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Observation and theory of the V-O-H$_2$ complex in silicon

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The interaction of hydrogen with radiation-induced defects (RD's) in Czochralski-grown silicon crystals has been studied by infrared-absorption spectroscopy and *ab initio* modeling. Hydrogen and/or deuterium was introduced into the crystals by indiffusion from H$_2$ (D$_2$) gas at 1200–1300 °C. The samples were subsequently irradiated with fast electrons ($E=2-4$ MeV) and annealed in the temperature range of 100–600 °C. The centers produced by the irradiation were the same in both the untreated and treated cases, namely the A-center, C$_i$-O$_i$ complex, and divacancy. A heat treatment of the H-treated samples resulted in the enhanced loss of these centers and the formation of centers containing hydrogen. The disappearance of the A centers in the temperature range of 100–150 °C is correlated with the appearance of three local vibrational modes (LVM's) at 943.5, 2126.4, and 2151.5 cm^{-1}. The isotopic shifts of these lines were obtained from measurements on the samples doped with hydrogen and deuterium. The lines are identified as related to stretching vibrational modes of a complex that consists of one oxygen and two hydrogen atoms sharing a vacancy site (V-O-H$_2$ complex). *Ab initio* calculations are used to explore the structures and properties of this defect. The origin of other LVM bands, which were observed upon annealing, is discussed.

I. INTRODUCTION

In silicon, practically all radiation-induced defects (RD's) associated with either single vacancies (V) or self-interstitial silicon atoms (I_{Si}) possess dangling bonds or weakly reconstructed Si–Si bonds. This suggests that strong interactions between the RD's and hydrogen atoms is to be expected, as hydrogen is known to eliminate (passivate) effectively the electrical activity of many extended and point defects in crystalline silicon.[1–3]

A considerable amount of evidence for the existence of these interactions has been obtained by means of electrical, optical, and magnetic measurements on Si samples into which RD's and H have been introduced in a variety of ways. These include hydrogenated samples, prepared by indiffusion or acid-etching, and subsequently irradiated with fast electrons, neutrons, or gamma rays, or samples exposed to a H plasma, or into which protons have been implanted.[1–15] However, so far only a few complexes consisting of primary radiation-induced defects (V and I_{Si}) together with hydrogen atoms have been unambiguously identified. The interaction of hydrogen with secondary RD's that can incorporate some impurity atoms in addition to vacancies and self-interstitials is much less understood.

In Czochralski-grown silicon (Cz-Si) crystals, one of the dominant defects induced by irradiation is known to be a vacancy-oxygen complex (A center). Some evidence for the interaction of hydrogen atoms with A centers was obtained by means of deep-level transient spectroscopy (DLTS) and infrared-absorption measurements.[13–15] Absorption bands at 870 and 891 cm^{-1} were identified as related to the oxygen-stretching vibrations for the partially and fully passivated A center, i.e., the V-O-H and V-O-H$_2$ complexes, respectively.[15] It would be expected that these complexes give rise to local vibrational modes (LVM's) related to Si-H stretch modes as well as a perturbed oxygen-related mode. However, no clear information for the existence of these bands was reported, making the assignment of the 891-cm^{-1} band uncertain.

In the present work we report our results, using infrared-absorption spectroscopy and *ab initio* modeling techniques, on the interaction of hydrogen with radiation-induced defects in Czochralski-grown Si crystals.

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II. EXPERIMENTAL DETAILS

Samples for this study were prepared from an *n*-type phosphorus-doped Cz-Si crystal ($\rho \approx 1\ \Omega\,\mathrm{cm}^{-1}$). The concentration of oxygen in the crystal was about $9.5\times10^{17}\ \mathrm{cm}^{-3}$ while the carbon concentration was below the detection limit of the optical-absorption method used ($\leqslant 5\times10^{15}\ \mathrm{cm}^{-3}$). Hydrogen (deuterium) was introduced into the samples by annealing at 1200 °C for 1 h in a H_2 (D_2) gas ambient at a gas pressure of about 1.5 atm., followed by quenching. Such a procedure leads to the incorporation of about $8.0\times10^{15}\ \mathrm{cm}^{-3}$ hydrogen atoms into the samples.[16] The hydrogenation treatment did not result in any noticeable changes in the oxygen-related 9-μm band.

Irradiation with fast (3 MeV) electrons, with a beam intensity of $5\times10^{13}\ \mathrm{cm}^{-2}\,\mathrm{s}^{-1}$, was performed at about 100 °C, with a radiation dose of $1.6\times10^{16}\ \mathrm{cm}^{-2}$. This value was chosen to create concentrations of radiation-induced defects close to that of hydrogen. Isochronal annealing experiments were carried out in an argon atmosphere in the range of 100–600 °C, in steps of 25 °C for 30 min each. Isothermal annealing experiments at 100 °C were also carried out.

