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1991 J. Phys.: Condens. Matter 3 9363

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J. Phys.: Condens. Matter 3 (1991) 9363–9370. Printed in the UK

The states of hydrogen in silicon

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Received 3 June 1991

Abstract. Isotope studies of states of atomic hydrogen in silicon are performed. It is shown that H is a bistable impurity: it has an equilibrium site at a tetrahedral interstitial site for H^+ and H^- and at a bond-centred site for H^0. It is found that, in the tetrahedral configuration, H has donor and acceptor levels in the gap, located close to $E_v + 0.3$ eV and $E_c - 0.2$ eV, respectively.

1. Introduction

The states of atomic hydrogen (H) in silicon (Si) have been studied intensively during the last few years owing to its ability to neutralize many defects and impurities [1]. The early theories [2, 3] predicted that the equilibrium H site is a tetrahedral (T) interstitial site and that H_T has a deep donor level. It was suggested [4] that the H_T level is located in the valence band but pushed out into the gap when H moves from the T site. H_T was not observed in experiments [5], but the T state of its muonium analogue (Mu_T) was discovered [6]. According to the modern point of view [7–10], the equilibrium site of H^0 is a bond-centred site, whereas the T site is metastable. This assumption was confirmed by electron and muon spin resonance [11, 12] and channelling [13]. Theory [10] predicted that H_{BC} has a donor level in the upper part of the gap, which is due to an antibonding combination of orbitals of two neighbouring Si atoms. In this model, H_{BC}^+ is a positively charged state of the 'Si–H–Si' defect, but not a proton. H_{BC}^+ is energetically preferable in comparison with H_{BC}^0. The existence of H_T^- in n-Si was also proposed.

The presence of H^+ and H^- was confirmed in experiments on the drift of H^+ and H^- in the electric field [14, 15]. According to the data on H diffusion in n- and p-Si [16–19], the donor and acceptor levels of H were expected to be situated close to the middle of the gap. However, the DLTS studies of the H states in n-Si [20, 21] and the precise analysis of the data on the H diffusion in heavily doped p-Si [22] show the presence of two different positions of the donor H level: at about $E_c - 0.16$ eV in n-Si and at about $E_v + 0.3$ eV in p-Si. This fact indicates that there is an unknown state of H, different from H_{BC}. Taking into account the data on the drift of H^+ in the electric field, one can propose that this unknown state of H is a proton at an interstitial site.

In this paper we present the results of the infrared (IR) absorption studies of the H states in proton- and deuteron-implanted Si. The H-related IR spectra of Si were studied in detail in the 500–800 cm^{-1} and 1900–2250 cm^{-1} ranges associated with the wagging and stretching vibrations of the Si–H single bonds in the vicinity of radiation defects [23–

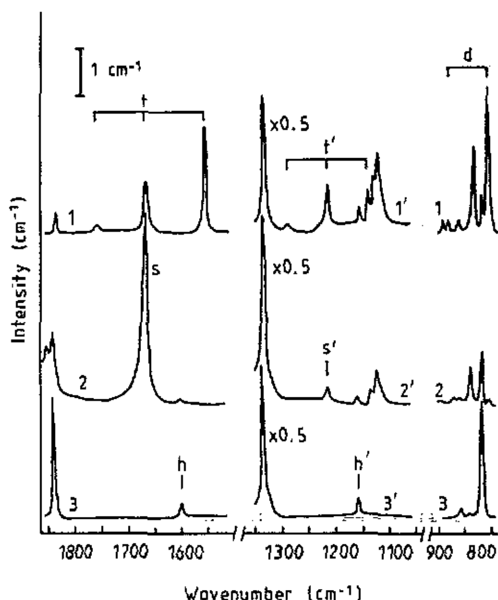

Figure 1. New H-related local vibrational bands in the spectra of the proton-implanted (curves 1, 2 and 3) and deuteron-implanted (curves 1', 2' and 3') Si crystals containing different concentrations of shallow impurities: curves 1 and 1', $N_{Sb} = 5 \times 10^{18}$ cm^{-3}; curves 2 and 2', $N_B \simeq 2 \times 10^{19}$ cm^{-3}; curves 3 and 3', $N_P \simeq 4 \times 10^{14}$ cm^{-3}. The concentrations of H and D are as follows: curve 1, 3×10^{18} H cm^{-3}; curve 2, 10^{19} H cm^{-3}; curve 3, 6×10^{18} H cm^{-3}; curves 1', 2' and 3', 5×10^{19} D cm^{-3}

