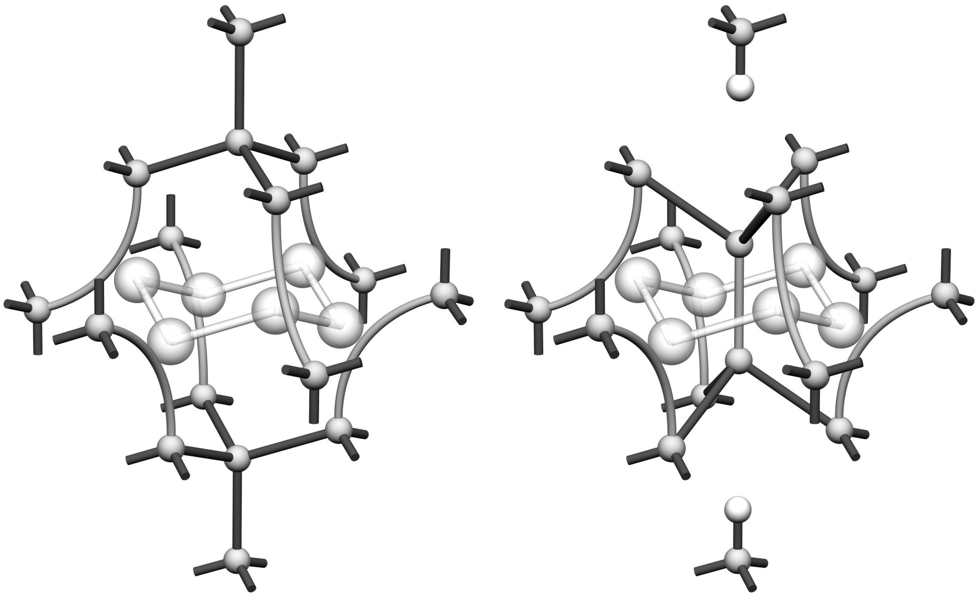
Workshop on Hydrogen in Semiconductors

April 15–16 Exeter, UK 1999

Organiser: R. Jones

Programme



V_6 and V_6H_2:
Models of the B^{4}_{80} (J-centre) and B_{41} optical centres in Si.

Co-sponsored by the European Science Foundation through the Ψ_k network and EPSRC through the CCP9 network

Organising Committee

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(School of Physics, Stocker Road, University of Exeter, Exeter EX4 4QL, UK)

Conference Location

The workshop is taking place on the main University of Exeter campus, accommodation is in the Birks Hall of residence and all lectures will take place in the main lecture theatre in the Harrison Building. The journey from Birks to the Harrison Building involves a steep climb, and will take about 20 minutes. Some participants will find the climb excessive. Please contact us if you want a lift from Birks to Harrison: a limited amount of car space is available.

The conference banquet will take place in Reed Hall (see enclosed map).

Delegates should wear the conference badges provided. Please remember to return your key to the Porter's Lodge when you vacate your room after the conference.

Registration and Conference Desk

There will be a conference desk in Room 102 of the Harrison Building on Thursday and Friday, from 08:30–09:30. The staff will be able to help with any queries, and can also confirm flight bookings, etc. if required.

Conference Staff

The following people will be happy to help you with any problems you may have during the conference: Bob Jones, Chris Latham, Jonathan Goss, António Resende, Ben Hourahine, James Coomer, José Coutinho and Simon Gay.

Conference Bar

There will be a conference bar in Birks Hall on Wednesday and Friday evening, at the times given below. On the evening of the banquet there will be a bar at Reed Hall open until midnight. Bar hours are as follows:

Wednesday	19:00 – 23:00	
Thursday	19:30 – 24:00	(Reed Hall)
Friday	19:00 – 23:00	

Banks and Shops

There is a National Westminster bank on campus, opposite the library (see map). Adjacent to this is the university shop where it is possible to buy phone cards, stamps, etc., as well as a 'Blackwells' book-shop.

Communicating

Telephone and Faxes

There is a public telephone at Birks Hall, and the telephone number for the Porter's Lodge is +44-1392-26 3395. In addition, urgent phone messages and faxes can be sent to the secretary of the Physics Department during the conference; the telephone number is +44-1392-26 4151, or FAX number +44-1392-26 4111. There are in addition several phone boxes dotted around the campus. The may be used with phone-cards, coins or some credit-cards. Telephone-cards may be purchased at the university shop. The phones are located:

1. In the corner of the main entrance lobby of Harrison
2. In Cornwall House opposite the Porters Lodge
3. In the car park outside the Great Hall
4. In Devonshire House next to the Ram Bar
5. In the lobby of the Northcott Theatre (this phone takes cash)
6. In the Newman lecture theatres, next to the Peter Chalk centre

Post

There is a post-box in the university shop, and another next to Reed Hall. We will also be happy to post items for you, if they are left at the reception desk.

E-mail and Photocopy facilities

It is expected that there will be e-mail facilities available for delegates use located in the Harrison building. Details will be announced at the beginning of the conference.

First Aid

The porters in both Birks and Harrison are trained in first aid, and in case of emergency please contact either a porter or one of the conference organisers. The porters in Harrison can be contacted on 3910 (263910 from an external phone), and in case of emergency the phone number for the Warden at Birks Halls is 263396.

Poster Sessions

All posters will be displayed throughout the duration of the conference in the bar area in Birks Hall. We would ask those delegates presenting posters to display them as soon as possible after registering on Wednesday the 14th. Fixings will be provided for attaching posters to the boards.

We regret that we cannot return any posters left behind after the conference.

Departure

Important: Please notify the conference desk of your time of departure so that we can organise transport.

Further information

Further information can be found on the Web at:

`http://newton.ex.ac.uk/research/theory/jones/hydrogen/`

Wednesday April 14

Participants arrive; a ferry service will run between
Exeter St. David's railway station and Birks Hall.

