to the deep level of $C_i-O_i^+$ that is observed by DLTS measurements, and which approaches the valence band with increasing x [2] however, this model would predict twice the shift rate for the C line that is observed.

With increasing x , the total vibronic band of the C_i-O_i centre is rapidly broadened. The shape can be understood very accurately by using an artificially broadened spectrum taken in crystalline Si data, showing that this broadening is predominantly due to composite disorder fluctuations in the alloy rather than discrete perturbations from nearby Ge atoms.

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Poster M-5

A deep level transient spectroscopy study of the negative bias temperature instability in metal insulator semiconductor structures

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Negative bias temperature instability (NBTI) is a major problem in the reliability of MOS and MIS devices. It is thought to be associated with point defect reactions and is often linked with hydrogen. We have conducted deep level transient spectroscopy (DLTS) measurements on silicon oxynitride MIS capacitors prior to and immediately after subjecting these devices to low field (1 MV cm^{-1}) stressing at $230 \text{ }^\circ\text{C}$ for 10 minutes. We report on significant degradation of the minority carrier generation lifetime as well as on a change in the dominant mechanism supplying minority carriers at the interface following the NBTI experiment. Moreover, we observed that the DLTS inversion layer peak progressively relaxes back to its initial (*i.e.* prior to the NBTI experiment) position, after a substantial time has elapsed. We propose a model that considers generation and motion of hydrogen-related species within the MIS structures in order to elucidate the aforementioned degradation and relaxation phenomena. Our experimental data support the belief that electrochemical reactions at the interface and/or diffusion of hydrogen-related species play a key role in detrimental NBTI effects.

Poster M-6

Neutron irradiation induced defects in silicon

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We present a study of defects states occurring in *n*-type (110) Czochralski-grown silicon after a high dose ($1 \times 10^{16} \text{ cm}^{-2}$) irradiation with fast neutrons and one hour isochronal annealing in N_2 from 500 °C to 700 °C with 50 °C steps. Deep-level transient spectroscopy (DLTS) measurements were used to identify the electrically active defects. We have observed several defects after annealing at 500 °C. Two of them have activation energies of $\sim 0.36 \text{ eV}$ with DLTS peaks which are wider than those typical of point defects. We associate these peaks with small interstitial clusters. We have observed that upon annealing at 600 °C the total defect concentration is very much reduced and all defects anneal out at 650 °C. However after an additional anneal at 700 °C a very wide DLTS peak is observed. We believe that this peak is associated with $\{311\}$ rod-like extended defects.

Poster M-7

Phase separation of amorphous $\text{SiO}_x/\text{SiO}_2$ superlattices to orderly-arranged Si nanocrystals

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The preparation of orderly-arranged Si quantum dots using a superlattice approach is presented. The different stages of phase separation and crystallisation are studied in detail by infrared absorption (IR), photoluminescence (PL), and transmission electron microscopy (TEM) as a function of annealing temperature from 300 to 1100 °C [1]. IR spectra show a continuous shift of the Si–O–Si asymmetric stretching mode to 1080 cm^{-1} which is a signature of Si and SiO_2 phase separation. Three PL bands are distinguished and correspond to the three stages of phase separation. A band centred at 560 nm is present in as-prepared samples and vanishes for annealing above 700 °C, which is clearly correlated to defects. The second band shifting from 760 nm to 890 nm is detected for annealing temperatures between 500 °C and 900 °C. A strong red luminescence due to quantum confinement is observed for annealing above 900 °C. Our results indicate that the different and seemingly contradictory PL observations in literature could originate from different states of network reorganisation during the phase separation and crystallisation processes. The origin of the different IR and PL bands, and the temperature dependence of PL, are discussed in comparison with bulk crystalline Si.

References:

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Poster M-8

High depth resolution profiling of the evolution and annealing of damage and the dopant redistribution of ultra shallow As implants in Si

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The relationship between ultra shallow damage formation / annealing and As profile redistribution has been investigated. Low energy As implants in Si were carried out at 2.5 keV to doses between $3 \times 10^{13} \text{ cm}^{-2}$ and $2 \times 10^{15} \text{ cm}^{-2}$ at room temperature. High depth resolution medium energy ion scattering (MEIS) was used to characterise the damage build up and As profiles as a function of implant dose and anneal temperature. Secondary ion mass spectrometry (SIMS) was also used to study the As profiles. The accumulation of the damage as a function of As dose does not follow the expected energy deposition function but proceeds from the surface, where it initially builds up as a 4 nm wide amorphous layer, inward with increasing dose. The observations are explained in terms of a mechanism involving interstitial migration to the oxide/Si interface and the subsequent layer-by-layer growth of the amorphous layer. For doses $\geq 4 \times 10^{14} \text{ cm}^{-2}$ arsenic depth profiles agreed well with TRIM calculations. However for lower doses As was observed to have a profile nearer to the surface, due to trapping in the narrow surface damaged layer, where it appears more easily accommodated. A control experiment involving low dose As implants into pre-amorphised Si did not show this anomalous behaviour.

Samples were annealed to temperatures between 600 and 1050 °C. Following epitaxial regrowth at 700 °C, MEIS showed that approximately 50% of the As has moved into substitutional sites, consistent with activation and / or the reported formation of inactive As_nV clusters ($n \leq 4$), while the remainder had segregated to and become trapped in a ≤ 1 nm wide layer clearly located on the Si side of the oxide / Si interface. Ultra low energy SIMS studies at normal incidence is able to resolve these ultra shallow peaks, including the As pileup following epitaxial regrowth. SIMS also confirmed that As retention was complete during dose build up and annealing.