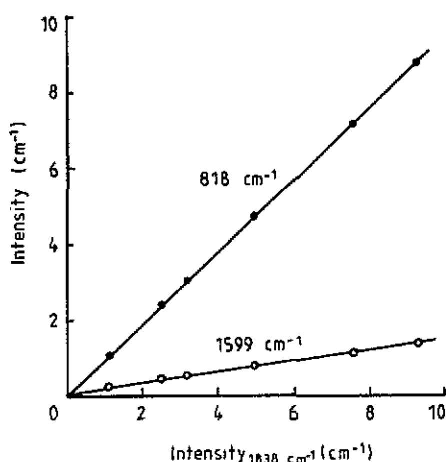

Figure 2. Intensity correlation for the 818 cm^{-1} (fundamental), 1599 cm^{-1} (overtone) and 1838 cm^{-1} bands related to the wagging and stretching vibrations of the Si^{-}–H^{+} dipole. The data were obtained from the spectra of the Si crystals implanted with different doses of protons.

28]. Some of the Si–H stretching bands were identified with the H-related vacancy-type complexes [29–32]. Therefore, the aim of the present investigation was the analysis of the origin of bands located in the 800–1900 cm^{-1} range. We have studied Si crystals with different contents of shallow donors and acceptors (P, Sb, B; $N_{dop} \simeq 10^{14}$–2×10^{19} cm^{-3}), implanted at about 300 K by protons and deuterons. Experimental details and some of the data have been published previously [30, 31, 33].

2. Results

Figure 1 shows the IR spectra of Si:P ($N_P \simeq 4 \times 10^{14}$ cm^{-3}), Si:Sb ($N_{Sb} \simeq 5 \times 10^{18}$ cm^{-3}) and Si:B ($N_B \simeq 2 \times 10^{19}$ cm^{-3}), measured at 80 K. The bands labelled h, h', d, t, t', s and s' were first observed in our previous investigation [33]. Their frequencies are presented in table 1, where the data for Si:P ($N_P \simeq 10^{19}$ cm^{-3}) are also included. The frequency ratios $\nu_{h,t,s}/\nu_{h',t',s'} \simeq 1.37$ are in good agreement with the isotopic shift of H-related vibrational bands due to the substitution of H by deuterium (D). This indicates that the h, t and s bands are connected with the H vibrations. In the case of the d bands we could not observe the isotopic frequency shift in the spectra of deuteron-implanted

Table 1. New H-related bands in the IR absorption spectra of proton- and deuteron-implanted Si.

Band	Shallow dopant	N_{dop} (cm^{-3})	Isotope of H	Frequency (cm^{-1}) at 80 K
h	B, P, Sb	$<10^{18}$	H	1599
h′	B, P, Sb	$<10^{18}$	D	1160
d	Sb	5×10^{18}	H	810, 880
d	P	10^{19}	H	806, 878
t	Sb	5×10^{18}	H	1562, 1670, 1764
t	P	10^{19}	H	1578, 1696, 1796 (≈1555)
t′	Sb	5×10^{18}	D	1144, 1220, 1292
s	B	2×10^{19}	H	1666
s′	B	2×10^{19}	D	1218

Si:Sb owing to a strong absorption by the free carriers at less than 700 cm^{-1} [33]. However, the IR studies [34] of Si:P, Si:As and Si:Sb treated at 120 °C in the H plasma show that the d bands are also connected with the H vibrations.

The h, d, t and s bands show different dependences upon N_{dop}, the implantation dose, the annealing temperature and the measurement temperature. The d, t and s bands appear only in the spectra of heavily doped samples ($N_{dop} > 10^{18}$ cm^{-1}). The h band is not observed in these spectra up to a dose of about 3×10^{17} H^+ cm^{-2}; it is well introduced in the case of low N_{dop}. In the dose range 3×10^{16}–8×10^{17} H^+ cm^{-2} the h band grows monotonically and its behaviour correlates with that of the 818 and 1838 cm^{-1} bands (figure 2). All these bands are annealed at temperatures of 180 °C or lower. The dose dependence of the d, t and s bands correlates with the behaviour of E_F around the divacancy levels situated at $E_c - 0.23$ eV and $E_v + 0.31$ eV; this can be seen from the absorption at 3.6 and 3.9 μm [35, 36]. The d and t bands show the same behaviour; they disappear at $E_F < E_c - 0.2$ eV and are annealed at 150 °C or lower. The annealing of these bands causes the changes in the Si–H stretching bands and correlates with the growth of the concentration of the H-passivated A centre [32] and with the strong increase in the free-carrier absorption. The s band disappears at $E_F > E_v + 0.3$ eV and is annealed at temperatures of 250 °C or above (the heat treatment of Si:B at 250 °C leads to strong absorption by free carriers).