17:00–20:00	Registration: Foyer of Birks Hall
19:00–21:00	Buffet Reception: Birks Hall
21:00–23:00	Registration: Foyer of Birks Hall
19:00–23:00	Bar Facilities available in Birks Hall

Thursday April 15

07:30–08:30	Breakfast: Birks Hall
09:00–09:15	Welcome (Harrison Building)

Session I – Chairman: P. Deák

09:15–09:40	*Glimpses of hydrogen in silicon via magnetic resonance studies,* G. D. Watkins
09:40–09:50	Discussion
09:50–10:20	*Optically active hydrogen dimers in Si*, B. Hourahine, R. Jones, A. N. Safonov, S. Öberg, P. R. Briddon, and S. K. Estreicher
10:20–10:30	Discussion
10:30–11:00	Coffee
11:00–11:45	*Microscopic properties of hydrogen-containing defects in Si from uniaxial stress studies of their vibrational spectra*, M. Stavola
11:45–12:00	Discussion
12:00–12:45	*Hydrogen interacting with intrinsic defects in Si*, S. K. Estreicher, J. L. Hastings, M. Gharaibeh and P. A. Fedders
12:45–13:00	Discussion
13:00–14:00	Buffet Lunch: Harrison Building, Rms. 101–103

Session II – Chairman: B. Bech Nielsen

14:00–14:45	*Interactions of hydrogen with silicon and consequences for devices*, C. G. Van de Walle
14:45–15:00	Discussion
15:00–15:45	*Energy levels for muonium in Si and Ge and electrical activity at high temperatures*, S. F. J. Cox, R. L. Lichti, K. H. Chow, E. A. Davis, T. L. Estle, B. Hitti, E. Mytilineou, C. Schwab, A. Amato, A. Schenck, M. Charlton and P. Donnelly
15:45–16:00	Discussion
16:00–16:30	Tea
16:30–17:15	*Effect of hydrogen on thermal donor formation in silicon*, L. I. Murin, V. P. Markevich, J. L. Lindström and T. Hallberg
17:15–17:30	Discussion
18:00–19:00	Poster Session: Birks
19:30–20:15	Reception: Reed Hall
20:15–24:00	Conference Dinner: Reed Hall

Friday April 16

07:30–08:30	Breakfast: Birks Hall

Session III – Chairman: S. K. Estreicher

09:00–09:45	*Hydrogen–defect complexes in silicon: Fact and speculation*, B. Bech Nielsen
09:45–10:00	Discussion
10:00–10:45	*Electrical properties of transition metal–hydrogen complexes in silicon*, J. Weber
10:45–11:00	Discussion
11:00–11:20	Coffee
11:20–12:00	*Defect profiles and the Feklisova-Yarykin conjecture*, J. Coomer, A. Resende, R. Jones, S. Öberg and P. R. Priddon
12:00–12:15	Discussion
12:15–12:50	*Acceptor-like hydrogen dimers in silicon*, B. Aradi and P. Deák
12:50–13:00	Discussion
13:00–14:00	Buffet Lunch: Harrison Building, Rms. 101–103

Session IV – Chairman: J. Weber

14:00–14:45	*Laplace transform DLTS studies of gold–hydrogen defects in silicon*, A. R. Peaker, J. Evans-Freeman and L. Dobaczewski
14:45–15:00	Discussion
15:00–15:45	*Electric field dependent structural and vibrational properties of the Si(100)–H(2×1) surface and its implications for STM induced hydrogen desorption*, K. Stokbro
15:45–16:00	Discussion
16:00–16:30	Tea
16:30–17:15	*Hydrogen-passivation of double donors in silicon: atomic and electronic structure*, P. T. Huy, C. A. J. Ammerlaan and T. Gregorkiewicz
17:15–17:30	Discussion
17:30–18:15	*Complexes of Group-VI Donors with hydrogen in GaP*, B. Clerjaud, D. Côte and W. Ulrici
18:15–18:30	Discussion
19:30–20:30	Dinner: Birks Hall
20:30–	Poster Session and Bar
20:00–23:00	Bar in Birks Hall

Saturday April 17

07:30–08:30	Breakfast: Birks Hall Ferry participants to station

Thursday April 15

GLIMPSES OF HYDROGEN IN SILICON VIA MAGNETIC RESONANCE STUDIES

G. D. Watkins

Department of Physics, Lehigh University, Bethlehem, PA 18015, USA

Magnetic Resonance studies have supplied several important bits of information concerning hydrogen in silicon, a few of which will be described. 1) A Pt–H_2 pair formed when substitutional Pt traps two hydrogen atoms has been successfully studied by electron paramagnetic resonance (EPR). Combined with local vibrational mode (LVM) studies, a rather complete picture of its lattice and electronic structure has emerged. 2) EPR studies of neutral bond-centered hydrogen (H^0_{BC}) by Gorelkinskii and Nevinny have measured the reorientation kinetics of the defect in its positive charged state. Reorientation is equivalent to a single diffusion jump, and the remarkable observation is that the results extrapolate accurately to the high temperature diffusion measurements made many years ago by Van Wieringen and Warmoltz, $\sim$ 18 decades away! A tempting conclusion is that diffusion over this wide temperature range is dominated by the defect in its positive charged state. 3) This conclusion is surprising, however, when one looks at what has been learned from muon (μ) studies in GaAs. There, μ (a light isotope of H) takes on all of the same configurations in the lattice as in silicon, and with similar relative stabilities, but detailed (SR studies have concluded that by far the most mobile species (by a factor of $\sim 10^{10}$ at room temperature) is the neutral defect in its metastable tetrahedral site (μ^0_T). 4) μSR studies in silicon have been able to estimate the electron emission and conversion kinetics from and between the various charge states of the two configurations and construct an almost complete configurational coordinate diagram for the defect. Almost complete because the energy difference between the neutral defect in the BC and H configurations remains undetermined, with the question of negative-U still uncertain. This uncertainty arises from the observation again in this study of the importance of metastable H^0_T, in this case in the emission and conversion kinetics. This may also turn out to be important in the interpretation of the electrical studies for hydrogen.

9:15

S I

1

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OPTICALLY ACTIVE HYDROGEN DIMERS IN SI

B. Hourahine, R. Jones, A. N. Safonov [†], S. Öberg [‡], P. R. Briddon [§], and S. K. Estreicher [♮]

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Photoluminescence experiments on silicon soaked in hydrogen, with subsequent irradiation and heat treatment, have revealed several optical centres with exceptionally low exciton binding energies. Studies using H and D mixtures demonstrated that some of these centres contain two hydrogen atoms: both ground and excited excitonic states in B_{41} and B^{1}_{71} are each split into three and four lines respectively showing that the defects contain *equivalent* and *inequivalent* pairs of hydrogen atoms. Magnetic field investigations demonstrate that these centres have trigonal symmetry. Other centres, such as B^{1}_{81} and B^{1}_{18} also contain two H atoms but have C_{1h} symmetry, while others B_{80} and B^{1}_{19} contain three and four H atoms respectively without any symmetry.