Poster M-9

Hydrogen molecules in 4H-SiC and GaN

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We present the results of theoretical calculations of the structure, diffusion and rotational energies, and the ro-vibrational modes of the molecule in hexagonal 4H-SiC and 2H-GaN. The molecule is stable and aligned along the *c*-axis. In both materials, its rotational barrier is sufficiently large that ortho- and para- forms have almost degenerate ro-vibrational modes. The origin of two modes at 4909 and 4110 cm⁻¹ attributed to molecules observed by multi-transmission FTIR experiments on Mg-doped insulating GaN grown by OMVPE is discussed [1].

References:

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Poster M-10

Oxygen-related radiation-induced defects in SiGe alloys

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Electronic properties of the vacancy-oxygen (V-O) complex and a pair of interstitial oxygen and carbon atoms (C_i-O_i) in unstrained $Si_{1-x}Ge_x$ crystals ($0 < x < 0.06$) have been studied by means of capacitance transient techniques. The SiGe crystals were grown by the Czochralski method and were doped with either phosphorus or boron during growth. The V-O and C_i-O_i centres were introduced into the crystals by room-temperature irradiation with 4 MeV electrons or with gamma-rays from a Co source.

The enthalpy of electron ionisation for the single acceptor level of the V-O centre relative to the conduction band edge, $H(c-VO)$, was found to increase with a rate $dH(c-VO)/dx = 0.56$ eV upon increase in Ge content. The enthalpy of hole ionisation for the single donor level of the C_i-O_i centre relative to the valence band edge, $H(p-C_iO_i)$, was found to decrease with a rate $dH(v-C_iO_i)/dx = -0.96$ eV upon increase in Ge content. For both the V-O- and C_i-O_i -related levels no significant changes in the values of electron (hole) capture cross section and entropy of ionisation with the changes in Ge content were observed.

Taking into account changes in the SiGe alloy band gap with the changes in chemical composition, we have calculated the rate of movement of the C_i-O_i -related donor level with respect to the conduction band edge upon the changes in Ge content, $dH(c-C_iO_i)/dx = 0.55$ eV. The obtained value is very close to that for the acceptor level of the V-O complex. Both the V-O acceptor and C_i-O_i donor levels are not pinned to the conduction band edge or to the valence band edge.

Possible reasons for the observed changes in electronic properties of the V-O and C_i-O_i complexes in $Si_{1-x}Ge_x$ crystals are discussed. It is argued that the value of enthalpy of V-O ionisation is very sensitive to the lattice parameter or Si-Si bond length, the larger these parameters the bigger the enthalpy of the ionisation.

Poster M-11

Divacancy annealing in silicon: A Laplace DLTS study

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Annihilation of divacancies (V_2) upon isochronal annealing has been studied in *n*-type Czochralski-grown (Cz) and float-zone-grown (FZ) Si crystals by means of high-resolution Laplace DLTS technique. Divacancies were introduced into the crystals by irradiation with 4 MeV electrons. Changes in the concentration of both the V_2 -related double and single acceptor levels were monitored.

Temperature ranges of the divacancy disappearance were found to be 225 – 275 °C in Cz-Si crystals and 300 – 350 °C in FZ-Si crystals upon 30-min. isochronal annealing. These results are consistent with those obtained previously by Watkins and Corbett [1]. Simultaneously with the V_2 disappearance in Cz-Si crystals a correlated appearance of two electron traps with activation energies for electron emission 0.23 eV $E(0.23)$ and 0.47 eV $E(0.47)$ was observed. It is argued that the main mechanism of the V_2 disappearance in Cz-Si crystals is related to the interaction of mobile divacancies with interstitial oxygen atoms. This interaction results in the formation of V_2O centres, which are responsible for the infrared absorption band at 833.4 cm^{-1} [2] and the $E(0.23)$ and $E(0.47)$ traps. Electronic properties of the V_2O complex were found to be very similar to those of V_2 but energy levels of the two defects could easily be separated using Laplace DLTS.

In FZ-Si crystals, a few electron traps appeared simultaneously with the V_2 annihilation. Small concentration of these traps compared to the V_2 concentration before annealing prevented their reliable identification.

Experimental results on the V_2 annihilation in Si crystals containing hydrogen are also discussed.

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Poster M-12

Ion implantation effects in silicon with high carbon content

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Keywords: silicon, carbon impurity, implantation, photoluminescence

Ion implantation is a vitally important tool for doping in the manufacture of silicon semiconductor devices. Its main drawback is that ion beam also introduces damages and related point defects. During annealing, these defects can agglomerate to form cluster and eventually extended defects, and are also responsible for transient enhanced diffusion (TED). Carbon impurity has been found to suppress TED by trapping and storing the excess interstitials. Edge-defined film-fed growth (EFG) silicon ribbon samples containing a high carbon concentration ($[C] \sim 2 \times 10^{18} \text{ cm}^{-3}$) were used in this study. They were implanted with 5.6 MeV Si ions in the amorphisation dose range ($10^{13} - 10^{15} \text{ cm}^{-2}$). The samples were annealed for 30 min. at each 100 °C step from 100 °C to 1000 °C. Photoluminescence (PL) and micro-Raman spectroscopy were used to monitor the development of defects during the annealing.

