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14.1 Introduction

Hydrogen, the most abundant substance in the universe, is also omnipresent on earth in the form of water, the most common liquid, following its name "hydro-gen". Being the first element in the periodic table of elements, hydrogen can show extreme properties. It is the smallest and lightest element of all. Consequently, hydrogen is frequently present as an impurity in crystals of every kind, and so too for silicon. When it is singly ionised only its nucleus, the bare proton, with dimensions of femtometres, is left. Without any core electrons, hydrogen is a unique impurity. The positively charged impurity will seek a position with maximum electron density, or lowest Coulomb potential, in the crystal, creating bonding in a typically ionic manner. In the neutral charge state, the hydrogen atom will have its 1s electron shell singly occupied. Using a different option, hydrogen can accept a second electron in this low-energy state offered by the 1s shell, which will become completely filled. This full shell is the typical form realised in covalent bonding. With these contrasting bonding schemes, the bonding of hydrogen in silicon is anticipated to be complex in its appearance. One cannot expect valid bonding models to be based on simple intuitive thinking. Rather, this is the domain of the most advanced theoretical computations. Such calculations, possible nowadays and undoubtedly possible with even greater precision in the future, have already shown the vital role of theory in the understanding of the behaviour of hydrogen in silicon. Maybe theory is having a larger impact than ever before on the physics of defects and impurities in semiconductors, with the obvious exception of shallow substitutional donors and acceptors and the celebrated effective-mass theory. Owing to its electronic structure, hydrogen is a highly reactive impurity. These expectations have been fully confirmed by the observation of interactions of hydrogen with a rich variety of impurities. including shallow and deep states, substitutional and interstitial impurities, and donor, acceptor and amphoteric impurities, from all rows and columns of the periodic table. A very special case is the interaction of hydrogen with itself in forming the H_2 molecule. This prototype of covalent bonding creates a molecule without any charge or dipole moment. In this reaction hydrogen has fully passivated its own electrical activity, a feature that hydrogen can also show in interactions with other impurities, such as acceptors and dan-

gling bonds. Several powerful experimental techniques, such as EPR, electron paramagnetic resonance, are not capable of observing passivated products, which creates a handicap for experimental investigations. Though possibly present in great quantities, hydrogen-passivated centres do not have any appreciable effect on material properties and are hard to detect. However, upon heat treatment, e.g. in device processing, passivated complexes may dissociate and reactivate the component impurities. In this way hydrogen can be responsible for unstable properties of silicon.

In the past two decades, intensive research on the effects of hydrogen in silicon has been conducted. Several methods for controlled intentional introduction of hydrogen have been developed, each with its own advantages and limitations. By exposing silicon wafers downstream from a plasma source of hydrogen atoms, silicon can be hydrogen-doped to a large concentration in a thin surface layer, typically 1 µm thick. Substrates are usually kept at an elevated temperature around 500°C. Another way to obtain shallow highly doped layers is chemical etching at room temperature, or even boiling in water, of silicon wafers. Treating samples in a wet atmosphere is a typical condition that also arises in standard IC processing. As a result, hydrogen can be introduced unintentionally and, if this is not realised, it can be responsible for unexpected phenomena and properties. A controlled introduction can be achieved by proton implantation. The range of introduction will depend on the implantation energy and can be up to several centimetres. The concentrations achieved are determined by the implantation dose and can vary widely as well. Implantation is accompanied by creation of radiation damage, with the usual requirement for thermal annealing of these defects. Diffusion at high temperatures, near 1200°C, for several hours can give uniform doping over millimetre distances.

For experimental research purposes, the method of hydrogen introduction selected will depend on the method of measurement envisaged. Shallow layers created by etching provide ideal samples for measurements by deep-level transient spectroscopy (DLTS). This sensitive technique yields concentrations and energy levels. Structural information is better obtained by spectroscopy in the infrared of vibrational modes of complexes involving the light hydrogen impurity. With two stable isotopes, the proton and deuteron, with a relative mass difference of a factor two, larger than for any other element, the identification of hydrogen modes can be safely performed. Local vibrational mode (LVM) spectroscopy is possible for all charge states of the defects. Even though this is not the case for magnetic resonance, this latter technique is still very suitable for detection and characterisation of hydrogen-related complexes if they are not fully passivated. Again, the availability of two isotopes is of great advantage for the identification of hydrogen in the centres. The different nuclear spins, $I_{\rm p} = 1/2$ for the proton and $I_{\rm d} = 1$ for the deuteron, give a clear distinction in the electron paramagnetic resonance (EPR) spectra. When electron-nuclear double resonance (ENDOR) can be performed, the different

nuclear magnetic moments, $\mu_{\rm p} = +2.79285 \,\mu_{\rm N}$ and $\mu_{\rm d} = +0.85744 \,\mu_{\rm N}$, allow an unambiguous identification of hydrogen. The crucial complementary role of theory has already been stressed.

Several reviews of hydrogen in silicon have been published in recent years [1–14]. These reviews include references to over a thousand original papers in the field, allowing one to follow the investigations in all details. This brief review will be limited to the discussion of four specific cases. First, single hydrogen atoms and molecules in silicon, as the basic structures, will be considered. The passivation of acceptor and donor impurities, is taken as the second and third examples. Finally, the interaction of hydrogen with transition metal impurities, as typical deep-level centres, is described.

14.2 Hydrogen Atoms and Molecules

Hydrogen is an amphoteric impurity in silicon. Depending on the Fermi level, as determined by the shallow dopants, it will assume either a positive or a negative charge state, or it may be neutral under nonequilibrium conditions. As an ionised donor, in the state H⁺, hydrogen will find its energetically most stable position in the region of highest electron density. This will be midway between two neighbouring silicon atoms, where the covalent bond between these atoms creates the highest electron density. Also, the neutral hydrogen atom will be bonded at this so-called bond-centred site, referred to as the BC site [15-23]. The negative hydrogen ion H⁻ [24-26], on the other hand, will prefer the region of lowest electron density, which is found in an interstitial space at the T site [20, 22]. The established structure models are given in Fig. 14.1 [27]. With hydrogen in the BC position, the two silicon neighbour atoms in the Si-H-Si three-centre bond move outwards from the hydrogen, possibly in an asymmetric way, to minimise the energy [15,17,19,21,22,28–30]. Theoretically calculated distances are indicated in Fig. 14.1 [22,27]. With the positive hydrogen ion situated in a region of high electron density, it is difficult to add one more electron to convert the impurity to the neutral state. In other words, a high Fermi level is required to create the neutral state, and the (+/0) donor level will be high in the bandgap. Using capacitancevoltage techniques, such as deep-level transient spectroscopy, the donor level of single hydrogen was determined as $E_{\rm d} = E_{\rm c} - 0.2 \, {\rm eV}$ [31–33]. In the earlier literature, this level, not yet identified as hydrogen-related, was labelled the E3' centre [34]. For negative hydrogen, firmly bonded on the T site with low electron density, similar arguments, but with opposite parameters, predict a lower energy for the level (0/-), where the centre will lose its electron. Experiment has determined this level to be $E_{\rm a} = E_{\rm c} - 0.56 \, {\rm eV}$, near the midgap position [35–37]. Both ions tend to be very stable, owing to the attractive electrostatic potentials in which they are accommodated. As such an option does not exist for hydrogen in its neutral state, the energy for H^0 is expected to be higher. In Fig. 14.2 [22], the energies for creation of H^- and H^+ ions



Fig. 14.1. Schematic illustrations of the location of (a) H^+ , (b) H^0 and (c) H^- in the silicon crystal. Relaxations of the silicon atoms, based on calculations presented in [22], are indicated. After Johnson and Van de Walle [27]

relative to the neutral H^0 are presented as a function of the Fermi energy, the energy which has to be transferred in an exchange of an electron with a reservoir [20-22, 29, 38]. As argued, the acceptor level $E_{\mathrm{a}}(0/-)$ is below the donor level $E_{\mathrm{d}}(0/+)$, which is reminiscent of centres with a negative correlation energy U. In the present case $U = E_{\mathrm{a}} - E_{\mathrm{d}} = -0.36 \,\mathrm{eV}$ [35], but the large energy gain is due to the different lattice sites occupied by hydrogen in its oppositely ionised states. This feature distinguishes the case of hydrogen from documented negative-U systems in silicon, such as the lattice vacancy and the interstitial boron impurity. In these latter cases energy is gained from Jahn-Teller-driven lattice distortions. Inspection shows that the energy





Fig. 14.2. Qualitative indication of the relative stability of different charge states of a hydrogen interstitial impurity in silicon. After Van de Walle et al. [22]

of H^0 is never the lowest, with the conclusion that H^0 is an unstable species. Neutral hydrogen atoms can lower their energy by following the option $2\mathrm{H}^0 \rightarrow \mathrm{H}^+ + \mathrm{H}^-$. Transitions between lattice sites forced by changes of charge state in the space charge region of a p-n junction have been observed [32]. The barrier height between BC and T sites was measured to be 0.29 eV. The transition rates for the proton and deuteron follow the square root of the mass ratio, indicating that the process just involves the jump of one hydrogen atom.