The high symmetry of B_{41} and B^{1}_{71} strongly restricts possible structures of the defects, particularly in the case of B_{41}, which although it is usually reported as possessing C_{3v} symmetry, actually requires the higher D_{3d} or D_3 symmetries necessary for equivalent hydrogen atoms. There are few defect structures with such high symmetry in silicon. If the defect possesses D_{3d} or D_3 symmetry, then here are only two sites in the diamond lattice at which 9:50
the centre of the defect can sit. These are the bond-centre and hexagonal lattice sites. The S I
obvious structure, consisting of two anti-bonded hydrogen atoms attached to the pair of silicon atoms surrounding a bond centred site must be discounted, since such defects should 2
be stable only at low temperatures.

The combined requirements of creation by irradiation and high thermal stability point towards a multivacancy–hydrogen complex. V_1 to V_5 can be excluded as these are not trigonal. As V_6 is centred on the hexagonal site and has D_{3d} symmetry, a plausible candidate is a complex between V_6 and hydrogen. From a consideration of the formation and stability of V_n defects with $n < 6$, V_6 is expected to form in irradiated material which is heated to $> 200\,^{\circ}$C.

Ab initio cluster calculations (AIMPRO) on V_6H_2 reveal that the stable defect involves an unexpected reconstruction (see cover). The properties of this complex are entirely consistent with the B_{41} centre. We therefore propose that this defect is responsible for the 1.1509 eV luminescence. Alternative structures are suggested for B^{1}_{71} and other H centres.

The calculations imply that the precursor, V_6, should also be optically active. It is suggested that this is the B^{4}_{80}, or J centre (1.107 eV), which forms in irradiated hydrogen-free material around 300–480 °C and is known to be trigonal. Stress alignment studies imply that it is vacancy related. These calculations suggest that the lowering in exciton binding energy arises from the release of tensile strain in the multi-vacancy defect consequent upon H attack.

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MICROSCOPIC PROPERTIES OF HYDROGEN-CONTAINING DEFECTS IN SI FROM UNIAXIAL STRESS STUDIES OF THEIR VIBRATIONAL SPECTRA

Michael Stavola

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11:00
S I
3

Vibrational spectroscopy has been an especially fruitful method for the study of hydrogen-containing complexes in semiconductors. The hydrogen vibrational bands provide an important fingerprint of the hydrogen-containing complexes, isotope shifts help identify the atoms in the complexes, and the vibrational frequencies are an important benchmark for theory. Uniaxial stress perturbations, when used in conjunction with vibrational spectroscopy, provide additional information about the microscopic properties of the defects. In favorable cases, the symmetry, reorientation kinetics, and ground state energy shift can be determined, revealing interesting physics that is not accessible to vibrational spectroscopy alone. The BH, AuH_n, and H_2 centers in Si will be discussed as examples.

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HYDROGEN INTERACTIONS WITH INTRINSIC DEFECTS IN SI

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† *Physics Department, Washington University, St. Louis, MO 63130, USA*

The interactions between hydrogen and intrinsic defects in silicon are systematically studied using *ab-initio* (tight-binding) molecular-dynamics simulations in supercells containing 64 and 216 host atoms and ab-initio Hartree-Fock calculations in clusters containing up to 100 Si atoms. The configurations, electronic structures, and binding energies of hydrogen bound to small vacancy aggregates are calculated. Both the vacancy and the self-interstitial efficiently dissociate interstitial H_2 molecules.[1] Vacancy-interstitial recombination at H_2 results in the formation of the H_2^* complex.[2] Ongoing research deals with the precipitation of H at defects. The very stable ring-hexavacancy,[3] an ellipsoidal void of diameter 7.8 Å and thickness 4.4 Å, is used as a model defect to study what happens when numerous H interstitials successively interact with such a defect. We also begun to study the interactions between self-interstitials, the formation of stable aggregates of $n = 2, 3, \ldots$ self-interstitials, and the trapping of H at such aggregates. This talk will begin with a summary of recently published results, continue with an overview of ongoing research, and conclude with a few speculation. Movies of molecular-dynamics simulations will be shown.

12:00
S I
4

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[1] S.K. Estreicher, J.L. Hastings, and P.A. Fedders, Phys. Rev. B **57**, R12663 (1998).
[2] S.K. Estreicher, J.L. Hastings, and P.A. Fedders, Phys. Rev. Lett. (in print).
[3] S.K. Estreicher, J.L. Hastings, and P.A. Fedders, Appl. Phys. Lett. **70**, 432 (1997).

INTERACTIONS OF HYDROGEN WITH SILICON AND CONSEQUENCES FOR DEVICES

Chris G. Van de Walle

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The recent resurgence of interest in the properties of hydrogen in semiconductors has been driven by a number of exciting developments: enhanced stability of defect passivation by using deuterium instead of hydrogen; hydrogen-induced exfoliation for producing silicon-on-insulator structures (the Smart-Cut® process); better control of hydrogen's influence on doping; and experimental observation of interstitial H_2 molecules.
A thorough understanding of the underlying mechanisms is essential for exploiting these processes. First-principles computations have significantly contributed to our body of knowledge about hydrogen-related phenomena; in this talk I will review our current understanding, and focus on recent work addressing the issues outlined above. The computational results have all been obtained using a state-of-the-art first-principles approach based on density-functional theory, *ab initio* pseudopotentials, and a supercell geometry. On the issue of stability of Si–H bonds, I will discuss the dissociation path and the connection to vibrational properties of the system; this immediately explains the enhanced stability of Si–D bonds. I will also discuss an exchange process between trapped and interstitial hydrogen that plays a significant role in diffusion processes. Relating to hydrogen-induced exfoliation, I will discuss current views on formation and structure of platelets. For hydrogen molecules, finally, I will describe the theoretical framework for understanding the physics of incorporation of a strongly bound molecule in a semiconducting environment.