The lowering of the measurement temperature from 300 to 80 K causes strengthening of the h, t and s bands by a factor of 2 or more. At the same time the d bands show an insignificant increase as in the case of the 818 cm^{-1} band.

3. Discussion

Figure 2 shows that the 818, 1599 (h) and 1838 cm^{-1} bands are connected with the vibrations of one and the same H atom. The frequency ratio of 1599/818 ≈ 1.95 and the intensity correlation indicate that the 1599 cm^{-1} h band is an overtone of the 818 cm^{-1} band. The behaviour of the 1838 cm^{-1} band correlates with that of the 2062 cm^{-1} band

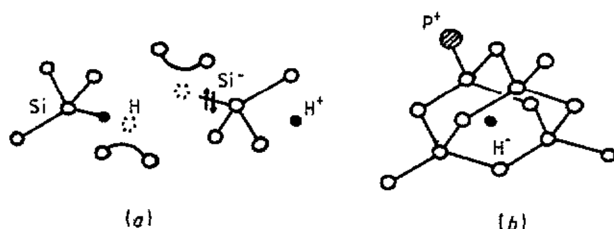

Figure 3. Proposed configurations of (*a*) the V_2HH^* centre and (*b*) the H-passivated shallow donor in Si.

[13, 23, 37] also. According to the uniaxial stress data [38], these bands were associated with the stretching vibrations of two different centres, each of which contains a single H atom. However, our previous study of the origin of the 1838 and 2062 cm^{-1} bands [31] shows that these bands are related to the V_2HH^* centre (figure 3(*a*); here H^* is H^+, which is located close to the T site and forms the Si^-–H^+ antibond). The 818 and 1838 cm^{-1} bands are connected with the Si^-–H^+ wagging and stretching vibrations, respectively, and the overtone absorption at 1599 cm^{-1} appears owing to the deformation of the Si^-–H^+ dipole charges.

The d and t bands in the Si : Sb and Si : P spectra have the same structures, but their frequencies slightly differ from each other (table 1). This indicates that the corresponding d centre contains a shallow donor atom (we label this atom by a letter P). Because the d-centre annealing correlates with the increase in free-carrier concentration and with the increase in the concentration of the H-passivated A centre (the last indicates that the H atoms in the passivated A centre originate from the d centre), one can conclude that the d centre is a neutral complex of H and P.

Some of the d and t bands were observed in the work reported in [34]. They are at 809.6, 1561.7 and 1671 cm^{-1} in the Si : Sb spectrum, at 809.8, 1561 and 1661 cm^{-1} in the Si : As spectrum and at 809.4, 1555.2 and 1647 cm^{-1} in the Si : P spectrum (we have observed a weak absorption at about 1555 cm^{-1} as a shoulder of the 1550 cm^{-1} band, showing more thermal stability than the d and t bands). The bands near 809 and 1560 cm^{-1} were identified as the wagging and stretching vibrations of the Si–H antibond in the vicinity of P. The additional band near 1660 cm^{-1} was assigned to a plasma-related defect. The following calculations [39–41] have shown that the global energy minimum configuration of the passivated donor is that involved in a very large lattice relaxation of the Si atom along the ⟨111⟩ axis containing P (the P–Si bond is broken, the H located close to the T site saturates the dangling Si bond and a lone pair of electrons on P is created). In such a configuration the calculated Si–H frequencies [40] are in agreement with the experimental values at about 809 and about 1560 cm^{-1}. However, is there a large lattice relaxation in the vicinity of the passivated donor in fact? Such a relaxation must cause changes in the lattice constant as in the case of the passivated acceptor [42].

If the assumption that the band at about 1660 cm^{-1} is connected with the plasma-related defect is valid, then in the case of a proton implantation this band must be stronger than that at about 1560 cm^{-1}. However, the ratio of intensities of the t bands at about 1560 and about 1670 cm^{-1} (figure 1) is comparable with that of the bands at about 1560 and about 1660 cm^{-1} observed in [34]. We have found that the structure of the d and t bands is similar to that of the vibrational transitions of a C_{3v} oscillator [43] originating from a T oscillator owing to the perturbation along the ⟨111⟩ axis. There are