In its neutral charge state the hydrogen atom, with its one unpaired electron, is paramagnetic and has been observed in magnetic resonance [30, 33, 39–41]. As H⁰ is unstable, illumination of the sample is required to produce the centre and its EPR spectrum, labelled Si-AA9. An important feature of the spectrum, as shown in Fig. 14.3 [40], is the doublet structure of the main line, which is the result of hyperfine interaction with one proton, nuclear spin $I_p = 1/2$. In deuterated material, the splitting is threefold since $I_{\rm d} = 1$, with a smaller splitting corresponding to the smaller nuclear magnetic moment of the deuteron. From the angular dependence, the centre symmetry has been determined as trigonal, providing confirmation of the BC site model. A close correspondence has been established between these EPR experiments on hydrogen and muon spin rotation studies of the positive anomalous muon and of the muonium atom [42-46]. The muon can be considered as a light isotope of hydrogen, with identical bonding behaviour in crystals of the diamond structure [47]. Table 14.1 summarises data for the two systems obtained by experiment and theory [41, 43, 48-51]. It has been concluded that hyperfine interactions with the proton and muon scale in proportion to the nuclear moments, giving a factor 3.17 for μ_{μ}/μ_{p} . The hyperfine interactions with the two equivalent silicon nearest-neighbour atoms in the Si- μ /p–Si bond are practically equal. This demonstrates the equivalence of the two cases and renders the muon a valuable substitute for hydrogen studies without the handicap of



Fig. 14.3. Electron paramagnetic resonance spectrum Si-AA9 of neutral hydrogen in silicon. Hyperfine interactions with ¹H and ²⁹Si are indicated by *arrows*. Observation conditions: sample illuminated, temperature 77 K, magnetic field parallel to $\langle 100 \rangle$, microwave frequency 37.47 GHz. After Gorelkinskii and Nevinnyï [40]

Table 14.1. Hyperfine parameters, obtained from EPR and μ SR experiments and from spin-density functional theory, for the centre $(H_{BC})^0$ and anomalous muonium, Mu^{*}. After Ammerlaan and Huy [52]

Centre	Nucleus	$A_{ }$	A_{\perp}	a	b	Method	Reference
		(MHz)	(MHz)	(MHz)	(MHz)		
$(\mathrm{H}_{\mathrm{BC}})^{0}$	$^{1}\mathrm{H}$	-6.2	-31.4	-23.0	8.4	EPR	[41]
Mu^*	Mu	-16.82	-92.59	-67.33	25.26	μSR	[50]
Mu^*	Mu	.9.6	-57.3	-35	22.3	Theory	[51]
$(H_{BC})^0$	²⁹ Si	-139.0	-72.9	-94.9	-22.0	EPR	[41]
Mu*	29 Si	-137.5	-73.96	-95.1	-21.2	μSR	[43]
Mu^*	²⁹ Si	-128	-63.5	-85	-21.5	Theory	[51]

requiring a paramagnetic state. The anisotropic part of the hyperfine interaction with the proton is understood as a dipole–dipole interaction with the electron spin density localised on the neighbouring silicon atoms. To account for the observed magnitude b = 8.4 MHz, a distance between the proton and the silicon of 1.65 Å is required [52]. Compared with the regular parameters of silicon, an outward relaxation by 0.47 Å is thus derived, in excellent agreement with theoretical results for this relaxation [27]. Both neutral and positive hydrogen are trigonal centres and are oriented along one of the four available

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 $\langle 111 \rangle$ crystal axes, with equal probability in the random case. Applying a uniaxial stress, in a suitably chosen direction, at a temperature where the hydrogen can jump between adjacent BC sites will induce a preferential alignment [30]. In the EPR spectrum, the concentrations of centres in the various distinct orientations can be monitored by the amplitudes of the corresponding resonances. Analysis of the repopulation in terms of a piezospectroscopic tensor for the trigonal case gives a negative energy per unit strain, confirming the outward relaxation of the silicon atoms with respect to the hydrogen [30]. From isochronal annealing studies carried out with samples in darkness, the reorientation process for H⁺ was found to follow first-order kinetics and an Arrhenius temperature dependence in the range 120 to 150 K. The frequency for jumps between BC sites is given by $\nu(T) = \nu(\infty) \exp(-E_{\rm a}/kT)$, where $\nu(\infty) = 2.3 \times 10^{12} \,\mathrm{s}^{-1}$ and $E_{\rm a} = 0.43 \,\mathrm{eV}$. It has thus been found that the energy barrier for reorientation, involving an elementary jump from one BC site to a neighbouring one, is essentially equal to the energy $E = 0.48 \,\mathrm{eV}$ observed for the permeation by positive hydrogen of a 2 mm thick wall at elevated temperatures in the range 1092–1200°C [53]. Figure 14.4 [54] summarises results obtained for positive-hydrogen diffusion by experimental and theoretical methods [29, 53, 55-57]. It can be concluded that a consistent



Fig. 14.4. Diffusivity of hydrogen H^+ in silicon from measurements at high temperatures by van Wieringen and Warmoltz [53], at low temperatures by Gorelkinskii and Nevinnyi [30] and at room temperature by Herring et al. [54]. After Herring et al. [54]



Fig. 14.5. Atomic structure of the H_2^* defect. After Holbech et al. [59]

set of data exists over an impressive range of temperatures and diffusion rates [54]. The solubility of atomic hydrogen at high temperatures is also given by an Arrhenius-type expression $S(T) = S(\infty) \exp(-E_s/kT)$, where $S(\infty) = 4.8 \times 10^{21} \text{ cm}^{-3}$ and $E_s = 1.87 \text{ eV}$ [53].

As in vacuum, H₂ molecules represent a stable form of hydrogen inside silicon as well. The molecule straddles the T site with almost degenerate energies for orientations along (100) and (111) but experiences a high barrier for diffusion [17, 20, 22, 23, 29, 58]. Another geometrical configuration of the hydrogen dimer consists of hydrogen atom near a BC site and a second atom on an AB site. This H^{*}₂ centre is illustrated in Fig. 14.5 [59]. It can be considered as being formed from the attraction of a single H⁺ ion on the BC site and an H^- ion on the T site [21, 23, 60–62]. It has a slightly higher formation energy than the molecule but diffuses more rapidly. As these forms of hydrogen have no gap levels and no dipole moment they are difficult to detect experimentally, and much of the modelling has come from theory. In experiments, local vibrational mode spectroscopy has been the most informative technique, both for the monatomic species and for the dimer, and has contributed to confirmation of the structural models. For H⁺ on the BC site, the reported stretch frequencies of the Si–H bond are $1990 \,\mathrm{cm}^{-1}$ for the proton and $1440 \,\mathrm{cm}^{-1}$ for the deuteron, scaling properly with mass [22, 63–65]. For the dimer H^{*}₂, the different frequencies observed for the Si-H stretch modes confirm the presence of a pair of inequivalent hydrogen positions in the defect [59, 62, 66]. Shifts induced by H/D isotope substitution can be interpreted consistently in the scheme of defects $H_{BC}\text{-}H_{AB},\ H_{BC}\text{-}D_{AB},\ D_{BC}\text{-}H_{AB}$ and $\mathrm{D}_{\mathrm{BC}}\text{-}\mathrm{D}_{\mathrm{AB}}$ and follow quite closely the square-root-of-mass dependence. Line splittings induced by uniaxial stress confirm the trigonal symmetry of the centre. In addition, the experimental frequencies are in good agreement with ab-initio local-density-functional cluster calculations.





Fig. 14.6. Spreading-resistance profiles of four boron-doped silicon samples hydrogenated at 122° C for 1 h for the lowest resistivity and 4 h for the other three resistivities. Note the different lower and upper depth scales and the greater penetration depths of atomic hydrogen for the lower boron concentrations. After Pankove et al. [69]

14.3 Passivation of Acceptors

The passivation, or neutralisation, of acceptor states has drawn attention strongly to the field of hydrogenation and to its drastic effects on semiconductor materials and device properties [67, 68]. Passivation of single substitutional acceptors in bulk single-crystalline silicon by ionised hydrogen donors H⁺ is observed in its most straightforward form as an increase of the resistivity in p-type material, as illustrated in Fig. 14.6 for the acceptor boron [69]. Passivation manifests itself also by a decrease of the free-carrier concentration [70, 71], a decrease of the photoluminescence of acceptor-bound excitons [72], the appearance of new local vibrational modes [70, 73-78] and an increase of carrier mobility [70, 71]. This latter effect distinguishes passivation from compensation. In the case of compensation, spatially unrelated donors and acceptors are present as dopants of opposite type, leading to a hole concentration $n(A^-) - n(H^+)$ and a concentration of ionised impurity scattering centres $n(A^-) + n(H^+)$. With passivation, the concentration of free carriers will be equal but the concentration of ionised impurities will be $n(A^{-}) - n(H^{+})$. At temperatures where ionised-impurity scattering governs the mobility (generally low temperatures), the passivation will thus enhance

the mobility. Passivation follows compensation through the attraction between negative substitutional acceptor impurities A^- and positive mobile hydrogen donors H^+ , but leads to new neutral centres which can be viewed, in the first instance, as donor-acceptor pairs. In this concept the donor level of hydrogen is raised into the conduction band by the nearby presence of the negatively charged acceptor. Likewise, the ionisation level of the acceptor is pushed to lower energy into the valence band by the repulsive force of the positive hydrogen donor. The bandgap is swept clean of levels, which is the essential feature of passivation. Most research has been performed on the shallow acceptor boron, with ionisation energy 45 meV, but neutralisation occurs likewise for the other group III acceptors Al, Ga, In and Tl, which have increasingly deeper acceptor levels [69, 72].