14:00

S II

1

I gratefully acknowledge collaborations with B. Tuttle, C. Herring, W. Jackson, N. Johnson, N. Nickel, and R. Street.

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ENERGY LEVELS FOR MUONIUM IN SILICON AND GERMANIUM AND ELECTRICAL ACTIVITY AT HIGH TEMPERATURES

S. F. J. Cox, R. L. Lichti [†], K. H. Chow [‡], E. A. Davis [§], T. L. Estle [♯], B. Hitti [♮], E. Mytilineou [§], C. Schwab [♭], A. Amato [¶], A. Schenck [⋄], M. Charlton [*] and P. Donnely [*]

ISIS Facility, Rutherford Appleton Lab (OX11 0QX) and University College London
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Investigations of the transitions between the various sites and charge states of muonium in Si and Ge are described and the inferences for hydrogen considered.
The experiments use the μSR techniques of muon spin rotation, relaxation and resonance. These are capable of detecting the charged (diamagnetic) and neutral (paramagnetic) muonium states with equal sensitivity on a microsecond timescale, generally before reaction and pairing with other defects, dopants or impurities. State conversions are most readily recognised via relaxation (depolarization) in longitudinal magnetic field: one-way reactions, spin-exchange and two-way reactions involving capture and loss of carriers can all be distinguished. Field scans identify the active neutral centre by determining the intermittent hyperfine constant. Radiofrequency resonance is uniquely valuable in analysing for the final state in a reaction sequence. In high transverse magnetic field a paramagnetic shift of the muon Larmor precession signal is observed in charge-exchange regimes which indicates that muonium spends a surprisingly high fraction of its time in the neutral state above 600K, despite the rapidity of electron capture and loss. 15:00 S II 2
A 4-state model (Mu^+_{BC}, Mu^0_{BC}, Mu^0_T and Mu^-_T) and corresponding configuration-coordinate diagram are consistent with the data and most theoretical input. Values for most of the relative energy levels and barriers, together with probabilities of site-change, ionization and carrier capture are available for Si. Preliminary values for Ge indicate that the potential energy surface for the neutral centres is much flatter than for Si, with the bond-centred (BC) and cage-centred (T) sites more nearly equal in energy than in Si and the barrier between them smaller. Both sites may be visited in the course of diffusion above 100K (contrary to Si, where only the T-site neutral is mobile); site changes without charge-state change remain slow at all temperatures in Ge so that the two single-site ionization energies may be measured separately. The BC site is the more stable by a small margin. The importance of both T and BC sites is also established in amorphous material.
The electrically active levels within the fundamental gap may be constructed from relevant level separations in the configuration coordinate diagram. (Since donor and acceptor levels involve energy differences, the isotope effects between muonium and hydrogen are expected to be relatively small.) The experiments are close to determining the site-change energies which are crucial to deciding whether muonium constitutes a negative-U centre in these materials.

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EFFECT OF HYDROGEN ON THERMAL DOUBLE DONOR FORMATION IN SILICON

L. Murin, V. P. Markevich, J. L. Lindström[†] and T. Hallberg[†]

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16:30
S II
3

We start with an overview of the previously published data on the problem. The main unanswered questions are noted and discussed. We report also some new information on the peculiarities of the very early stages of oxygen clustering in hydrogenated Si. The data are obtained from the studies of the formation kinetics at 350–400 °C of small oxygen clusters (dimers, trimers and the first TDD species) in Czochralski-grown Si crystals pre-heat-treated at high temperature in the hydrogen gas. It is argued that hydrogen affects the migration ability not only of the interstitial oxygen atoms but of the small oxygen aggregates as well. With this in mind the possible TDD formation schemes are considered.

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Friday April 16

HYDROGEN-DEFECT COMPLEXES IN SILICON: FACT AND SPECULATION

B. Bech Nielsen

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9:00
S III
1

The atomic structure of the complexes formed when hydrogen becomes trapped by intrinsic defects in silicon can be investigated by structure sensitive techniques and *ab initio* theory. In particular, FTIR spectroscopy has been widely applied to study the local vibrational modes of hydrogen, which depend critically on the atomic structure of such complexes. From comparison of the observed modes with those calculated by *ab initio* theory, it has been possible to identify specific complexes in several cases. Moreover, valuable information about the electronic structure of a few hydrogen-defect complexes has recently been obtained by EPR, and a detailed picture has emerged from these correlated studies.
In this talk, an overview of our major findings on hydrogen-vacancy, hydrogen-interstitial, and hydrogen-impurity complexes will be presented and a few new results will be presented. At the end of the talk, it will be discussed how local mode frequencies may be assigned to specific structural units. On basis of this, tentative assignments will be suggested and their implications for diffusion and trapping of hydrogen will be briefly discussed.

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ELECTRICAL PROPERTIES OF TRANSITION METAL-HYDROGEN COMPLEXES IN SILICON

J. Weber

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10:00
S III
2

Our recent studies on the properties of hydrogen in silicon doped with transition metals (TM) are summarized. In particular, we will concentrate on the substitutional TMs with their simple vacancy-like structure. Hydrogen was incorporated in the samples by wet chemical etching at room temperature or by hydrogen plasma treatment at elevated temperatures. Deep-level-transient spectroscopy (DLTS) on Schottky diodes reveals many new levels which are associated with transition metal-hydrogen complexes. The analysis of the deep level profiles gives valuable information about the number i of hydrogen atoms in the TM–H_i complexes and in addition gives evidence for electrically passive complexes. All hydrogen related features disappear after heat treatments above 600 K for several hours. Systematic trends in the TM–H_i level positions are discussed and compared to available experimental data and theory.