two components of the fundamental transition and four components of the first overtone, all of which are IR active. The increase in the perturbation must cause [43] the degeneracy of two of four overtone components. Indeed, the t bands (figure 1 and table 1) involve three components (in the case of Si : P there are four component, if a weak absorption near 1555 cm^{-1} is taken into account). It is seen that the splitting of the t bands is twice that of the d bands. This is in agreement with the predictions for the C_{3v} oscillator [43]. It is necessary to note that the strong temperature dependence of the t band intensities correlates with such a dependence of the overtone absorption bands related to a substitutional H^- in $CaF_2:H^-$ [44], which is an example of a T oscillator. Thus, our data allow us to assign the d and t bands to the fundamental and overtone vibrational transitions of the passivated P^+H^- centre, the configuration of which is shown in figure 3(*b*). In this model the donor passivation is due to a donor–acceptor pairing. Such a configuration simulated in [40, 45] without the lattice relaxation has allowed calculation of both the stretching and the wagging frequencies of the H vibrations: about 600 cm^{-1}. This value is in agreement with the fundamental frequency of about 810 cm^{-1}.

The charges of the P^+–H^- dipole are expected to be larger than those of the Si^-–H^+ dipole and therefore the overtone t bands are expected to be strong. Indeed, the intensities of the t bands are comparable with those of the d bands (figure 1), while the intensity of the 1599 cm^{-1} h band is sufficiently small in comparison with that of the 818 cm^{-1} band.

Thus, H_T^+ and H_T^- located in the vicinity of the V_2HH^* and P^+H^- centres, respectively, create the fundamental and overtone absorption bands in the same ranges at about 810 and about 1670 cm^{-1}. This allows us to propose that the 1666 cm^{-1} s band in the spectrum of Si : B is due to an overtone vibration of a single H_T^+ (the absence of the s-band splitting indicates that the symmetry of the H^+ environment is tetrahedral [43, 44]). H_T^+ is expected to be a compensating donor-type centre in Si : B. Indeed, the annealing of the s band at 250 °C or above correlates with the strong increase in the free-carrier concentration. In the Si : B spectrum there was no absorption due to the fundamental vibration of H_T^+. This may be explained by the large charge of H_T^+ in comparison with the Si^-–H^+ and P^+–H^- charges.

Let us now consider the dependence of the d, t, s and h bands upon the E_F positions in the gap.

The d and t bands are not observed at $E_F < E_c - 0.2$ eV. This indicates that firstly the P^+H^- centre does not appear at $E_F < E_c - 0.2$ eV and secondly there is the P^+H^- decay due to interactions with the minority carriers created during implantation (this conclusion is in agreement with the data in [46]). Because H has an acceptor level in the gap [15], one can conclude that this level is related to H_T^- and is situated near $E_c - 0.2$ eV.

According to [6], Mu_T is converted into a diamagnetic muon μ^+ at temperatures above 400 K. Therefore, H_T^0 is expected to have a very deep donor level and to interact with P. However, the P^+H^- centre does not appear at $E_F < E_c - 0.2$ eV and, therefore, one can conclude that H_T^0 is metastable. This conclusion is in agreement with the data in [5]. It may be proposed that, at $E_F < E_c - 0.2$ eV, H_T^0 transforms at first into the H_{BC}^0 state and then into the H_{BC}^+ state (because the H_{BC}^0 level is located at $E_c - 0.16$ eV [20, 21]). The interaction between H_{BC}^+ and P^+ is expected to be insignificant. This explains the low efficiency of the shallow-donor passivation [47]. The data presented lead us to conclude that the reaction for the shallow-donor passivation is $P^+ + H^- \rightarrow P^+H^-$.

The s band disappearing at $E_F > E_v + 0.3$ eV indicates that H_T^0 has a donor level near $E_v + 0.3$ eV. Indeed, this assumption is confirmed by the data on analysis of the H diffusion in heavily doped p-Si [22]. Therefore, it may be concluded that H_{BC}^+ predominates at $E_c - 0.2$ eV $> E_F > E_v + 0.3$ eV. Because H_{BC}^+ has an energy barrier for

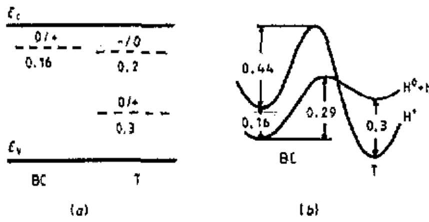

Figure 4. Schematic diagrams of (*a*) the electronic levels and (*b*) the configuration coordinates for the different states of a single H in Si.

diffusion of about 0.44 eV and is a fast-diffusing species at above 210 K [20], it can effectively interact with acceptor-like defects. This explains the effect of strong passivation of shallow acceptors [1] and the dependence of the 818, 1599 (h) and 1838 cm^{-1} bands upon E_F (the V_2HH^* is expected to be a result of the interaction of H_{BC}^+ with the acceptor-type V_2H centre).