With hydrogen migrating in p-type silicon as H^+ via bond-centred sites BC, the most likely structure for a BH complex is an H^+ ion trapped on a BC site next to an acceptor A^- . This structure of a hydrogen inserted between the acceptor and a nearest-neighbour silicon atom along a bonding $\langle 111 \rangle$ direction has received much support from extensive theoretical and experimental investigations [21,73–75,78–99]. The defect model is given in Fig. 14.7a [84], with Fig. 14.7b detailing the relaxations taking place to accommodate the extra atom [99]. Numerical values of the bond lengths and displacements obtained from various theoretical calculations and from experiment are given in Table 14.2 [81,82,85,86,90,93,99–102]. One may note that in some results the Si–H distance is shorter than the B–H distance, indicating a structure where the hydrogen passivates the dangling bond on the silicon atom and trivalent boron forms more planar bonds with three silicon neighbours. Both parts are



Fig. 14.7. (a) Schematic model of the B–H complex in silicon. After Bergman et al. [84]. (b) Equilibrium configuration of the B–H centre. *Dashed circles* indicate unrelaxed positions. After Zhou et al. [99]

Table 14.2. Equilibrium geometries of the Si–H–B complex in silicon from various calculations. Si_s and B_s indicate positions in an undistorted silicon lattice. All distances in units of Å. In experiments, the boron displacement B–B_s was measured to be 0.22 Å [82], 0.28 Å [86], or 0.3 Å [102]. After Zhou et al. [99]

H–Si	H–B	$\rm Si-Si_{s}$	$B-B_s$	Reference
1.56	1.51	0.16	0.55	[100]
1.46	1.59	0.22	0.48	[81]
1.44	1.66	0.26	0.49	[93]
1.49	1.53	0.16	0.47	[101]
1.63			0.47	[85]
1.65	1.36	0.24	0.42	[90]
1.64	1.35	0.33	0.31	[99]

fully covalently saturated and have no electrical activity. In other calculations the hydrogen atom is moved more towards the boron atom and a three-centre bond is formed. There exists general, but not unanimous, agreement that the hydrogen in the BH centre is on the $\langle 111 \rangle$ axis, forming a centre of trigonal symmetry, even though the energy surface in directions perpendicular to $\langle 111 \rangle$ is very flat [84,93,102–104]. For the acceptors Al, Ga and In, with larger covalent radii, the hydrogen atom is pushed off the axis [84, 93, 95, 105–108]. In an alternative model, the hydrogen atom is placed on the antibonding site of the acceptor, on the $\langle 111 \rangle$ axis, near the interstitial T site, the position of which is indicated in Fig. 14.1c [106,109–111]. However, in most other calculations this site is found to have a larger energy than the BC site and to form a saddle point on the total-energy surface [80, 88, 90, 91, 93]. Experimental results obtained by perturbed $\gamma – \gamma$ angular correlation suggest that hydrogen can be found in both positions [112–114]. Also, the back-bonding site of a silicon neighbour of the acceptor has been suggested as a suitable hydrogen position, similar to what is shown in Fig. 14.8a for the AsH complex [115]. Most of the quantitative modelling is based on theoretical study; experiment has yielded information on the site geometry by alpha particle channelling and nuclear-reaction studies [82,83,86,114]. The experimentally most fruitful technique for studying these passivated centres has been optical absorption related to local vibrational modes [70, 74, 77, 116]. Uniaxial stress has been applied to induce level splitting and draw conclusions about the symmetry, and to induce defect reorientations and study defect kinetics [84, 117]. Dichroism has been used to uniquely monitor specific orientations. For the reorientation of the BH centre, when the hydrogen atom jumps from one BC site to another neighbouring site of the same boron atom, a potential barrier of 0.19 eV was measured [87, 117], in excellent agreement with the activation energy of $0.22 \,\mathrm{eV}$ obtained in an anelastic relaxation experiment [118] and with calculated potential profiles [88,90,91]. A deviation from Arrhenius behaviour observed at low temperatures was related to the process of thermally assisted tunnelling [119, 120]. Isotope effects have been observed that



Fig. 14.8. (a) Schematic model of the AsH complex in silicon as an example of the structure of donor-hydrogen complexes. After Bergman et al. [84]. (b) Equilibrium configuration of the P-H centre. *Dashed circles* indicate unrelaxed positions. After Zhou et al. [99]

unequivocally verify the model of one acceptor and one hydrogen atom. The high-resolution results for the stretch mode vibrations are 1905.2 cm^{-1} for ${}^{10}\text{B}{-}^{1}\text{H}$, 1904.4 cm^{-1} for ${}^{11}\text{B}{-}^{1}\text{H}$, 1393.9 cm^{-1} for ${}^{10}\text{B}{-}^{2}\text{H}$ and 1390.6 cm^{-1} for ${}^{11}\text{B}{-}^{2}\text{H}$, and provide severe test data for the theory [78,111]. The remarkably strong boron isotope effect in the deuterated complex was explained as the result of a Fermi resonance [96]. The local-mode phonons due to the stretch mode and the less-studied lower-energy wagging modes [108,121] were also observed in the Raman spectra [76, 102–104].

The acceptor-hydrogen complexes are quite stable centres, with binding energies of 1.28 eV for BH, 1.44 eV for AlH, 1.40 eV for GaH and 1.42 eVfor InH between the two elements [95]. With respect to the H₂ molecule, the energy per hydrogen atom is 0.6 eV [21,85] or 0.3 eV [23]. The thermal annealing of complexes depends sensitively on the external conditions, such as the illumination level, the carrier concentration and the presence of hydrogen traps, but typically occurs near 150°C [72,76,112,113,122–125].

Double acceptors offer the interesting option of partial or full passivation, probably correlated with the binding of one or two hydrogen atoms to the dopant impurity. Experiments on beryllium have demonstrated tunnelling motion of one hydrogen around the acceptor atom, leading to a complex ground state and complex optical spectra. From experiment it was concluded that the energy minima for hydrogen are in the $\langle 111 \rangle$ directions, as for single acceptors, leading to a tetrahedral rotor [97, 126–128]. Theory has indicated energy minima in $\langle 100 \rangle$ directions and consequently an octahedral rotor [89, 91]. Similar data for the double acceptor cadmium, provided by perturbed-angular-correlation spectroscopy, were interpreted as thermally activated tunnelling with an activation energy of 0.21 eV [129]. For the double acceptor zinc, the experiments have identified optical spectra for Zn itself, and for the hydrogen complexes ZnH and ZnH₂ [130–133]. In deep-level transient spectroscopy, the effective passivation of zinc acceptors, reducing their concentration by at least two orders of magnitude, has been observed [134]. It was shown that thermal annealing at 470°C regenerates the acceptors back to their original concentration, with a reactivation energy of 2.2 eV.

14.4 Passivation of Donors

Confirming its power as a universal passivation agent, hydrogen is also capable of neutralising dopants of donor character. It has to be noted, however, that the passivation of the shallow donors phosphorus, arsenic and antimony in silicon is less effective, compared with the figures quoted for acceptors, with maximum donor passivation efficiencies reported as 80% [135,136]. Donor activity can be reactivated by thermal annealing around 150°C, with binding energies of 1.32 eV for PH, 1.43 eV for AsH and 1.43 eV for SbH [135, 136]. The energy of a hydrogen impurity bound to a donor is only 0.1 eV lower than in the hydrogen molecule H_2 , explaining the low stability [85]. Again applying a simple donor-acceptor pairing model, the negatively charged hydrogen ion H⁻, occupying interstitial T sites, is attracted by the positive donor D⁺. The passivated donor then consists of a donor on a substitutional site and hydrogen on a nearby interstitial site. Such a model is fully confirmed by advanced theoretical analyses, which all agree on the interstitial site being antibonding to a silicon nearest neighbour of the donor [85,99,137-141]. The atomic structure of the trigonal centres, with D-Si-H ordering along a (111) axis, is illustrated in Fig. 14.8 [84,99]. Quantitative information on the relaxation around the centre, given in Table 14.3 [99, 138-140], shows that both the donor and the silicon neighbour move in the same direction, in contrast to some of the earliest results, in which opposite directions of relaxation were calculated [93, 142, 143]. The first experimental evidence of donor passivation was based on an increase of the resistivity and Hall mobility upon hydrogenation of phosphorus- and arsenic-doped silicon [137, 144]. Substantial support for the defect model was provided by infrared absorption spec-

Table 14.3. Equilibrium geometries of the H–Si–P complex in silicon from various calculations. Si_s and P_s indicate positions in an undistorted silicon lattice. All distances in units of Å. After Zhou et al. [99]

H–Si	Si-P	$\rm Si-Si_{s}$	$P-P_s$	Reference
1.69	2.84	0.66	0.18	[140]
1.66		0.59	0.14	[139]
1.65	2.72	0.52	0.14	[138]
1.62	2.81	0.56	0.10	[99]

troscopy through the observation of local vibrational modes [84,135]. The line splittings under uniaxial stress of the AsH pair confirm the trigonal symmetry [84,117]. The silicon-hydrogen stretch-mode wavenumbers of 1555 cm^{-1} for PH, 1561 cm⁻¹ for AsH and 1562 cm^{-1} for SbH depend hardly at all on the donor mass, supporting a model in which hydrogen is not a direct neighbour of the donor itself. A hydrogen/deuterium isotope effect with a ratio of the vibration frequencies of about 1.37 for both stretching and wagging modes corresponds to an ordinary global minimum in the potential-energy surface. Mössbauer experiments have revealed that Sb donors can bind two hydrogen atoms [136, 145, 146]. Also, on the basis of theoretical calculations, multiple trapping of hydrogen at shallow acceptors and donors, notably by the formation of BH₂, PH₂ and SbH₂ complexes, has been predicted [141, 147, 148].