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DEFECT PROFILES AND THE FEKLISOVA–YARYKIN CONJECTURE

J. Coomer, A. Resende, R. Jones, S. Öberg † and P. R. Briddon ‡

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‡ *Department of Physics, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU*

Deep level transient spectroscopy (DLTS) is a technique which allows the activation energies for the emission of carriers from deep levels to band edges to be measured. In many cases the energy level of the defect can then be extracted. However, a major drawback with the technique is that the chemical composition of the defect cannot be obtained and the types of atoms which make up the defect are then assumed to reflect the composition of the crystal. This of course does not provide any indication of the number of impurity atoms in the defect. This problem is particularly acute for H related defects where, for example, it is known from infrared absorption spectroscopy carried out on mixed H and D implanted material that vacancies in Si and Ge can be decorated from 1 to 4 H atoms. Feklisova and Yarykin have recently suggested a way in which mapping the concentration profile of the defect might yield its composition. They investigated the trapping of two defects created by electron irradiation, namely the VO defect (*A* centre) and a complex involving O and possibly C called the K centre. The former has a $(-/0)$ level at $E_c - 0.17$ eV and the latter acts as a hole trap with a level of unspecified character at $E_v + 0.33$ eV. This is close to the level for C_iO. H was introduced at room temperature using a wet chemical etch. New defects were then created and, in particular, E4 and E5 which are VO–H_n and C_iO_i–H_n defects respectively with levels at $E_c - 0.32$ and $E_c - 0.36$ eV. In addition, two unspecified hole traps H3, H4 lie at $E_v + 0.16$ and $E_v + 0.27$ eV. Now the profiles demonstrated that the concentrations of E4 and E5 behaved as $e^{-2x/L}$ and $e^{-x/L}$ respectively from which it was concluded that E4 was VOH_2 and E5 possesses only one H atom. With the above assignment this is then the C_iO_iH defect. However, the VOH_2 defect is expected to contain only saturated bonds and thus be inactive. This raises serious questions over the Feklisova and Yarykin analysis.

11:20
S III
3

In order to investigate this, we have carried out first principles calculations with an empirical correction to ascertain the electrical levels of these defects. We find that the VOH_2 defect is inactive but VOH has a deep acceptor level.

We suggest that a better test of the Feklisova and Yarykin conjecture are depth profiles of V_2H_n defects with $n = 1, 2, 3, 4$ and 5. The structures and levels of these defects are reported.

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ACCEPTOR-LIKE HYDROGEN DIMERS IN SILICON

B. Aradi and P. Deák

Technical University of Budapest, Department of Atomic Physics,
Budapest, Budafoki út 8, H-1111, Hungary

12:15
S III
4

Recently it has been shown that luminescence at 1.151 and 1.138 eV in crystalline silicon is due to the recombination of excitons bound to isoelectronic acceptors containing two hydrogen atoms. Both centers are trigonal — in one of them the hydrogens are in equivalent positions, in the other one they are inequivalent. Both centers give rise to acceptor levels near the conduction band edge. The results of LDA-calculations on various hydrogen dimers will be presented to explain these observations.

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LAPLACE TRANSFORM DLTS STUDIES OF GOLD-HYDROGEN DEFECTS IN SILICON

A. R. Peaker, J. H. Evans-Freeman and L. Dobaczewski[†]

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We have used the technique of high resolution DLTS to study hydrogen-related complexes in silicon. Instead of using the rate window DLTS techniques pioneered by Lang, we have applied methods analogous to an inverse Laplace Transform to analyse carrier emission transients. In practice we use a form of Tikhonov regularisation (optimised for our experimental set up) to averaged isothermal carrier emission transients. With a signal to noise ratio of 1000:1 (in the averaged spectrum) we can routinely separate exponentials with a time constant ratio of 2:1. In practical terms this means we can achieve an order of magnitude improvement in resolution over conventional DLTS provided we have a suitable concentration of the defect (typically $0.1\,(N_d - N_a) > N_T > 0.01\,(N_d - N_a)$) and there are no other complicating factors (e.g. strong field dependence of the emission rate). This brings the technique into a regime where it is possible to quantify the effects, for example, of uniaxial stress or the local environment (e.g. in alloys) on carrier emission properties of a deep state. Over the last year we have used the technique to examine the properties of gold-hydrogen defects in silicon. We have diffused gold into n- and p-type material and then introduced hydrogen by wet etching. The high resolution DLTS measurements have been carried out on Schottky diodes.

14:00
S IV
1

Our results at low hydrogen concentration are in good agreement with previous conventional DLTS studies, and furthermore, we are able to separate quite clearly the gold acceptor and G4 and conclude from capture measurements that G4 is an acceptor. At higher hydrogen concentrations we see evidence of another state with electron emission characteristics close to G4 which we call G4′. From the dependence on hydrogen concentration it seems that this is AuH_2 assuming the previous assignment of G4 to the $-/0$ charge state of AuH to be correct. The state referred to as G1 which is believed to be the double acceptor ($=/-$) of AuH shows no fine structure in high resolution DLTS, even at high hydrogen concentrations. We observe two additional defect signatures in n-type material in high hydrogen layers, which are quite undetectable at low hydrogen concentrations. These states are also in high hydrogen material that does not contain gold but the defect states appear to be present in lower concentrations. Work is currently in progress to try to identify these hydrogen-related deep levels.

In p-type material the situation is somewhat more complicated. Hole emission is observed from the state assigned G2 by previous workers which is thought to be the donor state of AuH (0/+). From our high resolution DLTS measurements, G2 seems to exist in two configurations dependent on the hydrogen concentration and the history of the sample. We have undertaken uniaxial stress measurements on this centre and see splitting which we associate with a metastable reorientation of the defect under stress.

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ELECTRIC FIELD DEPENDENT STRUCTURAL AND VIBRATIONAL PROPERTIES OF THE SI(100)-H(2×1) SURFACE AND ITS IMPLICATIONS FOR STM INDUCED HYDROGEN DESORPTION

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15:00
S IV
2

I will report a first principles study of the structure and the vibrational properties of the Si(100)–H(2×1) surface in an electric field. From the calculations one can extract parameters which can be used to model the vibrational modes in the presence of the electric field corresponding to a realistic STM tip-surface geometry. Such models show that local one-phonon excitations have short lifetimes (10 ps at room temperature) due to incoherent lateral diffusion, while diffusion of multi-phonon excitations are suppressed due to anharmonic frequency shifts and have much longer lifetimes (10 ns at room temperature). The implications for current induced desorption of H are calculated using a recently developed first principles model of electron inelastic scattering. The calculations show that inelastic scattering events with energy transfer $n\hbar\omega$, where $n > 1$, play an important role in the desorption process.