The PL spectra of defect-induced centres anneal out at temperatures dependent on the implant dose, increasing from 700 °C for samples implanted with 10^{13} cm^{-2} to over 1000 °C for samples of 10^{15} cm^{-2} . In all these samples, at the anneal-out temperature range, the expected characteristic PL line at 903 meV of the {113} self-interstitial aggregates was not observed. This implies that a high content carbon can prevent the formation of this kind of rod-shaped aggregate.

The micro-Raman mapping analysis of small-angle chamfered samples revealed that there is a strain layer consistent with the projected ion-implantation range. The widths of the 520 cm^{-1} Raman line vary from 6 cm^{-1} to 12 cm^{-1} , indicating the stress effects from the damage. Raman spectra taken at the location of the broadened Raman peak show that some amorphous domains are present in the high-dose as-implanted samples. These amorphous domains can grow with increasing anneal temperature and act as quantum dots to enhance the PL emission at low energy broad band in the 500 – 800 °C anneal range.

Poster M-13

Hydrogen in dilute SiGe alloys

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Hydrogen atoms in a dilute SiGe alloy are considered theoretically. Structural, vibrational and electronic properties for crystalline alloys containing ~ 1.5 at. % Ge complexed with hydrogen are considered. The behaviour of bond-centred hydrogen is found to be weakly perturbed, when compared to hydrogen in pure Si.

Poster M-14

First-principles calculations on the structure of H-induced platelets in silicon and diamond

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Hydrogen is a common and widely studied impurity both in silicon and diamond. In particular, hydrogen ion implantation leads to the formation of planar microdefects in (111) and (100) planes – H-induced platelets, as confirmed by many experiments in Si [1,2]. There is evidence for the formation of such platelets in diamond [3]. IR measurements indicate that several structures of platelets exist depending on temperature [2].

We investigate possible structures of platelets in silicon and diamond and their stabilities, concentrating on incipient small-size platelets [4]. We regard finite-size platelets as bounded by dislocations and calculate the contributions to the total energy of platelets due to the elastic strain field of bounding dislocations and due to the hydrogen binding energy.

In addition to the studies of the (111) platelets, we investigate possible structures of the H-induced platelets in the (100) plane.

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Poster M-15

Erbium in silicon

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The doping of silicon by erbium has shown some amazing properties that can be exploited to create performance Si-based light emitters at the minimum of adsorption of optical fibres. The light emission comes from the inter- f transition in Er that is very weakly dependant on the surrounding crystal field. Nevertheless, only a small proportion of the introduced Er in Si behaves like light emission centres. The exact local structure of these sites is still quite unknown.

So, in this theoretical work we have computed (using density functional theory) different possible sites for Er in Si and studied the influence of co-dopants like oxygen. A wide range of structures was found and their electronic structures were calculated, giving some insights into this complex problem.

Poster M-16

Optical and electrical activity of B defects in Si

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Density functional theory is used to investigate boron interstitial clusters, the boron vacancy defect and defects formed with carbon, oxygen and hydrogen. Using data from experimental techniques such as DLTS, EPR, PL and IR we are able to assign structures to many observed centres and begin to develop a series of reaction paths for the evolution of B with annealing temperature depending on the relative concentrations of impurities.

Amongst other results we demonstrate that a metastable defect composed of two B interstitials and a self-interstitial has symmetry, vibrational modes and an electronic structure consistent with the I2 photoluminescence centre, also known as the Y centre. We also demonstrate that the B-V defect in Si is a bistable defect which can be converted between next-nearest neighbour and third-nearest neighbour configurations.

7.2 Diamond-related (Tuesday)

Poster T-1

Modelling of diamond detectors: effects of the trapping and detrapping phenomena on the detector's response

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Diamond detectors can be fabricated from Chemical Vapour Deposition (CVD) polycrystalline diamond films. The main advantage of the CVD diamond compared to the other detector material is its radiation hardness. This property is of immense interest for the detector development for high energy physics experiments.

The detection mechanism is by induction to the electrodes of the device due to the movement of the carriers. Using CVD techniques for growing diamond, there is a limited control over the defects and impurities. Defects and other inhomogeneities related to the polycrystalline structure degrade the material properties. They can also influence the movement of the carriers and consequently stop or delay the accumulation of the total induced charge on the electrodes. Therefore the trapping and detrapping can have a profound effect upon the performance of the detector.

We have built up a computer simulation of the detection mechanism in diamond detectors and, in particular, of these crucial problems. Previous simulations of the trapping-detrapping phenomena in diamond detectors have generally been restricted to simple detector geometries. We consider different configurations of electrodes, including a parallel plate, strip-pad, and interdigitated strip geometry. The diamond film (diamond detector) is simulated by a grid. We apply a spatial and time discretisation, regulated by the grid resolution and, by using the Shockley-Ramo theorem, we calculate the signal induced on the electrodes. In this paper, we calculate the effect of trapping/detrapping, recombination or scattering of carriers bulk defects on the signals detected.