The interaction of hydrogen with the chalcogen deep double donors sulphur, selenium and tellurium, leads to partial passivation of those centres. with the formation of shallow single donors. In infrared absorption spectroscopy, typical effective-mass-like excitation spectra were observed and three sulphur-hydrogen donors were identified, with electron binding energies of 92, 135.07 and 135.45 meV [149, 150]. The spectral shifts upon deuterium substitution prove the presence of one hydrogen atom. Taking advantage of the absence of full passivation, also magnetic resonance could also be applied to the new chalcogen-hydrogen complexes in their neutral paramagnetic states. For both sulphur and selenium, two such complexes were described as spin S = 1/2 centres, with trigonal symmetry, consisting of one substitutional chalcogen and one or two interstitial hydrogen atoms [151-156]. One of the selenium centres is interpreted in the most straightforward manner as a selenium-dihydrogen complex. By applying electron-nuclear double resonance (ENDOR), the nuclear spins and magnetic moments of the atoms in the centres were determined for the constituent nuclei ¹H or ²H and ³³S or ⁷⁷Se, resulting in their unambiguous identification. From the hyperfine interactions, the spin-density distributions in the complexes were established as being spatially very extended, consistent with their shallow-donor nature. Models allocating the hydrogen atoms to the possible BC, Si-AB or S/Se-AB sites on the $\langle 111 \rangle$ trigonal defect axis were proposed. The complete passivation of chalcogen donors by one hydrogen atom, with removal of all bandgap levels by better than a factor of 100, was concluded from DLTS [157–159]. The relevant spectra, as shown in Fig. 14.9 [157], demonstrate the absence of new levels, but shallow states may have escaped detection by this technique. Tellurium centres TeH and a tellurium-multi-hydrogen complex were observed by Mössbauer spectroscopy [146]. In the DLTS and EPR experiments, the chalcogen-hydrogen complexes were found to be stable up to 500°C [153, 157, 159–161]. The reactivation energies were determined as 1.61 eV for SH and 1.39 eV for both SeH and TeH [159]. Theoretical ab-initio modelling studies indicate configurations where hydrogen occupies sites antibonding to a nearest-neighour silicon atom as the most stable





Fig. 14.9. Passivation of the chalcogen elements S, Se and Te, measured by deeplevel transient spectroscopy, also showing reactivation of the dopants after thermal annealing at 538°C for 10 min. *Dashed-line* spectra were recorded on a reference sample, *solid curves* after hydrogenation and *dottet curves* after thermal reactivation. After Pensl et al. [157]

complex [141,162–164]. For sulphur, however, the complex with hydrogen on the BC site has an energy only 0.1 eV higher, and is, taking into account the error limits in the calculations, an additional option. For Se and Te, where the BC site has an energy higher by 0.3 and 0.8 eV, respectively, this form of complex can be excluded. Also, sites antibonding to the chalcogen atom are energetically unrealistic. All the singly hydrogenated complexes have trigonal symmetry and are predicted to be shallow donors. Doubly hydrogenated chalcogen impurities are predicted to be electrically inert. In contrast to an earlier theoretical treatment [165], modern computations provide good agreement with experimental results, in particular those from EPR.

The family of oxygen-related thermal double donors (TDDs) has an unparalleled long history of research aimed at the unravelling of its structure. At an early stage it was concluded from infrared absorption, resistivity measurements and DLTS that these complex donors with an extended core structure are also passivated by hydrogen [166, 167]. In particular, the smaller, earlier species are passivated, resulting in an effective shift of the overall ionisation energy to a shallower level. A nearly complete passivation could be achieved [168]. Thermal annealing in the range 100 to 200°C reactivates the donors, again with the earliest two species showing a behaviour that deviates from that of the later ones [168-171]. Observations made by EPR reveal quite different aspects of hydrogenation. In the EPR spectrum of the centre Si-NL10(H), the presence of hydrogen as a structural component was conclusively demonstrated by ENDOR [172, 173]. A typical spectrum, in which ENDOR transitions were recorded at frequencies symmetrically around the nuclear Zeeman frequency of hydrogen, is shown in Fig. 14.10 [172]. Taking into account the similarities between the Si-NL8 centre, commonly identified with the thermal double donor as defined by the IR absorption spectrum, and the Si-NL10(H) centre, the latter one is most readily interpreted as a hydrogenated thermal donor [174]. But it must be noted that the Si-NL10(H) centre is formed by heat treatment at 450°C, a temperature at which the TDDs passivated at low temperature have already been reactivated [171]. A solution can be found by the acceptance of two different varieties of passivated TDD with hydrogen incorporated at different sites in the complex. With the precise structure of the thermal donor still unknown, the structure of the passivation product is also not yet resolved. It will be a complex centre with low, probably triclinic, symmetry [174]. On the basis of a theoretical study, a partial passivation of the TDDs by binding one hydrogen atom has been reported [175]. An infrared absorption spectrum of one particular family of shallow thermal donors, i.e. STD(H), can possibly be associated with this single donor [176, 177]. Magnetic resonance and infrared absorption have established a link between the presence of STD(H) and Si-NL10(H) centres, suggesting their identity [178].





Fig. 14.10. (a) Hydrogen ENDOR spectrum observed after heat treatment at 470°C for 55 h of Czochralski-grown aluminium-doped silicon; (b) shift of the ENDOR frequency with magnetic field, identifying the proton nuclear g factor. After Martynov et al. [172]

14.5 Transition-Metal-Hydrogen Complexes

Common transition metals possess electronic states belonging to the 3d, 4d or 5d shell. As such states do not exist for silicon atoms or crystals, entirely new hybrid electronic structures can be created. Transition-metal impurities, therefore, unlike shallow dopants, form a strong perturbation in the electronic structure of silicon, creating deep potentials that provide options for binding electrons or holes in deep bandgap levels. Trapping and releasing carriers via these states is a relatively fast process, rendering the transition metals active recombination centres, governing carrier lifetimes. For hydrogen also, and for several other impurities as well, the transition metals are strongly attractive centres, with the result that impurity complexes are abundant. The high diffusivity of, especially, the later transition elements in the 3d, 4d and 5d series (iron, copper, silver and gold), together with their natural presence adds to the reality of such defect formation processes, either intentional or as the result of insufficient control over contamination in the environment.

In recent years extensive ab-initio theoretical calculations have been performed on the existence of transition-metal-hydrogen complexes, notably for gold, silver, palladium and platinum [179–185]. Using spin-polarised wave





Fig. 14.11. Structure and corresponding electrical levels of platinum and its complexes with hydrogen in silicon, from experiment [199, 204, 205] and theory [182]. Experimental and calculated levels are represented by *solid* and *dashed lines*, respectively. After Jones et al. [185]

functions and the local-density formalism, the stability and electronic levels of transition metals in clusters containing over 100 silicon atoms were calculated. It was found that these transition elements can bind from one to four hydrogen atoms, creating new electrically active centres of donor, (multiple) acceptor or amphoteric character. Unlike the shallow dopants, the transition elements are not passivated. For platinum, the calculated electronic levels of the isolated impurity and its hydrides PtH_n , with n = 1, 2, 3 and 4, are indicated in Fig. 14.11 [185].

Extensive experimental investigations of the electronic structure have also been carried out using DLTS. Recent results for Pd, Ag, Pt and Au, which are not always in agreement with data obtained in earlier days [186–192], are included in Fig. 14.11 as well [193–207]. A special analysis based on depth profiles has allowed the determination of hydrogen atom numbers [208]. Though in general good agreement is claimed, several discrepancies are apparent. In the experiments, no levels were detected for the TM–H₄ complexes, leading to the conclusion that four hydrogen atoms passivate all these transition metals. Also, the coincidence of calculated and experimentally measured levels is far from satisfactory at present, asking for further upgrading. Another interesting feature is provided by the different donor and acceptor level positions for gold and silver in the theory, whereas in the experiments they are reported to be equal within the error margin, handicapping the distinguishing of these impurities [185].

Experimental investigations of 3d transition metals have revealed the formation of several hydrogenated but still electrically active complexes, with up to nine new levels in the bandgap for cobalt, for example. Detailed studies by DLTS were carried out for titanium [191, 202, 209], vanadium [191, 210, 211],

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chromium [191,210–212], iron [189,190], cobalt [202,213–215], nickel [188,189, 202,216] and copper [188,189,217]. In addition, for the 4d element rhodium, the hydrogen complexes RhH_1 and RhH_2 were reported, both with two levels [218]. Complexes dissociate, recreating the isolated transition metals, at temperatures typically below 300°C. Information on the atomic and electronic structure from experiment has been provided by observations of local vibrational modes in optical absorption and from the Zeeman effect and hyperfine interactions in magnetic resonance.

By far the most thorough investigations were performed on the Pt- and Au-related complexes, in particular on the centre identified as PtH_2 [52,219-222]. This centre can be produced as a bulk defect, allowing IR and EPR measurements to be made, by hydrogenation treatment for 24 to 72 hours at 1000 to 1250°C of silicon doped with platinum. The magnetic resonance spectrum was analysed with the electron spin S = 1/2 and shows the angular dependence of a centre with the orthorhombic-I symmetry. Atomic constituents were identified on the basis of the observed hyperfine splitting patterns. The presence of one platinum atom was demonstrated by resolved hyperfine structure in three components with an intensity ratio of 0.25:1:0.25, as expected for natural platinum, where the isotope ¹⁹⁵Pt has a nuclear spin I = 1/2and 33% abundance. Two hydrogen atoms (nuclear spin I = 1/2, abundance 100%) on symmetry-equivalent positions were revealed by hyperfine structure with a ratio 1:2:1 in each of the platinum lines. Such an EPR spectrum is shown in Fig. 14.12 [223]. If the hydrogen is replaced by deuterium, spin I = 1, the number of hyperfine lines will increase to five, with



Fig. 14.12. EPR spectra of the centres $Si:PtH_2$ and $Si:PtH_3$. Hyperfine interactions with the platinum isotopes and with hydrogen characterise the structure of the spectra, indicated by *dashed arrows* for PtH_2 and *solid arrows* for PtH_3 . After Huy and Ammerlaan [223]

an intensity ratio of 1:2:3:2:1, but their mutual separation is too small to be resolved and only the appropriate line broadening is observed. Local vibrational modes at $1888.2 \,\mathrm{cm}^{-1}$ and $1901.6 \,\mathrm{cm}^{-1}$ were identified as the anti-symmetric and symmetric hydrogen stretching-mode vibrations, respectively, of PtH_2 in its paramagnetic state [222]. The observation of isotope shifts in the vibration frequencies for the centres PtHD and PtD₂ confirms the presence of two hydrogen atoms in the centre [224]. Unlike EPR, vibrational spectroscopy is not restricted to the paramagnetic state $(PtH_2)^-$ of the centre and hence the corresponding vibrations for two other diamagnetic charge states of the centre have also been reported [224, 225]. The simultaneous loss of both LVM and EPR spectra upon thermal annealing at 600°C indicates the association of the spectra with the same centre [219]. Careful investigations were made of the charge state of the centre by monitoring the presence of spectra as the Fermi level was varied. As a result it was concluded that the paramagnetic state of the complex corresponds to $(PtH_2)^-$ and that a level $(PtH_2)^2 / (PtH_2)^-$ lies between $E_c - 0.045 \,\mathrm{eV}$ and $E_c - 0.1 \,\mathrm{eV}$. The first acceptor level $(PtH_2)^-/(PtH_2)^0$ is positioned between $E_c - 0.23 \,\mathrm{eV}$ and $E_{\rm v} + 0.32 \, {\rm eV}$. These results are consistent with the DLTS data presented in Fig. 14.11. It must be concluded that hydrogenation of platinum-doped silicon leads to the formation of a double acceptor, and hence no electrical passivation. In the defect model the two hydrogen atoms have an interstitial position in an (011) plane through the substitutional platinum atom. In the analysis of the data a preference was deduced for silicon antibonding positions, outside the nearest silicon neighbours of the Pt atom. The position inside the nearest-neighbour cage, more of BC character, however, cannot be excluded yet.