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HYDROGEN-PASSIVATION OF DOUBLE DONORS IN SILICON: ATOMIC AND ELECTRONIC STRUCTURE

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Over the last ten years, the full passivation by hydrogen of shallow single donors and acceptors in silicon has been extensively investigated, both by experimental and theoretical methods as a result these passivated dopants have become well-understood defects. In some contrast, the understanding of the more complex and varied processes of passivation of deep electronic center is still not on a satisfactory level. The structure and corresponding electrical activity of hydrogen complexes with deep centers have proven to be intriguing results are controversial in several cases. The interactions of hydrogen with the chalcogen double donors are good examples of this situation. Experiments using deep level transient spectroscopy (DLTS),[1] infrared absorption[2] and magnetic resonance[3] showed that hydrogen can passivate the sulfur double donor in silicon. However, there still is dispute about the number of hydrogen atoms participating in the passivation process and about the question whether a single hydrogen complex will behave as a, possibly shallow, single donor. In our experiments the hydrogen passivation of the chalcogen double donors sulfur and selenium was studied. New results, to be reported, were obtained for selenium they will be put in perspective by comparing to the experimental[1−3] and theoretical[4] data available for the sulfur-hydrogen system. For selenium two new electron paramagnetic resonance (EPR) spectra, labeled Si-NL60 and Si-NL61, were observed. The spectra, both revealing trigonal symmetry, have been investigated in detail by ENDOR (electron-nuclear double resonance) and FSE (field-scanned ENDOR). By the use of both natural and isotopically enriched selenium (isotope ^{77}Se, nuclear spin $I = \frac{1}{2}$, natural abundance 7.6%, enriched 99.1%) the involvement of one selenium in the passivated centers was conclusively established. From the hyperfine structure due to hydrogen or deuterium, using heavy water with 99.95%, the presence of hydrogen was concluded. The Si-NL60 spectrum displays the nuclear interaction with one hydrogen atom. From the hyperfine and quadrupole interactions its is concluded that the corresponding center is very similar to the sulfur-hydrogen pairs (EPR spectra Si-NL54 and Si-NL55). The paramagnetic state most probably corresponds to the neutral charge state of a Si:SeH single donor. The other spectrum, Si-NL61, reveals hyperfine interaction with two inequivalent hydrogen atoms. For this Si:SeH2 center no corresponding sulfur-two-hydrogen pair was reported in preceding magnetic resonance experiments. The electronic and nuclear spin-Hamiltonian parameters of the Si-NL60 and Si-NL61 centers were determined by EPR and ENDOR. Models for atomic and electronic structure will be discussed on the basis of this information. Thermal annealing studies showed the centers to be stables up to temperatures around 600 °C. This result confirms the more stable bonding of hydrogen to double donors compared to the single ones. Measurements of annealing and conversion kinetics, applying uniaxial stress as well, are in progress.

16:30
S IV
3

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COMPLEXES OF GROUP-VI DONORS WITH HYDROGEN IN GAP

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Photoluminescence measurements on sulfur-doped GaP performed before and after exposure to a radio frequency hydrogen plasma[1,2] suggested that hydrogen neutralizes group- VI donors in GaP. However, to our knowledge, group-VI donor-hydrogen complexes have not been directly evidenced until now in this material.

Sulfur, selenium and tellurium doped LEC grown GaP samples have been investigated by local vibrational mode (LVM) spectroscopy; as it is always the case for this type of material, hydrogen is also present in the samples with a concentration in the 10^{15}–10^{16} cm^{-3} range. LVM's at 2204, 2210 and 2217 cm^{-1} at 5 K are due to complexes of hydrogen with sulfur, selenium and tellurium respectively; sulfur doped deuterated samples have also been investigated and the LVM due to the sulfur-deuterium complex is at 1617 cm^{-1}. These wave numbers indicate that hydrogen binds one of the host phosphorus atoms which are next
17:30 nearest neighbors of the group-VI donor. It has to be noted that no bending modes of the
S IV complexes could be observed.

4 Experiments under uniaxial stress have been performed. Their results cannot be interpreted in the frame of the conventional models.[3,4] A new model has been developed. It shows that the complexes have C_s symmetry and that the symmetry planes of the complexes are (110) and equivalent planes. The precise orientation of the induced electric dipole moment of the LVM in this plane is determined for each complex. The P–H bond is not along one of the main crystallographic axes as it is usually the case for hydrogen-shallow dopant complexes. A complete microscopic description of the complexes is given.

It comes out that the group-VI donor-hydrogen complexes in GaP are completely different from those observed in GaAs and AlSb where hydrogen binds one of the host group-III atoms nearest neighbors to the donor.

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POSTERS

HYDROGENATION OF ELECTRON IRRADIATION DAMAGE IN SILICON

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Using high resolution Laplace DLTS, we have measured the electron emission characteristics of the di-vacancy and related defects in electron irradiated silicon. The irradiation was with 2 MeV electrons. A comparison has been made before and after room temperature diffusion of atomic hydrogen from the surface, which was introduced by wet chemical etching.

P 1 We identify the reaction products of hydrogen and the A centre as an electron trap with an activation energy of ~ 0.31 eV and in addition one or more inert species. By comparison with *ab initio* calculations we also assign Laplace DLTS features to the reaction products of the di-vacancy and hydrogen. These defects are very close in emission characteristics to the states previously assigned to the divacancy, but can be clearly separated using the Laplace technique.

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HYDROGEN INTERACTION WITH DISLOCATION SOLITONS IN SI

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It is well known that hydrogen interacts with dislocations in silicon. For example, dislocation velocity in the presence of hydrogen plasma is enhanced with the barrier to motion dropping from 2.2 eV to 1.2 eV.[1] However the nature of these interactions are not well understood. Dislocation motion can proceed either through reconstructed kink formation and migration, through the formation and propagation of reconstruction defects ("solitons"), or a combination of the two. It has been proposed that solitons are responsible for, amongst other things, kink relaxation dynamics.[2] Therefore a thorough understanding of the behaviour of solitons is crucial to understanding the mechanisms of dislocation motion.

P 2 In order to understand the interaction between hydrogen and solitons, we examine several possible bonding configurations between the two. We find that hydrogen can bond strongly to isolated solitons. We determine the vibrational characteristics of such hydrogen-soliton centres, and discuss the implications of soliton-hydrogen interactions for dislocation motion.