Acknowledgement:

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Poster T-2

Incorporation of sulphur into hydrogenated amorphous carbon films

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Amorphous hydrogenated carbon (a-C:H) films are increasingly being suggested for use in potential carbon based electronic devices. Adding dopant elements to the films can alter their mechanical and electrical properties dramatically. Addition of larger percentage levels of second elements (such as N, P or S) may lead to new solid state binary compounds, such as carbon nitrides, phosphides and sulfides. Radio frequency plasma enhanced chemical vapour deposition (RF-PECVD) has been used to deposit sulphur containing a-C:H films from a CH₄/H₂S gas mixture. These a-C:H:S films were deposited on Si using various process pressures (10 – 50 mTorr), DC biases (100 – 400 V) and H₂S proportions in the gas mixture (0 – 27%). Films were analyzed by X-ray photoelectron spectroscopy (XPS), secondary ion mass spectrometry (SIMS) and laser Raman spectroscopy. XPS revealed that the a-C:H:S films had a surface S:C ratio of up to 1:4 (*i.e.* 25% S) and that the sulfur content was inversely proportional to the DC bias and also chamber pressure. SIMS depth profiling shows the films to be homogeneous in composition. The $I(D)/I(G)$ ratio from 514 nm Raman spectroscopy was used to compare the structure of the doped and undoped films. The doped films had an $I(D)/I(G)$ ratio of ~ 0.6 compared to ~ 0.4 for the undoped films, suggesting that the presence of sulphur in the film or plasma aided the formation of small graphitic regions within the film.

Poster T-3

Impedance spectroscopy of diamond films

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Impedance spectroscopy has been widely utilised to study the conduction paths within a range of conducting and less-conducting materials, but its application to diamond films is relatively new. This technique allows the contributions to the overall conductivity from the grains, grain boundaries and electrodes to be isolated. Thus it can be used as a powerful tool for researching methods for reducing problems within diamond technology that are associated with grain boundaries and poor metallic contacts.

In this paper we will discuss our recent work on undoped polycrystalline CVD diamond films, where we have investigated the different conduction paths and impedance values associated with film quality ('black' *vs.* 'white', 'hot filament' *vs.* 'MWPECVD') and grain size (nanocrystalline films *vs.* polycrystalline films with grain sizes of several tens of microns). In addition we have looked at the effect of homoepitaxial growth on these films. Results from studies on doped single crystal material will also be described. For example, we will report the first measurement of frequency dependence impedance on boron-doped single crystalline diamond films within the range 0.1 Hz to 10 MHz with the temperature ranging from -100 °C up to 300 °C. The Cole-Cole (Z' *vs.* Z'') plots are found to be well fitted to a RC parallel circuit model and the equivalent Resistance and Capacitance for the diamond films have been estimated using Z -view curve fitting.

The potential of this under-used technique for diamond film analysis will be discussed.

Homoepitaxial growth for the control of carrier mobility in diamond

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It is well established that hydrogen-terminated diamond surfaces can support a thin p -type layer, an effect often referred to as ‘surface conductivity’. The origin of this effect has been controversial, but a consensus is now emerging around the idea that the carriers emerge because of an upward band-bending process induced by surface charge transfer reactions. Surface conductivity has been observed on a wide range of diamond materials, including CVD-grown polycrystalline diamond, CVD-grown homoepitaxial layers and natural type IIa stones. In fact, it appears that only in the case of the presence of nitrogen within the diamond does surface conductivity not arise following hydrogenation. This p -type layer has been utilised for the fabrication of unipolar device structures, such as Schottky-like diodes and field-effect transistors.

We have previously reported carrier transport characteristics, based upon Hall effect measurements, for surface conductive layers on single crystal material, polycrystalline ‘white’ CVD diamond and even black ‘thermal management’ grade CVD diamond. What is interesting is the relative insensitivity of the measured characteristics to these strongly differing diamond types, with mobilities in the range $20 - 60 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, and sheet carrier concentrations of the order 10^{13} cm^{-2} being typical. Our measurements at temperatures as low as 0.3 K have not shown carrier ‘freeze-out’, and a thermal activation energy of around $5 - 10 \text{ meV}$ can be suggested. To design effective devices using this p -type layer it would be highly advantageous to not only improve the carrier mobilities, but also to be able to control the carrier concentration in each layer. We have therefore initiated a programme based upon homo-layer growth on both polycrystalline and single crystal diamonds with just these aims. The results are exciting; single crystal type Ib (HPHT, Sumitomo) material does not show surface conductivity, but homoepitaxial layers grown on this material do. Moreover, the carrier transport characteristics can be controlled by varying the thickness of the homoepitaxial layer. Using this approach we have achieved the highest carrier mobility yet reported in this type of layer at a carrier concentration useful for device fabrication, at $240 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. In addition, we have grown homo-layers on both black and white polycrystalline diamond films, considerably enhancing the properties in both cases. This paper will present a comprehensive overview of the carrier transport characteristics that we have measured for more than one hundred homo-layers and demonstrate, for the first time, a clear methodology for controlling these characteristics. AFM and STM images will also be presented, illustrating the influence of surface roughness on both carrier concentrations and mobilities.

Poster T-5

Diamond UV photodetectors

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It is well established that diamond can be a useful material for the fabrication of deep UV photodetectors. Indeed, diamond photoconductive devices fabricated by the UCL team have been commercialised by U.K. industry. In addition to being 'blind' to visible light, these detectors can be both fast (operation in the MHz regime has been demonstrated), and sensitive (gain levels of several thousand have been measured). Less well developed are diamond-based imaging arrays. We have previously reported a 'proof-of-principle' 1-D imaging array with eight active pixels each of $\sim 150 \mu\text{m}$. This paper concerns the fabrication of devices with smaller pixel dimensions and greater density. Results will be shown for 1-D arrays with 30 – 120 pixels of $50 \mu\text{m}$ dimensions. The use of these arrays within biotechnology will be discussed.