The optical-absorption spectra were measured by a Fourier-transform infrared (FT-IR) spectrometer at 10 and 295 K in the range of 400–4000 cm^{-1} with a spectral resolution of 0.5 or 1.0 cm^{-1}.

III. EXPERIMENTAL RESULTS

A band at 1075.1 cm^{-1} with a shoulder at 1075.8 cm^{-1} was observed at 10 K in the as-grown hydrogenated samples. Replacement of hydrogen by deuterium led to a shift of both lines to 1076.0 and 1076.6 cm^{-1}. These lines were assigned previously to LVM's related to asymmetrical stretching vibrations of an interstitial oxygen atom perturbed by the presence of a H_2 (D_2) molecule (O_i-H_2 complexes).[17–19] Weak traces of the bands at about 817, 1838.5, and 2062.3 cm^{-1} were also observed in hydrogenated samples. According to a previous study,[20] all these bands are related to LVM's of the H_2^* complex consisting of two hydrogen atoms on the same trigonal axis, with one H atom at a bond-centered interstitial site and another one at a nearby antibonding site.[20–22]

We now turn to the results found in irradiated samples. The dominant centers produced by irradiation were found to be the same in both Si:O,H and the as-grown material: namely *V*O, C_i-O_i, and V_2. Figure 1 shows fragments of the infrared-absorption spectra of the as-grown and hydrogenated samples after irradiation. The intensities of the bands at 885.3 and 2766.3 cm^{-1}, which are known to originate from the VO^- and V_2^- (Ref. 23 and 24) are practically the same in both spectra. The integrated absorption intensity of a band at 865.8 cm^{-1}, which is related to the C_i-O_i complex,[25] in the hydrogenated samples was found to be about 75% in the as-grown samples. Additionally, in the hydrogenated irradiated samples, two close bands at 1987 and 1990 cm^{-1}, due to $I_{Si}H_2$,[5,32] and weak traces of the bands at 943.5, 2126.4, and 2151.5 cm^{-1} were detected. A small increase in the intensities of the lines of H_2^* complex was also observed. The band at 1075.1 cm^{-1}, due to the O_i-H_2 complex, was found to decrease in intensity by about 10–15 % after the irradiation.

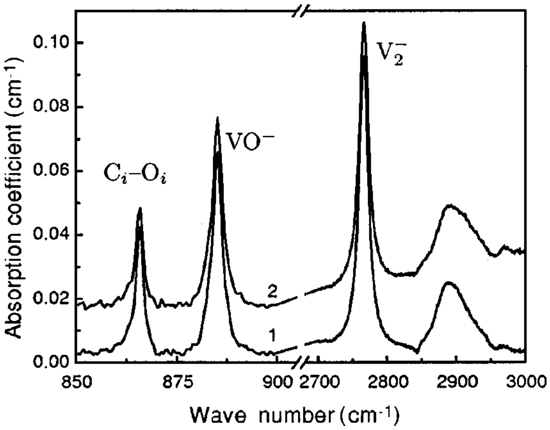

FIG. 1. Absorption spectra measured at 10 K for (1) as-grown and (2) hydrogenated Cz-Si samples which were irradiated with fast electrons. The spectra are arbitrarily positioned on the absorption axis for presentation.

In contrast to the modest influence of the hydrogenation treatment on the radiation-induced defects, profound effects were revealed in the annealing behavior of the RD's. An enhanced disappearance of all RD's occurred in the hydrogenated samples. As an example, Fig. 2 shows the changes in the integrated intensities of the band due to negatively charged *A* centers after isochronal annealing of H-soaked and as-grown samples. The isothermal annealing study of an irradiated Si:O,H sample showed that the radiation-induced defects started to disappear at temperatures as low as 100 °C. Simultaneously to the elimination of RD's, a substantial decrease in H_2 concentration was monitored by the strength of the line at 1075.1 cm^{-1}. Curves 1 and 2 in Fig. 3 show that a substantial decrease in intensity of the lines at 1075.1 cm^{-1} (O_i-H_2) and 885.3 cm^{-1} (*A* center) were found during isothermal anneals, at 100 °C, of the hydrogenated samples.