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[1] Y. Yamashita, F. Jyobe, Y. Kamiura, K. Maeda, Phys. Stat. Solidi A **171**, 27 (1999).

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DONOR FORMATION IN GERMANIUM BY HYDROGEN PLASMA TREATMENT

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A spreading resistance probe analysis of hydrogen-plasma-treated Ge crystals with different concentrations of shallow dopants and oxygen is presented. The samples were treated in dc H-plasma at 260, 300 and 350 °C for 0.5 and 1.5 hours. An enhanced formation of donor centers was observed in all the treated samples. The appearance of *p*-*n* junctions was revealed in *p*-type Ge.

The formation of O–H complexes and oxygen-related thermal donors is suggested to occur in Ge:O crystals under H-plasma treatment.

P 3

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SHALLOW DONOR CENTERS IN HYDROGENATED CZ-SI CRYSTALS

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The results of EPR and infrared absorption studies of shallow donor centers which are introduced into hydrogenated Cz-Si crystals as a result of electron irradiation and/or heat-treatments in the temperature range of 300–500 °C are reported. It is shown that the same shallow donor species are generated in both the pre-irradiated and non-irradiated Cz-Si:H crystals during heat-treatments at about 470 °C. Preliminary irradiation was found to result in enhanced formation of the donors. The possible atomic structures and formation mechanisms of the shallow donors in hydrogenated Cz-Si crystals are discussed.

P 4

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MUONIUM AS A HYDROGEN ANALOGUE IN SILICON AND GERMANIUM; QUANTUM EFFECTS AND HYPERFINE PARAMETERS

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P 5

We present an all–electron theoretical study of muonium and hydrogen impurities in silicon and germanium. The electron–electron interactions are described within density functional theory using the local density approximation and a generalized gradient approximation. A double adiabatic approximation is employed and we minimize the energy of muonium or hydrogen at the bond–centred site with respect to all degrees of freedom. At this level of approximation the relaxations of the host atoms are different for the muon and proton. The extra relaxations of the silicon and germanium atoms due to the zero–point motion of a muon at the bond centred site are quite small, while those for the proton are even smaller. The zero–point energy for a muon at the bond centred site is considerably larger than at the tetrahedral site. When zero–point motion is included the muon is more stable at the tetrahedral site than at the bond–centre. The hyperfine and superhyperfine parameters are calculated as averages over the motion of the muon, and are compared with previous calculations and with experiment.

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AB INITIO SIMULATION OF HYDROGEN IN SILICON

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P 6

We present the results of ab initio path integral molecular dynamics calculations of hydrogen in silicon. The technique used is based on the Feynman path integral formulation of quantum mechanics, which is used to treat the atomic nucleus as a quantum object. Standard DFT techniques are used to treat the electrons in an ab initio fashion. This combined approach enables us to properly treat quantum fluctuations such as tunneling and zero point motion of the hydrogen atom.

The detailed properties of hydrogen are often probed experimentally by the muSR technique. Although muonium is chemically identical to hydrogen, it has a smaller mass and may therefore be substantially affected by quantum nuclear fluctuations, such as zero point motion and tunneling. There is therefore a need to simulate the properties of both hydrogen and muonium in silicon and test the effect of such fluctuations. Similar calculations for muonium are underway.

The results that we present show that these nuclear quantum fluctuations can make a significant difference to the energetics and structures formed. This therefore has important implications for the interpretation of experimental results and our basic understanding of the properties of hydrogen-like atoms in silicon.

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A NOVEL VACANCY-RELATED MUON SPECIES IN CRYSTALLINE SILICON

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The positive muon (μ^+) can be considered as light isotope of hydrogen from the viewpoint of solid-state physics. It is an ideal tool for the study of isolated centres in semiconductors which are analogous to hydrogen centres. Low-temperature investigations of positive muons (μ^+) in crystalline silicon by means of two different techniques provide us with evidence of a novel paramagnetic muon species with weak, anisotropic hyperfine interaction (Solid State Comm. **107**, 395 (1998)). It adds to the list of known muon species, i.e. normal (tetrahedral position, $\mathrm{Mu_T}$) and anomalous (bond-centered position, $\mathrm{Mu_{BC}}$, analogous to the AA9 hydrogen centre) muonium and the diamagnetic muon species. The signatures of the novel species $\mathrm{Mu_V}$ are found in intrinsic but not in doped samples (dopant concentration about 10^{16} cm^{-3}). Longitudinal field quenching experiments reveal that $\mathrm{Mu_V}$ is not formed promptly. It results from a reaction in which normal muonium transforms into $\mathrm{Mu_V}$, the reaction rate at $T = 10$ K was found to be about 10^6 s^{-1}. The hyperfine coupling of $\mathrm{Mu_V}$ is determined from zero-field muon spin precession experiments. The hyperfine tensor is found to be axially symmetric with the components $A_\mathrm{x} = A_\mathrm{y} = -12.0$ MHz and $A_\mathrm{z} = 28.75$ MHz, with the z axis pointing into the $\langle 110 \rangle$ crystallographic direction. It corresponds, after rescaling, to the hyperfine tensor of the hydrogen centre termed VH, which was discovered recently by Bech Nielsen *et al.* (Phys. Rev. Lett. **79**, 1507 (1997)) and which has been attributed to hydrogen trapped in vacancies. This novel muon species $\mathrm{Mu_V}$ is tentatively interpreted as muonium trapped in vacancies, which are created during deceleration of the implanted muon close to the end of its stopping track.

P 7

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NEUTRAL FRACTION OF MUONIUM AND HYDROGEN IN SILICON AT ELEVATED TEMPERATURES

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P 8

Measurements of a paramagnetic shift of the muon Larmor frequency in silicon indicate that muonium — and by inference hydrogen — defect centres spend a surprisingly high proportion of their time in the neutral charge state above 600 K, despite the rapidity of electron loss (ionization) and recapture. The data should allow determination of the relevant electrically active energy level.