The annealing behaviour of the s band shows that H_T^+ is stable up to 250 °C or above and is a slowly diffusing species in the heavily doped p-Si. H_T^+ can trap an electron from the valence band and transforms into H_{BC}^0. Both H_{BC}^+ and H_T^+ can passivate the shallow acceptors by direct compensation [48]. This mechanism is expected to predominate at $E_F < E_v + 0.3$ eV.

The data presented allow us to propose the following transitions between the different states of a single H in Si:

$$H_{BC}^0 \Leftrightarrow H_T^0 \quad (1)$$

$$H_{BC}^0 \Leftrightarrow H_{BC}^+ + e^- \quad (2)$$

$$H_{BC}^+ \Leftrightarrow H_T^+ \quad (3)$$

$$H_T^+ + e^- \Leftrightarrow H_T^0 \quad (4)$$

$$H_T^0 + e^- \Leftrightarrow H_T^-. \quad (5)$$

According to the data in [20], the energies of the right-directed reactions (1), (2) and (3) are about 0.29 eV, about 0.16 eV and about 0.44 eV, respectively. The right-directed reaction (4) is a transition of an electron from the valence band to the donor level of H_T, with an energy of about 0.3 eV. Reaction (5) describes the electron transitions between the conduction band and an acceptor level of H_T and has an energy of about 0.2 eV. These data are summarized in figures 4(*a*) and 4(*b*), where the scheme of the electronic states of H in the gap and the configuration coordinate diagram are presented. The curves in figure 4(*b*) are expected to cross because H_T^0 is metastable and, therefore, the energy of the left-directed reaction (1) must be less than 0.29 eV. This allows us to estimate a barrier for the left-directed reaction (3) to be about 0.7–0.8 eV. It is interesting that this value is in agreement with the binding energy of H at the substitutional carbon [21] and boron [49] sites. It may be proposed that H can leave these sites as H_T^+ only.

The model proposed is in good agreement with the data of the recent radio-frequency study of muons in Si and GaAs [50]. It was found [50] that in Si both Mu_T and anomalous Mu_{BC}^* are converted to a final μ_{BC}^+ at about 300 K and about 150 K, respectively. The right-directed reaction (2) is related to the $Mu_{BC}^* \rightarrow \mu_{BC}^+$ transition and the $Mu_T \rightarrow \mu_{BC}^+$ transition may be described by the left-directed reaction (1) and the right-directed

reaction (2). Mu_T cannot directly transform into μ_T^+ (left-directed reaction (4)) owing to the very deep localization of the corresponding donor level. Furthermore, our data allow us to account for the apparent decrease in the transverse field μ^+ asymmetry between 320 and 420 K [6, 50] as due to the contributions of the right-directed reactions (3) and (4). We believe also that the large diamagnetic fraction (about 100%) in the heavily doped n-Si and p-Si [6] is due to μ_T^- and μ_T^+, respectively.

Figure 4(*b*) shows that in a Si crystal containing a large supply of electrons and holes a single H can migrate by a mechanism similar to the Bourgoin–Corbett [51] mechanism (a difference is that there are the barriers for the left-directed reaction (1) and the right-directed reaction (3)). This mechanism is expected to predominate at high temperatures. Indeed, the energy of the right-directed reaction (3) is in good agreement with that of the H diffusion at high temperatures [52]. The high mobility of H in n-Si at less than 200 °C [53] may be explained by the contribution of reaction (2). We have estimated the energy of the low-temperature stage of H diffusion in n-Si [53] to be about 0.3 eV. One can see that this value is also in agreement with the barrier for the right-directed reaction (2).

In n-Si the reactions (2)–(5) can lead to the formation of a pair of neighbouring H_{BC}^+ and H_T^-, which is expected to be an H_2^* molecule [16]. Indeed, a stable configuration of H_2^* was simulated to be $H_{BC}^+ + H_T^-$, [54].

4. Conclusion

These studies show that in Si the single H^+ and H^- both have a global equilibrium site at a T site and act as the compensating centres. The corresponding donor and acceptor levels are located close to about $E_v + 0.3$ eV and about $E_c - 0.2$ eV, respectively. At $E_c - 0.2\,\mathrm{eV} > E_F > E_v + 0.3\,\mathrm{eV}$ a metastable H_T^0 transforms to H_{BC}^0, but at temperatures above 150 K the last state is converted to H_{BC}^+ owing to the ionization of the corresponding donor level at about $E_c - 0.16$ eV [20, 21]. The transitions between the different H states cause the complex dependence of the H behaviour upon the dopant concentration, temperature, etc.

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