EPR observations were also made of the PtH₃ complex, with trigonal symmetry [52,223,226,227]. The presence of three symmetry-equivalent hydrogen atoms is deduced from the characteristic hyperfine splitting into four components with intensities in the ratio 1:3:3:1 as observed for hydrogen, and as illustrated in Fig. 14.12. Another similar centre is $Au_s(H_i)_2$, the gold analogue of PtH₂, identified by the EPR spectrum Si-NL64 [52, 223, 226-228]. For this centre, the presence of one gold atom is indicated by four equal-amplitude resonances, reflecting the ¹⁹⁷Au isotope with its 100% abundance and nuclear spin I = 3/2. Figure 14.13 [228] shows a recorded resonance with the combined gold and hydrogen hyperfine interactions leading to the structure (1:2:1):(1:2:1):(1:2:1):(1:2:1). In LVM spectroscopy, the monohydride complexes PtH_1 and AuH_1 were identified as electrically active defects, in agreement with findings from theory and DLTS [224, 229, 230]. Remarkably, EPR spectra corresponding to these complexes have escaped detection for as yet unknown reasons. For all three EPR centres discussed, the isotropic part of the hydrogen hyperfine interaction is near 10 MHz. On comparing this strength with the coupling of an electron in the 1s state of hydrogen, with $a \approx 1400 \text{ MHz}$, one concludes that spin density on hydrogen in the complexes is very low. This can correspond to no electron in the 1s orbital and a positive hydrogen ion, or to a full 1s shell with two electrons of opposite spin and hydrogen as a negative ion. It appears that the neutral charge state H^0 is avoided, and one is tempted to conclude that the negative-U effect for isolated hydrogen, rendering H^0 unstable, is active in TM-H complexes as well.



Fig. 14.13. Part of the EPR spectrum Si-NL64 of the AuH₂ centre in silicon. The fourfold splitting is due to hyperfine interaction with the ¹⁹⁷Au isotope (abundance 100%, nuclear spin I = 3/2), the additional 1:2:1 structure reveals the presence of two hydrogen atoms. After Huy and Ammerlaan [228]

14.6 Conclusion

This review has demonstrated the activity of the hydrogen impurity in silicon for a few important cases. The treatment of the subject has been far from exhaustive. Some topics not dealt with are the interactions of hydrogen with the intrinsic crystal defects (multi)vacancies and interstitials, produced by radiation and implantation; the effect opposite to passivation manifested by the activation by hydrogen of isoelectronic impurities, such as C; the phenomenon of hydrogen-enhanced diffusion of impurities, as observed for aluminium and oxygen; the formation of hydrogen-related shallow donors; the impact of hydrogen at the Si/SiO₂ interface, at grain boundaries and its interaction with P_b centres; and hydrogen in amorphous silicon, with its application in improving solar cell materials. For these subjects, reference should be made to the literature.

References

- 1. S.J. Pearton, J.W. Corbett, T.S. Shi: Appl. Phys. A 43, 153 (1987)
- J.I. Pankove, N.M. Johnson (eds.): Hydrogen in Semiconductors, Semicond. Semimetals 34 (1991)
- M. Stutzmann, J. Chevallier (eds.): Hydrogen in Semiconductors: Bulk and Surface Properties, Physica B 170, 1–581 (1991)
- S.M. Myers, M.I. Baskes, H.K. Birnbaum, J.W. Corbett, G.G. DeLeo, S.K. Estreicher, E.E. Haller, P. Jena, N.M. Johnson, R. Kirchheim, S.J. Pearton, M.J. Stavola: Rev. Mod. Phys. 64, 559 (1992)
- S.J. Pearton, J.W. Corbett, M. Stavola: Hydrogen in Crystalline Semiconductors (Springer, Berlin 1992) pp. 1-363
- 6. S.K. Estreicher: Mater. Sci. Eng. Rep. R 14, 317 (1995)
- N.H. Nickel, W.B. Jackson, R.C. Bowman, R.G. Leisure (eds.): Hydrogen in Semiconductors and Metals (Materials Research Society, Warrendale 1998) pp. 1–455
- 8. N.H. Nickel (ed.): Hydrogen in Semiconductors II, Semicond. Semimetals 61 (1999)
- M. Stavola: Hydrogen diffusion and solubility in c-Si. In: Properties of Crystalline Silicon, EMIS Datareviews Series No. 20, ed. by R. Hull (INSPEC, IEE, London 1999) pp. 511–521
- M. Stavola: Hydrogen-containing point defects in c-Si. In: Properties of Crystalline Silicon, EMIS Datareviews Series No. 20, ed. by R. Hull (INSPEC, IEE, London 1999) pp. 522–537
- J. Weber, A. Mesli (eds.): Defects in Silicon: Hydrogen, Mater. Sci. Eng. B 58, 1–183 (1999)
- R. Jones, B.J. Coomer, J.P. Goss, B. Hourahine, A. Resende: Solid State Phenom. 71, 173 (2000)
- 13. J. Chevallier, B. Pajot: Solid State Phenom. 85-86, 203 (2002)
- 14. C.A.J. Ammerlaan, P.T. Huy: Solid State Phenom. 85-86, 353 (2002)
- 15. S. Estreicher: Phys. Rev. B 36, 9122 (1987)
- 16. B. Bech Nielsen: Phys. Rev. B 37, 6353 (1988)
- P. Deák, L.C. Snyder, J.L. Lindström, J.W. Corbett, S.J. Pearton, A.J. Tavendale: Phys. Lett. A 126, 427 (1988)
- 18. P. Deák, L.C. Snyder, J.W. Corbett: Phys. Rev. B 37, 6887 (1988)
- 19. G.G. DeLeo, M.J. Dorogi, W.B. Fowler: Phys. Rev. B 38, 7520 (1988)
- 20. C.G. Van de Walle, Y. Bar-Yam, S.T. Pantelides: Phys. Rev. Lett. 60, 2761 (1988)
- 21. K.J. Chang, D.J. Chadi: Phys. Rev. B 40, 11644 (1989)
- 22. C.G. Van de Walle, P.J.H. Denteneer, Y. Bar-Yam, S.T. Pantelides: Phys. Rev. B 39, 10791 (1989)
- 23. C.G. Van de Walle: Phys. Rev. B 49, 4579 (1994)
- 24. A.J. Tavendale, S.J. Pearton, A.A. Williams: Appl. Phys. Lett. 56, 949 (1990)
- 25. J. Zhu, N.M. Johnson, C. Herring: Phys. Rev. B 41, 12354 (1990)
- 26. N.M. Johnson, C. Herring: Phys. Rev. B 46, 15554 (1992)
- N.M. Johnson, C.G. Van de Walle: Isolated Monatomic Hydrogen in Silicon. Semicond. Semimetals 61, 13 (1999)
- 28. C.H. Chu, S.K. Estreicher: Phys. Rev. B 42, 9486 (1990)
- 29. C.G. Van de Walle: Physica B 170, 21 (1991)