Poster T-6

The incorporation and properties of hydrogen in single crystal CVD diamond

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Hydrogen is believed to be a common impurity in diamond, but unlike other group-IV materials, there is little detailed information about how hydrogen is actually incorporated into the lattice. Muon implantation experiments in diamond [1] and theory both indicate that neutral hydrogen is metastable at a tetrahedral interstitial site, with its lowest energy configuration consisting of hydrogen at or around the bond centre. However, the equivalent hydrogen centres have not been identified. Experimental progress has been somewhat disappointing, and theoretical predictions have driven the field [2] without the necessary experimental facts to confirm many of the predictions.

Single crystal diamond grown by chemical vapour deposition (CVD) is now becoming available and the incorporation of hydrogen during growth or via post growth treatment (plasma processing, implantation *etc.*) can be systematically studied in this material. Infrared studies have shown that hydrogen is incorporated into single crystal CVD diamond, but in this work no models were proposed for the hydrogen related defect centres [3]. It has been shown that hydrogen can compensate the boron acceptor in bulk diamond, and studies suggest that hydrogen diffuses readily only in the positive charge state [4]. A nitrogen-hydrogen complex has been identified by electron paramagnetic resonance (EPR) studies on as-grown single crystal CVD diamond, and characterised in detail [5]. These data will be reviewed and new data on hydrogen incorporation in bulk CVD diamond will be presented.

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Poster T-7

Production of crystalline carbon phosphide by laser ablation of phosphorus at the solid-liquid interface in various carbon containing solvents

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Crystalline carbon phosphide (or phosphorus carbide) has never been previously reported in any literature, although it is theorised that it will have several interesting and potentially lucrative properties, such as being mechanically hard, and being a wide band gap semiconductor. We have performed a study of the products formed from the pulsed laser ablation (PLA) of solid phosphorus immersed in various carbon containing solvents. The PLA occurs at the solid-liquid interface, and the ablated phosphorus particles form a high energy plasma, and combine with the solvent to produce various crystalline and amorphous C/P-containing products. Results will be presented that indicate that one of these products may be a crystalline phase of carbon phosphide. Several techniques will be used to provide evidence for this, including Transmission Electron Microscopy, electron diffraction, energy dispersive X-ray spectroscopy, Secondary Ion Mass Spectrometry, and optical emission spectroscopy of the plasma.

Poster T-8

Protective and anti-thrombogenic DLC coating

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DLC coatings produced by plasma assisted chemical vapour deposition from hydrocarbon precursor gases consist of carbon and hydrogen, two of the main constituents of living organisms. *In-vitro* tests have shown DLC to be biocompatible [1]. The coating is wear resistant, lubricious, and chemically inert with very low permeability, making it a versatile coating for a range of biomedical implants. By virtue of these properties, the coating has been used as protection on articular prosthesis (knee) with the additional advantage of preventing allergic reactions. *In-vivo* tests indicate that the coating is also haemocompatible. Flow accelerators used in conjunction with vascular stents, uncoated and coated with heparin, phosphoryl choline and DLC were implanted in a porcine artery for eight weeks. Fibrin and platelet deposition on the device coated with DLC was less by a factor of about 10 compared with the other coatings; the thrombogenic response was therefore much reduced. In addition, because of its atomic density, the coating acts as an effective diffusion barrier, preventing metallic ions from the implant entering the body and protecting the implant from attack by the biological environment. The coating can also be applied to soft tissue, for example to collagen. Collagen can readily be incorporated in the body [2], but in contact with blood, causes thrombus formation, which may be avoided with the DLC coating. An application would be the construction of collagen conduits, internally coated with DLC to provide surgical vascular replacement in *e.g.* bypass operations. In gastro-intestinal "patches", a DLC coating will reduce permeation through the collagen. In general, the use of DLC could prevent post-surgical adhesion of prostheses and other forms of implanted devices to associated or local tissues.

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Poster T-9

What to do when Fowler-Nordheim theory fails: a model for carbon field emitters

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Classic theory for cold field emission due to Fowler and Nordheim (FN) is shown to violate the criteria for the validity of WKB for applied fields in the region of $F > 1 \text{ V } \mu\text{m}^{-1}$. Particular problems are shown to arise when the barrier height is significantly lowered, either via image effects, negative electron affinity, dielectric screening or otherwise. By examining the complete Schrödinger's equation for the full image problem, we have found an analytical solution close to the top of the barrier. A comparison with experimental data for carbon field emitters shows excellent agreement, with our theory giving many orders of magnitude improvements over the FN theory.

Poster T-10

Do isolated interstitial atoms occur in diamond? A re-examination of the EPR defects
NIRIM-1 and NIRIM-2

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All of the EPR and optical data relating to some of the basic nickel-related defects in diamond have been compared, as well as previously little-considered information about the effect of spin-orbit coupling and the magnitude of the crystal field. New models are proposed for the EPR defects, which are found in synthetic diamond grown at high pressure and high temperature with getters to reduce the content of nitrogen impurity: NIRIM-1 and NIRIM-2, which some authors have attributed to isolated interstitial nickel at an undistorted, or distorted, T_d site, respectively. It is suggested that NIRIM-1 is more likely to be substitutional Ni(+), $3d^5$, at a T_d site, than the previously suggested interstitial Ni(+), $3d^9$, and that NIRIM-2 is interstitial Ni(+), $3d^9$, pinned at a site 0.308 nm along $\langle 111 \rangle$ from a substitutional B(-) impurity, beyond one of its nearest C neighbours. This supports the suggestion that isolated interstitial Ni is mobile.