Furthermore, it was found that the absorption spectra due to defects that are formed upon annealing differ significantly for the H-soaked and as-grown samples. Figure 4 shows fragments of absorption spectra of the samples at different stages of isochronal annealing. Consistent with the results of

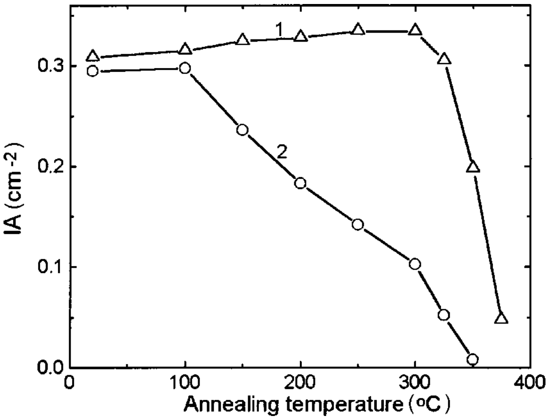

FIG. 2. Isochronal (30 min) annealing behavior in the integrated absorption intensity of the 885.3-cm^{-1} band due to *A* centers in electron-irradiated (1) as-grown and (2) hydrogenated Cz-Si samples.

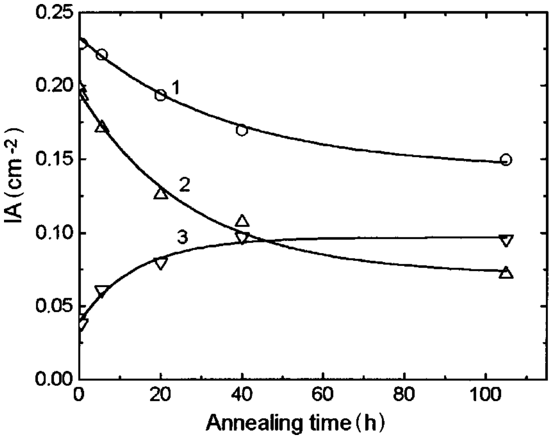

FIG. 3. Changes in the integrated absorption intensities of bands at (1) 885.3, (2) 1075.1, and (3) 943.5 cm^{-1} with isothermal annealing at 100 °C for an *e*-irradiated hydrogenated Cz-Si sample. The sample was kept at room temperature for one year before the isothermal annealing which produced the increase in intensity of the 943.5-cm^{-1} band.

previous studies,[26,27] the disappearance of the *A* centers in as-grown samples was accompanied by the formation of centers which give rise to a band at 895.3 cm^{-1} (VO_2).[26,27] In contrast, in the annealed hydrogenated material the band at 895.3 cm^{-1} was not detected. However, other lines were observed. The most intense among them were the lines at 943.5 and 891.5 cm^{-1} [Fig. 4(b)]. In addition, a number of lines in the wave-number range 1900–2250 cm^{-1} were found and those at 2126.4 and 2151.5 cm^{-1} were among the strongest ones. This range is characteristic for Si-H stretch modes.[1–3] No lines in this range were observed in the isochronally annealed as-grown samples.

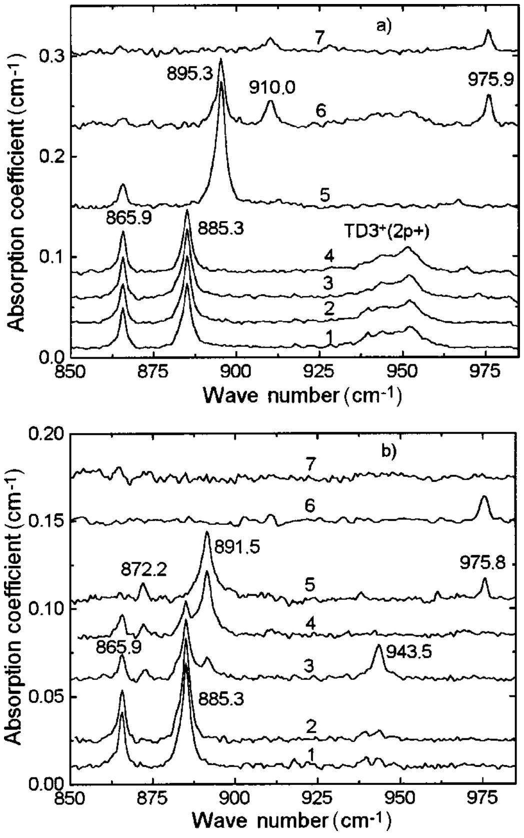

FIG. 4. Development of absorption spectra, measured at 10 K, for *e*-irradiated (a) as-grown and (b) hydrogenated Cz-Si samples with temperature, after 30-min isochronal anneals: 1, as-irradiated; 2, 100 °C; 3, 200 °C; 4, 300 °C; 5, 400 °C; 6, 500 °C; 7, 600 °C. The spectra are baseline corrected and arbitrarily positioned on the absorption axis for presentation.