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HIGH FIELD EPR & ENDOR MEASUREMENTS ON V_NH COMPLEXES IN SILICON

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P 9

Proton irradiated silicon samples have been studied with magnetic resonance. The EPR experiments have been conducted at X, K, and D microwave bands of 9, 23, and 140 GHz, respectively.
Hyperfine interactions have been carefully followed by ENDOR. The measurements were performed at different temperatures and microwave power levels.
The obtained spectra and their angular dependences are compared with simulations based on the existing models of V_nH centers (VH, V_2H, V_3H).

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HYDROGEN-RELATED COMPLEXES IN SIC

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Hydrogen is the main impurity in silicon carbide (especially in CVD-grown layers) which is the most promising semiconductor at present for high power/temperature/frequency applications. *Ab initio* LDA calculations have been used to study hydrogen related defects in intrinsic SiC. Relative stabilities, occupation levels and vibrational modes have been calculated and compared to existing experimental data. Interesting differences with respect to H in Si have been found.

P 10

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A MUON STUDY OF CZOCHRALSKI SILICON AT HIGH TEMPERATURES

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Czochralski silicon contains high levels of oxygen, which, during anneals between 570–820 K, forms thermal donor complexes. Complex formation is enhanced by the presence of hydrogen which is believed to catalyse the oxygen diffusion, although the precise mechanism for this is still a matter of investigation.

Much of our knowledge of isolated hydrogen behaviour in silicon has come from studies of the behaviour of its light isotope muonium, formed by implanting spin polarised positive muons. Above room temperature, the muon polarisation decay follows a simple exponential, and this is believed to be due to a charge exchange (CE) reaction involving repeated ionisation of muonium followed by electron capture.

In this study we present results from muon investigations of Czochralski silicon at high temperatures. A sample heat treated to precipitate the oxygen shows very similar behaviour to float zone material when the CE model is applied; the CE model seems to describe untreated material much less satisfactorily, and this is attributed to the presence of oxygen. Observation of the muon behaviour in this latter case provides information on the nature of the muon species involved and may help elucidate the role of hydrogen in oxygen diffusion.
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P 11

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LOCAL VIBRATIONAL MODE BANDS OF V-O-H COMPLEXES IN SILICON

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P 12

Infrared absorption study of formation and annealing of radiation-induced defects in hydrogenated Czochralski-grown silicon crystals have been performed. Hydrogen and/or deuterium was introduced into the crystals by in-diffusion from H_2 (D_2) gas at 1200–1300 °C. The samples were irradiated with fast electrons ($E = 2$-4 MeV) and annealed in the temperature range of 100–600 °C. The dominant centres produced by irradiation were found to be the same in both Si:O,H and as-grown materials: *A* centre, C_i-O_i complex and divacancy. A profound effect of hydrogen was revealed in the annealing behaviour of radiation-induced defects. The disappearance of them in hydrogenated crystals occurred at lower temperatures beginning from 100 °C and was followed by a creation of a number of new infrared absorption bands in wavenumber regions characteristic for the oxygen- and hydrogen-related local vibrational modes (LVMs) in silicon. Disappearance of A centres in the temperature range of 100–150 °C was found to correlate with the appearance of three LVM bands at 943.5, 2126.4 and 2151.5 cm^{-1}. Substitution of hydrogen by deuterium resulted in a shift of the lines to 943.2, 1549.1 and 1567.4 cm^{-1}. In the samples co-doped with H and D in addition to these lines two other ones were observed at 1557.3 and 2140.6 cm^{-1}. It was suggested that the lines are related to LVMs of a complex V-O-H_2. The complexes are formed by the interaction of mobile hydrogen molecules with the A centres. The V-O-H_2 complex is stable up to 200 °C. Simultaneously with the disappearance of the LVM bands due to V-O-H_2 complex at higher temperatures an absorption band at 891.5 cm^{-1} was developed. A line at the same position was observed in deuterated samples. No correlation was found between the appearance of this band and the development of any bands in the range which is characteristic for stretching vibrations of hydrogen (deuterium) atoms in Si. The line at 891.5 cm^{-1} is preliminary identified as related to the stretching vibrations of oxygen atoms in a complex VO_2 with a hydrogen molecule in the vicinity.

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VIBRATIONAL MODES OF VOH_2 IN SI

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The structure and vibrational modes of VO–H_2 defect in Si are calculated using a first principles cluster method (AIMPRO). The calculated modes are compared with those reported by Markevich *et al.* at this conference. P 13

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THE ELECTRICAL PROPERTIES OF TRANSITION METAL HYDROGEN COMPLEXES IN SILICON: A THEORETICAL STUDY

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The electrical levels of various combinations of transition metal–H_n defects in Si are calculated and compared with recent transient capacitance measurements. Spin-polarised local density functional cluster theory is used. The shifts of these levels with H can be understood through a displacement and splitting of the gap t_2 manifold of states due to the impurity. Passive defects are identified. The similarities between Au– and Ag–H defects, and Pt– and Pd–H defects are discussed. P 14

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THEORETICAL INVESTIGATION OF THE STRUCTURAL, VIBRATIONAL AND ELECTRICAL PROPERTIES OF MULTI-HYDROGEN VACANCY DEFECTS IN SILICON

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Large H-terminated clusters ($Si_{181}H_{116+n}$) are used to simulate the properties of VH_n defects with $n = 1$ to 4 within the framework of the local spin density functional theory.

P 15

Our calculations have shown that for VH_1 and VH_2, the reconstructed bond across two Si neigbours of the vacancy plays an important role on the their vibrational and electrical properties.

The H-stretch mode frequencies are calculated within an error bar of 0.1–0.5% relatively to the observed ones. The vibrational properties of VH_3 are compared with those of V_2H_6, together with recent electron paramagnetic resonance and Fourier transform infra-red spectroscopic studies.

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NITROGEN-HYDROGEN DEFECTS IN GAP

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P 16

Models of the nitrogen-hydrogen defect in GaP, which contain one and two H atoms, are investigated using *ab initio* density functional cluster theory. We find that a single H atom binding to N possesses two infrared absorption frequencies close to those attributed to an NH_2 defect. The shift in the modes with charge state is consistent with the photo-sensitivity found for the defect. A third mode observed for this centre is assumed to be an overtone of the bend mode. The isotope shifts of the calculated modes are in excellent agreement with experiment in contrast with the model which contains two H atoms

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