Electrical activity of chalcogen and pnictogen hydrogen defects in diamond

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It has been suggested that S-H defects in diamond possess electrical donor levels shallower than isolated substitutional sulphur [1,2] and mirror what has been found in silicon [3]. Now in silicon, it is believed that the donor levels of Se-H and Te-H defects are shallower than that of S-H and that this may also be true in diamond. We report first-principle calculations of the donor levels of S, Se and Te defects in diamond as well as their complexes with hydrogen, together with levels calculated for similar defects considering the pnictogens P, N, As and Sb.

The calculations find that the most stable S-H defect has a donor level 1.00 eV below the conduction band minimum (CBM) in diamond, 0.43 eV shallower than the value calculated for isolated substitutional sulphur. The most stable Se-H complex has a donor level 0.70 eV below the CBM, while the most stable Te-H complex is predicted to be a very shallow donor indeed with a level 0.42 eV below the CBM.

Calculations considering the pnictogens suggest that substitutional As and Sb may be shallow donors, although N and all pnictogen-hydrogen complexes are predicted to have very deep donor levels. The case is made for the doping of diamond with arsenic.

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Poster T-12

Cathodoluminescence study of H-implanted B-doped diamond samples

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Keywords: diamond characterisation, cathodoluminescence, ion implantation, B-H complexes.

The interactions between hydrogen and boron in *p*-type diamond have been investigated in the last few years in particular there has been interest in the study of the B-H complexes, leading to the passivation of the boron. Several techniques were employed to determine the influence of the hydrogen on the sample characteristics, such as carrier concentration and carrier mobility [1]. The present work reports a cathodoluminescence study of B-doped diamond samples implanted with hydrogen. A B-doped diamond sample was prepared by HPHT synthesis. It was cut into a 50 mm thick slice such that three different growth sectors could be identified and the boron concentration, determined by infrared spectroscopy, was 1, 5 and 15 ppm in the three sectors. Subsequent hydrogen ion implantation was carried out: four doses of $2.5 \times 10^{15} \text{ cm}^{-2}$ were implanted with energy between 30 and 300 keV, in an area with the highest acceptor concentration, giving a nearly constant hydrogen concentration to a depth of 1.5 mm. Cathodoluminescence analysis was performed using varying energies of the electron beam, which allows us to investigate different depths in the samples [2].

Peaks related to the lattice damage due to ion implantation (*i.e.* TR12) were detected in the CL spectra taken with low beam energy (that is, in the implanted surface layer). With higher beam energies (beyond the implanted layer), the blue band, typical of undoped diamond, was observed, indicating that the boron is passivated outside the range of the implantation. The analysis of this data takes into account the distribution of excitation produced by the cathodoluminescence, and thus can give a good indication of the depth distribution of the defects themselves.

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Transition metals in diamond

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Two models are commonly put forward to explain the electronic structure of substitutional transition metal (TM) defects in diamond: the Ludwig-Woodbury model [1] and the vacancy model [2]. *Ab-initio* Hartree-Fock calculations presented here suggest that these two models are extremes that are not met in practice. The complete set of orbitals expected to be found in the band gap of diamond are those derived from the transition's metals *d*-orbitals, and vacancy-like orbitals formed from the 'dangling bonds' of the transition metal's nearest neighbours.

The two models differ in their description of the roles of these two sets of orbitals. The Ludwig-Woodbury model considers the vacancy-like orbitals to be of low energy and completely full - remaining electrons are placed into the metal's *d*-orbitals which then determine the properties of the complex. Conversely the vacancy model pictures the metal *d*-orbitals to be of low energy and fully occupied, and additional electrons to be housed in the vacancy-like orbitals. The composition of the complex's valence orbitals has important consequences for the interpretation of experimental data. EPR measurements particularly will be affected, where *g*-values and hyperfine structure will be strongly sensitive to the valence electrons being centred on carbon nearest neighbours or on the transition metal itself [3].

The electronic structures of small transition metal clusters were examined with the *ab-initio* package GAMESS [4,5] and it was found that in all cases these two sets of orbitals have an appreciable interaction. It is also found that the electronic structures of the transition metal clusters change smoothly from being best described using the Ludwig-Woodbury model, to the vacancy model, as the atomic number of the transition metal in the cluster increases. In some cases the energies of the two sets of orbitals were found to be very close, and a hybrid of the two models incorporating both sets of orbitals had to be invoked to explain the electronic configurations calculated.

Our calculations show that the electronic structure of TM defects in diamond will be qualitatively different as the transition series is crossed. Most clusters are well described by one of the accepted models, but in some a hybrid of the two schemes must be used as both vacancy and metal orbitals contribute strongly to the valence orbitals.

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Radiation damage centres in type-Ib diamond

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In this work we used *ab-initio* (AIMPRO) modelling to investigate the structures and electronic properties of possible nitrogen-carbon aggregates in low-temperature-irradiated type Ib diamond, in an attempt to relate the observed optical absorption to energy levels calculated from the models.