- 30. Yu.V. Gorelkinskii, N.N. Nevinnyi: Mater. Sci. Eng. B 36, 133 (1996)
- 31. K. Irmscher, H. Klose, K. Maass: J. Phys. C: Solid State Phys. 17, 6317 (1984)
- 32. B. Holm, K. Bonde Nielsen, B. Bech Nielsen: Phys. Rev. Lett. 66, 2360 (1991)
- B. Bech Nielsen, K. Bonde Nielsen, J.R. Byberg: Mater. Sci. Forum 143–147, 909 (1994)
- L.C. Kimerling, P. Blood, W.M. Gibson: Defect states in proton-bombarded silicon at T < 300 K. In: Defects and Radiation Effects in Semiconductors 1978, ed. by J.H. Albany (Institute of Physics, Bristol 1979) pp. 273-280
- 35. N.M. Johnson, C. Herring, C.G. Van de Walle: Phys. Rev. Lett. **73**, 130 (1994)
- 36. N.M. Johnson, C. Herring, C.G. Van de Walle: Phys. Rev. Lett. 74, 4566 (1995)
- C.H. Seager, R.A. Anderson, S.K. Estreicher: Phys. Rev. Lett. 74, 4565 (1995)
 P. Deák, L.C. Snyder, J.W. Corbett: Phys. Rev. B 43, 4545 (1991)
- 39. Yu.V. Gorelkinskii, N.N. Nevinnyi: Sov. Tech. Phys. Lett. **13**, 45 (1987) [Pis'ma Zh. Tekh. Fiz. (USSR) **13**, 105 (1987)]
- 40. Yu.V. Gorelkinskii, N.N. Nevinnyi: Physica B 170, 155 (1991)
- Yu.V. Gorelkinskii: Electron Parametric Resonance Studies of Hydrogen and Hydrogen-Related Defects in Crystalline Silicon. Semicond. Semimetals 61, 25 (1999)
- V.A. Gordeev, Yu.V. Gorelkinskii, R.F. Konopleva, N.N. Nevinnyi, Yu.V. Obukhov, V.G. Firsov: Preprint 1340, Leningrad Nuclear Physics Institute, Academy of Sciences of the USSR (1987), pp. 1–30
- R.F. Kiefl, M. Celio, T.L. Estle, S.R. Kreitzman, G.M. Luke, T.M. Riseman, E.J. Ansaldo: Phys. Rev. Lett. 60, 224 (1988)
- 44. R.B. Gel'fand, V.A. Gordeev, Yu.V. Gorelkinskii, R.F. Konopleva, S.A. Kuten', A.V. Mudryi, N.N. Nevinnyi, Yu.V. Obukhov, V.I. Rapoport, A.G. Ul'yashin, V.G. Firsov: Sov. Phys. Solid State **31**, 1376 (1989) [Fiz. Tverd. Tela **31**, 176 (1989)]
- 45. V.A. Gordeev, R.F. Konopleva, V.G. Firsov, Yu.V. Obukhov, Yu.V. Gorelkinskii, N.N. Nevinnyi: Hyperfine Interact. **60**, 717 (1990)
- 46. B. Hitti, S.R. Kreitzman, T.L. Estle, E.S. Bates, M.R. Dawdy, T.L. Head, R.L. Lichti: Phys. Rev. B 59, 4918 (1999)
- 47. T.L. Estle, S. Estreicher, D.S. Marynick: Phys. Rev. Lett. 58, 1547 (1987)
- B.D. Patterson, A. Hintermann, W. Kündig, P.F. Meier, F. Waldner, H. Graf, E. Recknagel, A. Weidinger, T. Wichert: Phys. Rev. Lett. 40, 1347 (1978)
- K.W. Blazey, J.A. Brown, D.W. Cooke, S.A. Dodds, T.L. Estle, R.H. Heffner, M. Leon, D.A. Vanderwater: Phys. Rev. B 23, 5316 (1981)
- 50. K.W. Blazey, T.L. Estle, E. Holzschuh, W. Odermatt, B.D. Patterson: Phys. Rev. B 27, 15 (1983)
- 51. C.G. Van de Walle, P.E. Blöchl: Phys. Rev. B 47, 4244 (1993)
- 52. C.A.J. Ammerlaan, P.T. Huy: Solid State Phenom. 85-86, 353 (2002)
- 53. A. van Wieringen, N. Warmoltz: Physica 22, 849 (1956)
- 54. C. Herring, N.M. Johnson, C.G. Van de Walle: Phys. Rev. B 64, 125209-1 (2001)
- 55. F. Buda, G.L. Chiarotti, R. Car, M. Parrinello: Phys. Rev. Lett. **63**, 294 (1989)
- P.E. Blöchl, C.G. Van de Walle, S.T. Pantelides: Phys. Rev. Lett. 64, 1401 (1990)

- 57. C. Herring, N.M. Johnson: Hydrogen Migration and Solubility in Silicon. Semicond. Semimetals **34**, 225 (1991)
- 58. N.M. Johnson, C. Herring: Phys. Rev. B 38, 1581 (1988)
- J.D. Holbech, B. Bech Nielsen, R. Jones, P. Sitch, S. Öberg: Phys. Rev. Lett. 71, 875 (1993)
- 60. K.J. Chang, D.J. Chadi: Phys. Rev. Lett. 62, 937 (1989)
- 61. S.B. Zhang, W.B. Jackson, D.J. Chadi: Phys. Rev. Lett. 65, 2575 (1990)
- 62. A.N. Safonov, E.C. Lightowlers, G. Davies: Phys. Rev. B 56, R15517 (1997)
- B.N. Mukashev, K.H. Nussupov, M.F. Tamendarov: Phys. Lett. 72A, 381 (1979)
- 64. H.J. Stein: Phys. Rev. Lett. 43, 1030 (1979)
- B.N. Mukashev, K.H. Nussupov, M.F. Tamendarov, V.V. Frolov: Phys. Lett. 87A, 376 (1982)
- 66. K.J. Chang, D.J. Chadi: Phys. Rev. B 42, 7651 (1990)
- J.I. Pankove, D.E. Carlson, J.E. Berkeyheiser, R.O. Wance: Phys. Rev. Lett. 51, 2224 (1983)
- 68. C.-T. Sah, J.Y.-C. Sun, J.J.-T. Tzou: Appl. Phys. Lett. 43, 204 (1983)
- 69. J.I. Pankove, R.O. Wance, J.E. Berkeyheiser: Appl. Phys. Lett. 45, 1100 (1984)
- 70. Y.-C. Du, Y.-F. Zhang, G.-G. Qin, S.-F. Weng: Solid State Commun. 55, 501 (1985)
- 71. A. Chari, M. Aucouturier: Solid State Commun. 71, 105 (1989)
- M.L.W. Thewalt, E.C. Lightowlers, J.I. Pankove: Appl. Phys. Lett. 46, 689 (1985)
- 73. G.G. DeLeo, W.B. Fowler: Phys. Rev. B 31, 6861 (1985)
- 74. N.M. Johnson: Phys. Rev. B **31**, 5525 (1985)
- J.I. Pankove, D.J. Zanzucchi, C.W. Magee, G. Lucovsky: Appl. Phys. Lett. 46, 421 (1985)
- 76. M. Stutzmann: Phys. Rev. B 35, 5921 (1987)
- M. Stavola, S.J. Pearton, J. Lopata, W.C. Dautremont-Smith: Appl. Phys. Lett. 50, 1086 (1987)
- B. Pajot, A. Chari, M. Aucouturier, M. Astier, A. Chantre: Solid State Commun. 67, 855 (1988)
- 79. G.G. DeLeo, W.B. Fowler: J. Electron. Mater. 14a, 745 (1985)
- 80. G.G. DeLeo, W.B. Fowler: Phys. Rev. Lett. 56, 402 (1986)
- A. Amore Bonapasta, A. Lapiccirella, N. Tomassini, M. Capizzi: Phys. Rev. B 36, 6228 (1987)
- 82. A.D. Marwick, G.S. Oehrlein, N.M. Johnson: Phys. Rev. B 36, 4539 (1987)
- 83. B. Bech Nielsen, J.U. Andersen, S.J. Pearton: Phys. Rev. Lett. 60, 321 (1988)
- 84. K. Bergman, M. Stavola, S.J. Pearton, T. Hayes: Phys. Rev. B 38, 9643 (1988)
- 85. K.J. Chang, D.J. Chadi: Phys. Rev. Lett. 60, 1422 (1988)
- A.D. Marwick, G.S. Oehrlein, J.H. Barrett, N.M. Johnson: The structure of the boron-hydrogen complex in silicon. In: *Defects in Electronic Materials*, ed. by M. Stavola, S.J. Pearton, G. Davies (Materials Research Society, Pittsburgh 1988) pp. 259-264
- 87. M. Stavola, K. Bergman, S.J. Pearton, J. Lopata: Phys. Rev. Lett. 61, 2786 (1988)

- C.G. Van de Walle, P.J.H. Denteneer, Y. Bar-Yam, S.T. Pantelides: Hydrogen diffusion and passivation of shallow impurities in crystalline silicon. In: *Shallow Impurities in Semiconductors 1988*, ed. by B. Monemar (Institute of Physics, Bristol 1989) pp. 405-414
- 89. E. Artacho, F. Ynduráin: Solid State Commun. 72, 393 (1989)
- 90. P.J.H. Denteneer, C.G. Van de Walle, S.T. Pantelides: Phys. Rev. B 39, 10809 (1989)
- P.J.H. Denteneer, C.G. Van de Walle, S.T. Pantelides: Phys. Rev. Lett. 62, 1884 (1989)
- P.J.H. Denteneer, C.G. Van de Walle, Y. Bar-Yam, S.T. Pantelides: Mater. Sci. Forum 38-41, 979 (1989)
- 93. S.K. Estreicher, L. Throckmorton, D.S. Marynick: Phys. Rev. B 39, 13241 (1989)
- T. Sasaki, H. Katayama-Yoshida: Mechanism of hydrogen passivation in silicon. In: Shallow Impurities in Semiconductors 1988, ed. by B. Monemar (Institute of Physics, Bristol 1989) pp. 395-404
- 95. T. Zundel, J. Weber: Phys. Rev. B 39, 13549 (1989)
- 96. G.D. Watkins, W.B. Fowler, M. Stavola, G.G. DeLeo, D.M. Kozuch, S.J. Pearton, J. Lopata: Phys. Rev. Lett. 64, 467 (1990)
- 97. K.R. Martin, W.B. Fowler, G.G. DeLeo: Mater. Sci. Forum 83-87, 69 (1992)
- 98. Dj.M. Maric, P.F. Meier, S.K. Estreicher: Phys. Rev. B 47, 3620 (1993)
- 99. Y. Zhou, R. Luchsinger, P.F. Meier: Phys. Rev. B 51, 4166 (1995)
- 100. G.G. DeLeo, W.B. Fowler: Computational Studies of Hydrogen-Containing Complexes in Semiconductors. Semicond. Semimetals 34, 511 (1991)
- 101. Dj.M. Maric, P.F. Meier: Helv. Phys. Acta 64, 908 (1991)
- 102. C.P. Herrero, M. Stutzmann, A. Breitschwerdt: Phys. Rev. B 43, 1555 (1991)
- 103. C.P. Herrero, M. Stutzmann: Solid State Commun. 68, 1085 (1988)
- M. Stutzmann, C.P. Herrero: Raman studies of hydrogen passivation in silicon. In: *Defects in Electronic Materials*, ed. by M. Stavola, S.J. Pearton, G. Davis (Materials Research Society, Pittsburgh 1988) pp. 271–276
- 105. A. Amore Bonapasta, P. Giannozzi, M. Capizzi: Phys. Rev. B 44, 3399 (1991)
- 106. A. Amore Bonapasta, P. Giannozzi, M. Capizzi: Phys. Rev. B 45, 11744 (1992)
- 107. Y. Zhou, R. Luchsinger, P.F. Meier: Mater. Sci. Forum 196-201, 885 (1995)
- 108. M. Stavola, S.J. Pearton, J. Lopata, W.C. Dautremont-Smith: Phys. Rev. B 37, 8313 (1988)
- 109. L.V.C. Assali, J.R. Leite: Phys. Rev. Lett. 55, 980 (1985)
- 110. L.V.C. Assali, J.R. Leite: Phys. Rev. Lett. 56, 403 (1986)
- 111. E.C.F. da Silva, L.V.C. Assali, J.R. Leite, A. Dal Pino Jr.: Phys. Rev. B 37, 3113 (1988)
- 112. A. Baurichter, S. Deubler, D. Forkel, M. Uhrmacher, H. Wolf, W. Witthuhn: Hydrogen passivation of indium acceptors in silicon. In: *Shallow Impurities in Semiconductors 1988*, ed. by B. Monemar (Institute of Physics, Bristol 1989) pp. 471–476