We now consider the processes that occur in the hydrogenated samples during irradiation and subsequent annealing. The high-temperature heat treatment of the silicon crystals in the H_2 ambient results in the incorporation of hydrogen atoms into the lattice up to the solubility limit at the treatment temperature.[16] Following a quench to room temperature, practically all the hydrogen introduced from the gas phase in moderately doped Si is found to be in the molecular form.[18,28] H_2 (D_2) molecules are quite mobile in Si at room temperature, and an activation energy for their migration was estimated and calculated to be 0.78 eV.[18,29,30] In Cz-Si crystals, oxygen atoms were found to be effective traps for mobile hydrogen molecules. The binding energy between the molecule and O_i was estimated to be only 0.28 eV.[18] In the absence of other traps, there is a dynamical equilibrium between both H_2 and O_i-H_2 species with the ratio $[H_2]/[O_i\text{-}H_2]$ depending on the temperature and oxygen content.

Recent *ab initio* molecular-dynamics calculations have shown that H_2 molecules are broken up by reactions with silicon vacancies and self-interstitials[31] leading to the formation of Si-H bonds. A similar process in which hydrogen molecules react with RD's having dangling bonds can also be expected.

The hydrogenated CZ-Si used here contained about 10^{18} cm^{-3} oxygen atoms, $\leqslant 5\times10^{15}$ cm^{-3} carbon atoms, and about $(3-4)\times10^{15}$ cm^{-3} hydrogen molecules before irradiation. The electron irradiation dose used should produce about 3×10^{15} cm^{-3} of separated Frenkel pairs (V and I_{Si}). Because of their high concentration, the interstitial oxygen atoms are the most effective traps for mobile vacancies, so practically the same amount of V-O complexes was induced by irradiation in H-soaked and as-grown samples. The concentration of hydrogen molecules was comparable with that of substitutional carbon atoms, so H_2 can compete with C_s in the capture of mobile I_{Si}. Indeed, the concentration of C_i-O_i complexes in hydrogenated samples was about 25% lower than in as-grown ones, showing that less C_i atoms were created in the Si:O,H samples. This is because irradiation-induced interstitials can be trapped by a hydrogen molecule giving the bands 1987 and 1990 cm^{-1}.[5,32] Our data are consistent with this assignment.

O_i-H_2 complexes are not stable at temperatures exceeding 50 °C in silicon, thus heating the Si:O,H crystals results in the appearance of mobile H_2 molecules that can interact with RD's, forming other complexes.[31] The particular interest of the present work is the interaction of these mobile hydrogen molecules with vacancy-oxygen centers. It appears that there is a correlation between the disappearance of the *A* centers and the development of a complex which gives rise to an IR absorption band at 943.5 cm^{-1} (see Fig. 3). Further, it was found that the lines at 2126.4 and 2151.5 cm^{-1} were formed at the same time as the 943.5 cm^{-1} band. Figure 5 shows the development of these three lines upon isochronal anneal-

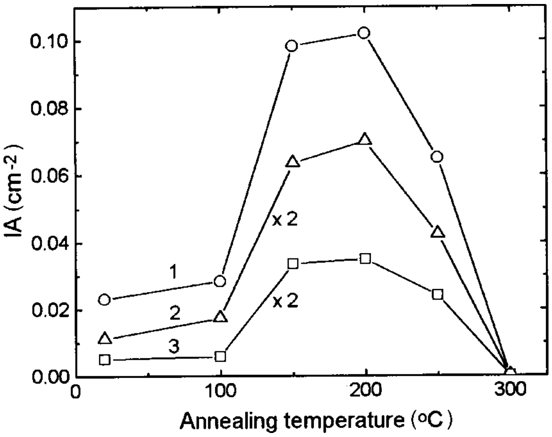

FIG. 5. Isochronal (30 min) annealing behavior in the integrated absorption intensity of the bands at (1) 943.5, (2) 2126.4, and (3) 2151.5 cm^{-1} with temperature for an *e*-irradiated hydrogenated Cz-Si sample.

ing. It seems likely that all these bands are related to the same defect. The lines at 2126.4 and 2151.5 cm^{-1} are in the wave-number range characteristic of Si-H stretch modes. As a rule, significant isotopic shifts of the lines in this range occur when hydrogen is substituted by deuterium.[1–3] Indeed, in deuterated samples the lines at 1549.1 and 1567.4 cm^{-1} were observed. Together with a line at 943.2 cm^{-1}, their growth upon annealing is similar to the lines at 943.5, 2126.4, and 2151.5 cm^{-1} found in H-soaked samples. In the samples co-doped with hydrogen and deuterium, additional lines were observed at 1557.3 and 2140.6 cm^{-1}. Figure 6 shows a fragment of the infrared-absorption spectra of a sample, which was co-doped with H and D and annealed for 105 h at 100 °C after electron irradiation.