Immediately after irradiation, two dominant absorption bands appear in the visible spectral region with zero-phonon lines (ZPL) at 2.367 eV (523.6 nm) and 2.535 eV (489.1 nm), respectively. These bands are believed to be due to transitions at an interstitial nitrogen-carbon complex with different atomic arrangements.

The 2.367 eV band is annealed at low temperature (~ 500 K), accompanied with a correlated increase in the absorption strength of the vibronic band with a ZPL at 2.535 eV. During the annealing of the 2.367 eV band there are no other significant changes in absorption lines in the visible and infra red regions that are related to the concentrations of nitrogen or self-interstitial atoms. On the other hand, the annealing of the 2.535 eV absorption band is directly correlated with a decrease in the concentration of positive nitrogen atoms, and an increase in the concentration of neutral nitrogen atoms, calculated from the absorption strengths at 1332 and 1344 cm^{-1} , respectively. Following the annealing of the 2.535 eV absorption band, there is a rapid increase in the concentration of the [001]-split carbon interstitial centres, calculated from the intensity of the absorption line at 1.859 eV.

Preliminary EPR measurements showed that the 2.367 eV and 2.535 eV absorption bands are not EPR active. This implies that, if the centre giving rise to either of the two absorption bands possesses a charge, then possible arrangements of a carbon-nitrogen aggregate must be charged. Other possibilities for atomic arrangements may involve only self-interstitial atoms in hexagonal, tetrahedral or bond-centred structures.

Possible arrangements of a carbon-nitrogen aggregate in diamond include carbon-nitrogen split, carbon-nitrogen bond-centred and a nitrogen atom trapped at a carbon atom in tetrahedral or hexagonal sites. A nitrogen atom, trapped at two interstitial carbon atoms split along the [110] direction, is also a possible arrangement.

Calculated models of a charged interstitial carbon-nitrogen defect, split along the [001] direction with a C_{2v} symmetry, produce a ground state of $a_2^1 a_2^2 b_0^1$, giving the centre a transformation of A_1 symmetry in the ground state. Excitation of electrons from a states to b states are dipole-allowed, and calculations give the $a_1^1 a_2^2 b_1^1$ transition energy as approximately 1.85 eV. This energy is in reasonable agreement with the observed 2.535 eV zero-phonon energy. A charged interstitial carbon-substitutional nitrogen atom bond-centred aggregate model was given C_s symmetry. Possible dipole-allowed transitions give a calculated energy of approximately 1.76 eV which is again comparable with that of the observed 2.535 eV absorption line.

The 2.367 eV centre has a ground state splitting of 3 meV; consequently these models with no ground state splitting cannot fully represent that transition. A neutral carbon interstitial atom in tetrahedral and bond-centred sites are calculated to have optical transitions in the visible region. However, a neutral carbon interstitial atom in hexagonal, tetrahedral or bond-centred models shows dipole-allowed transitions in the visible region.

Poster T-15

Investigation of deposition and etching in a DC arc-jet reactor

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We will summarise results from two concurrent lines of study involving the DC arc-jet reactor at the University of Bristol - namely, the characterisation of $\text{CH}_4/\text{H}_2/\text{Ar}$ plasmas used for polycrystalline and nanocrystalline diamond growth, and etching of high-quality polycrystalline CVD deposited films by nitrogen plasmas. The plasma diagnostics are complemented by modelling of the gas phase chemistry in the arc jet reactor by Mankelevich at Moscow State University. Plasma diagnosis involves a combination of both absorption (cavity ring down) spectroscopy and optical emission spectroscopy (OES).

Recent studies have shown that diamond films may be etched in the DC arc-jet reactor using an $\text{Ar}/\text{H}_2/\text{N}_2$ gas mixture. We have investigated the use of this plasma to etch three distinct types of CVD diamond surface provided by Element Six Ltd.: (i) the as-deposited growth surface of a polycrystalline film, (ii) an equivalent surface after lapping, and (iii) the back (nucleation) surface of such films. Pre- and post- etching surfaces have been characterised using stylus profilometry, scanning electron microscopy and micro-Raman spectroscopy. The plasma in the region of the surface has also been characterised using the spectroscopic techniques applied to the deposition plasma.

Cavity ring-down spectroscopy (CRDS) is a sensitive, non-invasive absorption technique that allows quantitative determination of absolute column densities. We have previously reported line-of-sight absorption measurements of $\text{C}_2(\text{a})$ and $\text{CH}(\text{X})$ radical species in the arc jet plume, which can be converted to absolute concentrations given certain assumptions about the spatial extent of the radical distribution within the plume [3]. Future work focuses on extension of such CRDS studies to include ground state $\text{C}_2(\text{X}^1\Sigma_g)$ radicals - which calculations [4] suggest may be a significant diamond growth species in such highly activated CVD environments - and on the design and implementation of an optical cavity that can be translated vertically so as to enable 2-D concentration profiling of the radical densities (and gas temperatures) within the plume.