- 113. T. Wichert, H. Skudlik, M. Deicher, G. Grübel, R. Keller, E. Recknagel, L. Song: Phys. Rev. Lett. **59**, 2087 (1987)
- 114. T. Wichert, H. Skudlik, H.-D. Carstanjen, T. Enders, M. Deicher, G. Grübel, R. Keller, L. Song, M. Stutzmann: Localization of hydrogen in B and In doped silicon by ion channeling and PAC. In: *Defects in Electronic Materials*, ed. by M. Stavola, S.J. Pearton, G. Davies (Materials Research Society, Pittsburgh 1988) pp. 265–270
- 115. J.M. Baranowski, J. Tatarkiewicz: Phys. Rev. B 35, 7450 (1987)
- 116. N.M. Johnson, C. Doland, F. Ponce, J. Walker, G. Anderson: Physica B 170, 3 (1991)
- 117. M. Stavola, K. Bergman, S.J. Pearton, J. Lopata, T. Hayes: The symmetry and properties of donor-H and acceptor-H complexes in Si from uniaxial stress studies. In: *Shallow Impurities in Semiconductors 1988*, ed. by B. Monemar (Institute of Physics, Bristol 1989) pp. 447-452
- 118. G. Cannelli, R. Cantelli, M. Capizzi, C. Coluzza, F. Cordero, A. Frova, A. Lo Presti: Phys. Rev. B 44, 11486 (1991)
- 119. M. Stavola, Y.M. Cheng: Solid State Commun. 93, 431 (1995)
- 120. M. Stavola, J.-F. Zheng, Y.M. Cheng, C.R. Abernathy, S.J. Pearton: Mater. Sci. Forum **196–201**, 809 (1995)
- 121. M. Stavola, Y.M. Cheng, G. Davies: Mater. Sci. Forum 143-147, 885 (1994)
- 122. C.H. Seager, R.A. Anderson: Appl. Phys. Lett. 59, 585 (1991)
- 123. T. Zundel, J. Weber: Phys. Rev. B 43, 4361 (1991)
- 124. T. Zundel, J. Weber, L. Tilly: Physica B 170, 361 (1991)
- 125. Y. Ohmura, K. Abe, M. Ohtaka, A. Kimoto, M. Yamaura: Mater. Sci. Forum **258–263**, 185 (1997)
- 126. K. Muro, A.J. Sievers: Phys. Rev. Lett. 57, 897 (1986)
- 127. E.E. Haller: Hydrogen-related effects in crystalline semiconductors. In: Shallow Impurities in Semiconductors 1988, ed. by B. Monemar (Institute of Physics, Bristol 1989) pp. 425–436
- 128. R.E. Peale, K. Muro, A.J. Sievers: Phys. Rev. B 41, 5881 (1990)
- 129. M. Gebhard, B. Vogt, W. Witthuhn: Phys. Rev. Lett. 67, 847 (1991)
- 130. M. Suezawa, R. Mori: Phys. Stat. Sol. (b) 210, 507 (1998)
- 131. M. Suezawa: Optical absorption study of hydrogen in Zn-doped Si. In: Hydrogen in Semiconductors and Metals, ed. by N.H. Nickel, W.B. Jackson, R.C. Bowman, R.G. Leisure (Materials Research Society, Warrendale 1998) pp. 357-362
- 132. R. Mori, M. Suezawa: Physica B 273–274, 220 (1999)
- 133. R. Mori, N. Fukata, M. Suezawa, A. Kasuya: Physica B 302-303, 206 (2001)
- 134. P. Stolz, G. Pensl, D. Grünebaum, N. Stolwijk: Mater. Sci. Eng. B 4, 31 (1989)
- 135. K. Bergman, M. Stavola, S.J. Pearton, J. Lopata: Phys. Rev. B 37, 2770 (1988)
- 136. Z.N. Liang, L. Niesen: Nucl. Instrum. Methods Phys. Res. B 63, 147 (1992)
- 137. N.M. Johnson, C. Herring, D.J. Chadi: Phys. Rev. Lett. 56, 769 (1986)
- 138. A. Amore Bonapasta, P. Giannozzi, M. Capizzi: Phys. Rev. B 42, 3175 (1990)
- 139. P.J.H. Denteneer, C.G. Van de Walle, S.T. Pantelides: Phys. Rev. B 41, 3885 (1990)
- 140. S.B. Zhang, D.J. Chadi: Phys. Rev. B 41, 3882 (1990)
- 141. Z.N. Liang, P.J.H. Denteneer, L. Niesen: Phys. Rev. B 52, 8864 (1995)

- 142. A. Amore Bonapasta, A. Lapiccirella, N. Tomassini, M. Capizzi: Phys. Rev. B **39**, 12630 (1989)
- 143. G.G. DeLeo, W.B. Fowler, T.M. Sudol, K.J. O'Brien: Phys. Rev. B 41, 7581 (1990)
- 144. N.M. Johnson, C. Herring: Hydrogen neutralization of shallow-donor impurities in single-crystal silicon. In: *Defects in Electronic Materials*, ed. by M. Stavola, S.J. Pearton, G. Davies (Materials Research Society, Pittsburgh 1988), pp. 277–280
- 145. Z.N. Liang, C. Haas, L. Niesen: Phys. Rev. Lett. 72, 1846 (1994)
- 146. Z.N. Liang, L. Niesen: Phys. Rev. B 51, 11120 (1995)
- 147. L. Korpás, J.W. Corbett, S.K. Estreicher: Mater. Sci. Forum 83-87, 27 (1992)
- 148. L. Korpás, J.W. Corbett, S.K. Estreicher: Phys. Rev. B 46, 12365 (1992)
- 149. S.P. Love, K. Muro, R.E. Peale, A.J. Sievers, W. Lo: Phys. Rev. B 36, 2950 (1987)
- 150. R.E. Peale, K. Muro, A.J. Sievers: Mater. Sci. Forum 65-66, 151 (1990)
- 151. I.S. Zevenbergen, T. Gregorkiewicz, C.A.J. Ammerlaan: Phys. Rev. B 51, 16746 (1995)
- 152. I.S. Zevenbergen, T. Gregorkiewicz, C.A.J. Ammerlaan: Mater. Sci. Forum 196–201, 855 (1995)
- 153. C.A.J. Ammerlaan, I.S. Zevenbergen, T. Gregorkiewicz: Passivation of electronic centres in silicon by hydrogen. In: *Physics of Semiconductor Devices*, ed. by V. Kumar, S.K. Agarwal (Narosa, New Delhi 1998) pp. 531–538
- 154. C.A.J. Ammerlaan, P.T. Huy: Solid State Phenom. 69-70, 583 (1999)
- 155. P.T. Huy, C.A.J. Ammerlaan, T. Gregorkiewicz; Physica B **273–274**, 239 (1999)
- 156. P.T. Huy, C.A.J. Ammerlaan, T. Gregorkiewicz, D.T. Don: Phys. Rev. B 61, 7448 (2000)
- 157. G. Pensl, G. Roos, C. Holm, E. Sirtl, N.M. Johnson: Appl. Phys. Lett. 51, 451 (1987)
- 158. G. Pensl, G. Roos, P. Stolz, N.M. Johnson, C. Holm: Hydrogen neutralization of chalcogen double donor centers in single-crystal silicon. In: *Defects in Electronic Materials*, ed. by M. Stavola, S.J. Pearton, G. Davies (Materials Research Society, Pittsburgh 1988) pp. 241–246
- 159. G. Roos, G. Pensl, N.M. Johnson, C. Holm: J. Appl. Phys. 67, 1897 (1990)
- 160. Yu.V. Martynov, I.S. Zevenbergen, T. Gregorkiewicz, C.A.J. Ammerlaan: Solid State Phenom. 47–48, 267 (1996)
- 161. I.S. Zevenbergen: Ph.D. thesis, University of Amsterdam (1998)
- 162. V.J.B. Torres, S. Öberg, R. Jones: Theory of hydrogen single passivated substitutional sulphur double donor in Si. In: *Shallow-Level Centers in Semi*conductors, ed. by C.A.J. Ammerlaan, B. Pajot (World Scientific, Singapore 1997) pp. 501–504
- J. Coutinho, V.J.B. Torres, R. Jones, A. Resende, P.R. Briddon: Phys. Stat. Sol. (b) 235, 107 (2003)
- 164. J. Coutinho, V.J.B. Torres, R. Jones, P.R. Briddon: Phys. Rev. B 67, 035205-1 (2003)
- 165. A.S. Yapsir, P. Deák, R.K. Singh, L.C. Snyder, J.W. Corbett, T.-M. Lu: Phys. Rev. B 38, 9936 (1988)
- 166. N.M. Johnson, S.K. Hahn, H.J. Stein: Mater. Sci. Forum **10–12**, 585 (1986)
- 167. N.M. Johnson, S.K. Hahn: Appl. Phys. Lett. 48, 709 (1986)

- 288 C.A.J. Ammerlaan
- 168. A. Chantre, S.J. Pearton, L.C. Kimerling, K.D. Cummings, W.C. Dautremont-Smith: Appl. Phys. Lett. 50, 513 (1987)
- 169. D.I. Bohne, J. Weber: Phys. Rev. B 47, 4037 (1993)
- 170. D.I. Bohne, J. Weber: Mater. Sci. Forum 143-147, 879 (1994)
- 171. J. Weber, D.I. Bohne: Passivation of thermal donors by atomic hydrogen. In: Early Stages of Oxygen Precipitation in Silicon, ed. by R. Jones (Kluwer Academic, Dordrecht 1996) pp. 123–140
- 172. Yu.V. Martynov, T. Gregorkiewicz, C.A.J. Ammerlaan: Phys. Rev. Lett. 74, 2030 (1995)
- 173. Yu.V. Martynov, T. Gregorkiewicz, C.A.J. Ammerlaan: Mater. Sci. Forum 196–201, 849 (1995)
- 174. C.A.J. Ammerlaan, I.S. Zevenbergen, Yu.V. Martynov, T. Gregorkiewicz: Magnetic resonance investigations of thermal donors in silicon. In: *Early Stages of Oxygen Precipitation in Silicon*, ed. by R. Jones (Kluwer Academic, Dordrecht 1996) pp. 61–82
- 175. P. Deák, L.C. Snyder, J.W. Corbett: Phys. Rev. B 45, 11612 (1992)
- 176. R.C. Newman, M.J. Ashwin, R.E. Pritchard, J.H. Tucker, E.C. Lightowlers, T. Gregorkiewicz, I.S. Zevenbergen, C.A.J. Ammerlaan, R. Falster, M.J. Binns: Mater. Sci. Forum 258–263, 379 (1997)
- 177. R.E. Pritchard, M.J. Ashwin, J.H. Tucker, R.C. Newman, E.C. Lightowlers, T. Gregorkiewicz, I.S. Zevenbergen, C.A.J. Ammerlaan, R. Falster, M.J. Binns: Semicond. Sci. Technol. **12**, 1404 (1997)
- 178. R.C. Newman, J.H. Tucker, N.G. Semaltianos, E.C. Lightowlers, T. Gregorkiewicz, I.S. Zevenbergen, C.A.J. Ammerlaan: Phys. Rev. B 54, R6803 (1996)
- 179. D.E. Woon, D.S. Marynick, S.K. Estreicher: Phys. Rev. B 45, 13383 (1992)
- 180. R. Jones, S. Öberg, J. Goss, P.R. Briddon, A. Resende: Phys. Rev. Lett. 75, 2734 (1995)
- 181. A. Resende, J. Goss, P.R. Briddon, S. Öberg, R. Jones: Mater. Sci. Forum 258–263, 295 (1997)
- 182. R. Jones, A. Resende, S. Öberg, P.R. Briddon: Mater. Sci. Eng. B 58, 113 (1999)
- 183. A. Resende, R. Jones, S. Öberg, P.R. Briddon: Mater. Sci. Eng. B 58, 146 (1999)
- 184. A. Resende, R. Jones, S. Öberg, P.R. Briddon: Phys. Rev. Lett. 82, 2111 (1999)
- 185. R. Jones, B.J. Coomer, J.P. Goss, B. Hourahine, A. Resende: Solid State Phenom. 71, 173 (2000)
- 186. S.J. Pearton, A.J. Tavendale: Phys. Rev. B 26, 7105 (1982)
- 187. S.J. Pearton, E.E. Haller: J. Appl. Phys. 54, 3613 (1983)
- 188. S.J. Pearton, A.J. Tavendale: J. Appl. Phys. 54, 1375 (1983)
- 189. A.J. Tavendale, S.J. Pearton: J. Phys. C: Solid State Phys. 16, 1665 (1983)
- 190. S.J. Pearton, A.J. Tavendale: J. Phys. C: Solid State Phys. 17, 6701 (1984)
- 191. R. Singh, S.J. Fonash, A. Rohatgi: Appl. Phys. Lett. 49, 800 (1986)
- 192. A. Mesli, E. Courcelle, T. Zundel, P. Siffert: Phys. Rev. B 36, 8049 (1987)
- 193. E.Ö. Sveinbjörnsson, O. Engström: Appl. Phys. Lett. 61, 2323 (1992)
- 194. H. Feichtinger, E. Sturm: Mater. Sci. Forum 143-147, 111 (1994)
- 195. E.Ö. Sveinbjörnsson, G.I. Andersson, O. Engström: Phys. Rev. B 49, 7801 (1994)

- 196. E.Ö. Sveinbjörnsson, O. Engström: Mater. Sci. Forum 143-147, 821 (1994)
- 197. E.Ö. Sveinbjörnsson, O. Engström: Phys. Rev. B 52, 4884 (1995)
- 198. J.A. Davidson, J.H. Evans: Semicond. Sci. Technol. 11, 1704 (1996)
- 199. J.-U. Sachse, E.Ö. Sveinbjörnsson, W. Jost, J. Weber, H. Lemke: Phys. Rev. B 55, 16176 (1997)
- 200. J.-U. Sachse, J. Weber, H. Lemke: Mater. Sci. Forum 258-263, 307 (1997)
- 201. N. Yarykin, J.-U. Sachse, J. Weber, H. Lemke: Mater. Sci. Forum 258–263, 301 (1997)
- 202. J. Weber: Electrical properties of transition metal hydrogen complexes in silicon. In: *Hydrogen in Semiconductors and Metals*, ed. by N.H. Nickel, W.B. Jackson, R.C. Bowman, R.G. Leisure (Materials Research Society, Warrendale 1998) pp. 345–356
- 203. L. Rubaldo, P. Deixler, I.D. Hawkins, J. Terry, D.K. Maude, J.-C. Portal, J.H. Evans-Freeman, L. Dobaczewski, A.R. Peaker: Mater. Sci. Eng. B 58, 126 (1999)
- 204. J.-U. Sachse, J. Weber, E.Ö. Sveinbjörnsson: Phys. Rev. B 60, 1474 (1999)
- 205. J.-U. Sachse, E.O. Sveinbjörnsson, N. Yarykin, J. Weber: Mater. Sci. Eng. B 58, 134 (1999)
- 206. J. Weber, S. Knack, J.-U. Sachse: Physica B 273-274, 429 (1999)
- 207. N. Yarykin, J.-U. Sachse, H. Lemke, J. Weber: Phys. Rev. B 59, 5551 (1999)
- 208. O.V. Feklisova, N.A. Yarykin: Semicond. Sci. Technol. 12, 742 (1997)
- 209. W. Jost, J. Weber: Phys. Rev. B 54, R11038 (1996)
- 210. T. Sadoh, H. Nakashima, T. Tsurushima: J. Appl. Phys. 72, 520 (1992)
- 211. T. Sadoh, M. Watanabe, H. Nakashima, T. Tsurushima: Mater. Sci. Forum 143–147, 939 (1994)
- 212. T. Sadoh, M. Watanabe, H. Nakashima, T. Tsurushima: J. Appl. Phys. 75, 3978 (1994)
- 213. W. Jost, J. Weber, H. Lemke: Mater. Sci. Forum 196-201, 927 (1995)
- 214. W. Jost, J. Weber, H. Lemke: Semicond. Sci. Technol. 11, 22 (1996)
- 215. W. Jost, J. Weber, H. Lemke: Semicond. Sci. Technol. 11, 525 (1996)
- 216. M. Shiraishi, J.-U. Sachse, H. Lemke, J. Weber: Mater. Sci. Eng. B 58, 130 (1999)
- 217. S. Knack, J. Weber, H. Lemke: Physica B 273-274, 387 (1999)
- 218. S. Knack, J. Weber, H. Lemke: Mater. Sci. Eng. B 58, 141 (1999)
- 219. P.M. Williams, G.D. Watkins, S. Uftring, M. Stavola: Phys. Rev. Lett. 70, 3816 (1993)
- 220. M. Höhne, U. Juda, Yu.V. Martynov, T. Gregorkiewicz, C.A.J. Ammerlaan, L.S. Vlasenko: Phys. Rev. B 49, 13423 (1994)
- M. Höhne, U. Juda, Yu.V. Martynov, T. Gregorkiewicz, C.A.J. Ammerlaan, L.S. Vlasenko: Mater. Sci. Forum 143–147, 1659 (1994)
- 222. P.M. Williams, G.D. Watkins, S. Uftring, M. Stavola: Mater. Sci. Forum 143-147, 891 (1994)
- 223. P.T. Huy, C.A.J. Ammerlaan: Solid State Phenom. 82-84, 133 (2002)
- 224. S.J. Uftring, M. Stavola, P.M. Williams, G.D. Watkins: Phys. Rev. B 51, 9612 (1995)
- 225. M. Stavola, S.J. Uftring, M.J. Evans, P.M. Williams, G.D. Watkins: Spectroscopy of transition-metal-hydrogen complexes in silicon. In: *Defect and Impurity Engineered Semiconductors and Devices*, ed. by S. Ashok, J. Chevallier, I. Akasaki, N.M. Johnson, B.L. Sopori (Materials Research Society, Pittsburgh 1995) pp. 341–352

- 226. P.T. Huy, C.A.J. Ammerlaan: Physica B 302-303, 233 (2001)
- 227. P.T. Huy, C.A.J. Ammerlaan: Physica B 308-310, 408 (2001)
- 228. P.T. Huy, C.A.J. Ammerlaan: Phys. Rev. B 66, 165219-1 (2002)
- 229. M.J. Evans, M.G. Gornstein, M. Stavola: Vibrational spectroscopy of gold hydrogen complexes in silicon. In: *Defects in Electronic Materials II*, ed. by J. Michel, T. Kennedy, K. Wada, K. Thonke (Materials Research Society, Pittsburg 1997) pp. 275–280
- 230. M.J. Evans, M. Stavola, M.G. Weinstein, S.J. Uftring: Mater. Sci. Eng. B 58, 118 (1999)