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Poster T-16

Effect of HPHT annealing on paramagnetic defects in diamond

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The formation and anneal-out conditions of paramagnetic defects in high-pressure and high-temperature diamond are investigated through a comprehensive annealing study of as-grown crystals. Diamond crystals are subjected to a sequence of heat treatments in the temperature range between 1550 °C and 2000 °C and the concentrations of paramagnetic defects is determined by electron paramagnetic resonance measurements after each annealing step. The quantitative data is analysed in the light of recently published results on the behaviour of nickel and/or nitrogen defects upon annealing. As with the P1 and W8 centres, the NIRIM-1 nickel-related defects show a strong decrease in their concentration after annealing at 1900 °C, whereas the NIRIM-2 centres seem to be rather stable. The evolution of the nickel-related centres concentration through the annealing sequence shows that not all W8 defects transform into the paramagnetic nickel-nitrogen complexes. Indeed, most of the W8 defects are transformed in other non-paramagnetic centres, with the AB1, AB3, and AB6 defects being probably a by-product of such process. The relatively low concentration of nickel-nitrogen paramagnetic complexes formed upon annealing shows that their formation does not play a fundamental role in the kinetics of the nitrogen aggregation during heat treatments.

Poster T-17

Investigating the deposition and gas-phase conditions of ultrananocrystalline diamond (UNCD) thin films

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Microwave plasma chemical vapour deposition (MPCVD) has been used to deposit nanocrystalline films from argon/methane/hydrogen plasmas. Film morphology has been assessed by scanning electron microscopy (SEM) and transition electron microscopy (TEM). Allotropic purity has been assessed by laser Raman spectroscopy (LRS). Historically in the group absolute mol fractions of methane, acetylene and methyl radical species have been measured by molecular beam mass spectrometry in conventional hydrogen/methane plasmas. Similar data will be presented monitoring species trends during the crossover from faceted microdiamond to nanocrystalline diamond growth by varying the plasma gas from 99% hydrogen to 99% argon with a constant 1% methane. Data will also be presented comparing UNCD growth conditions with ballas and other related nanodiamond phases. Mechanistic chemistry will also be explored through computational simulation.

Poster T-18

Chemical vapour deposition of diamond coatings onto metallic substrates

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Diamond films have been deposited onto metallic substrates such as molybdenum using a modified Hot Filament Chemical Vapour Deposition (HFCVD) with a vertical filament arrangement. The deposition of adherent diamond onto metallic substrates is difficult to achieve due to the thermal mismatch between the diamond and metallic substrates. Several methods have been proposed in order to overcome adhesion problems including the use of interlayer materials, chemical treatments and substrate biasing.

In this paper we present a combination of surface pre-treatment techniques in order to improve substrate-film adhesion and film quality. Negative biasing has been used in combination with conventional substrate pretreatment methods *i.e.* mechanical abrasion or acid etching in an ultrasonic bath. Scanning electron microscopy (SEM) and Raman spectroscopy results show that improvements in the morphology, crystallite size, phase purity and adhesion can be achieved with the use of surface pre-treatments methods.

Keywords: Adhesion, Nucleation, Substrate biasing, Chemical Vapour Deposition (HFCVD)

Impact of inert gases on the structure, properties and growth of nanocrystalline diamond films deposited by hot filament chemical vapour deposition

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Recently, nanocrystalline diamond (NCD) has attracted considerable scientific interest for use in biomedical, microelectromechanical (MEMS) devices and aerospace mechanisms. For biomedical applications, diamond has potential for use in orthopaedic implantation as it exhibits both haemocompatibility and histocompatibility characteristics, it is chemically inert, and it does not degrade. For biomedical and electronic applications, it is highly desirable to deposit much smoother films with crystals size in the nanoscale range.

In this paper we present experimental results of CVD diamond growth from methane, fixed at 1 vol. %, with incremental substitution of hydrogen with helium or argon gases, the concentrations of the inert gases were varied between 0 and 98 vol. %. Results show that initially the addition of either argon or helium increases the growth rate and significantly alters the film structure and crystallinity up to 60 vol. %. With additions of argon or helium greater than 60 vol. % in the gas phase the growth decreases and there is degradation of the crystal structure. In general, nanocrystalline diamond has been deposited at dilutions in excess of 90 vol. % helium or argon.

Keywords: Diamond, growth and characterisation, nanocrystalline, biocompatibility, chemical vapour deposition (CVD)

Poster T-20

Diamond coatings on dental cutting tools

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Diamond coatings on Co cemented tungsten carbide (WC-Co) hard metal tools are widely used for cutting non-ferrous metals. It is difficult to deposit diamond onto cutting tools, which generally have a complex geometry using a single step growth process. This paper focuses on the deposition of polycrystalline diamond films onto dental tools, which possess 3D complex or cylindrical shape employing a novel single step CVD growth process. The diamond deposition is carried out in a hot filament chemical vapour deposition (HFCVD) reactor with a modified filament arrangement. The filament is mounted vertically with the drill held concentrically within the filament coils, as opposed to the commonly used horizontal arrangement. This is an uncomplicated and inexpensive filament arrangement for coating substrates with a cylindrical symmetry.

In addition, the problems associated with adhesion of diamond films on WC-Co substrates are amplified in dental tools due to very sharp edges and unpredictable cutting forces. The presence of Co, used as a binder in hard metals, causes poor adhesion of diamond to the substrate. By applying surface treatments the amount of metallic Co on the surface can be reduced. A two-step pre-treatment employing Murakami etching followed by an acid treatment was used with the WC-Co dental tools. The CVD diamond films are examined in terms of the growth rate, morphology, adhesion and cutting efficiency.

Keywords: Cutting tools, adhesion, WC-Co, dental tools, chemical vapour deposition (CVD)

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