It is likely that *V*-O-H_2 complexes formed by the interaction of mobile H_2 molecules with *A* centers are the centers responsible for the lines at 943.5, 2126.4, and 2151.5 cm^{-1}. The positions and isotopic shifts of the bands in Si:O,H and Si:O,D samples are consistent with those expected for *V*-O-H_2, in which an oxygen atom and two hydrogen atoms share a vacancy. For such a complex, the 943.5 cm^{-1} line can be assigned to an oxygen stretching LVM, and the 2126.4 and 2151.5 cm^{-1} lines to the vibration of two Si-H units. These suggestions were then investigated by an *ab initio* modeling scheme.

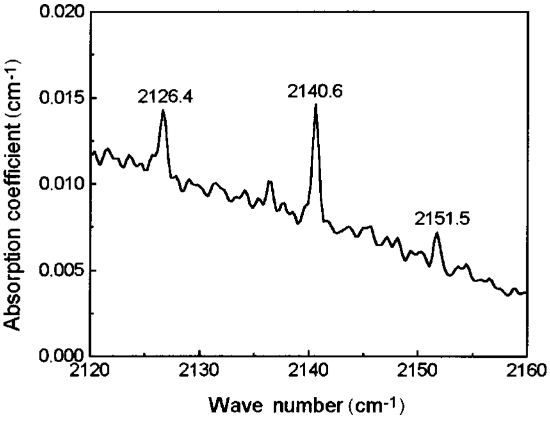

FIG. 6. Infrared-absorption spectrum, measured at 10 K, for a Cz-Si sample which was co-doped with hydrogen and deuterium, irradiated with fast electrons, and annealed at 100 °C for 105 h.

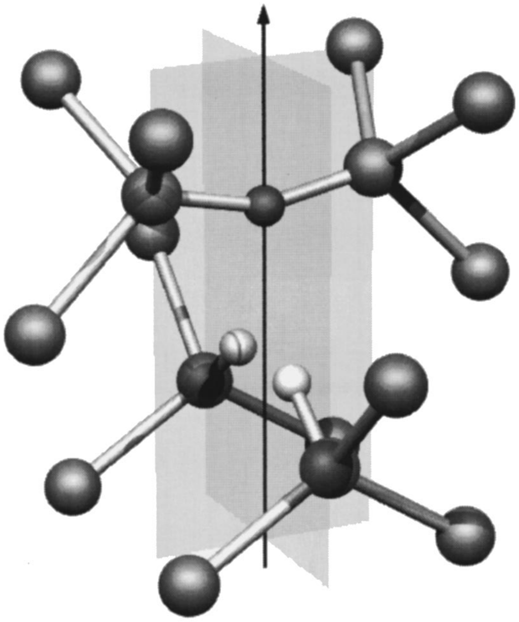

FIG. 7. Calculated ground-state structure for the *V*-O-H_2 center in silicon. Oxygen is over the C_2 axis, and the white atoms represent hydrogen.

IV. THEORETICAL CALCULATIONS

We carried out local-density-functional cluster calculations using the *Ab Initio* Modeling Program (AIMPRO),[33] to determine the structure and vibrational modes of *V*-O-H_2 defects. Clusters containing 133 atoms, with the composition $Si_{70}H_{62}O$, were used. The oxygen atom was placed at the center of the cluster within the vacancy, bridging two Si atoms. The two remaining silicon dangling bonds were allowed to interact with the hydrogen atoms.

The valence electronic wave functions were expanded in a set of *s* and *p* Gaussian orbitals placed at the atomic nuclei and at bond centers. The charge density was fitted to a sum of Gaussian functions placed at the same sites. Norm-conserving pseudopotentials of Bachelet *et al.*[34] were used to eliminate the core electrons. Full details of the method have been described elsewhere.[33] Previously the method has been used to describe the structure and vibrational modes of vacancy-oxygen defects[35] and oxygen dimers in silicon.[36]

Two configurations of the *V*-O-H_2 defect were investigated. In the first both hydrogen atoms were placed inside the vacancy (see Fig. 7 and Table I) in a manner similar to VH_2.[4] In the second configuration they lay outside, at antibonding sites, as in NiH_2.[37] Both configurations have C_{2v} symmetry. We found that the second configuration was

TABLE I. The ground-state structure of the *V*-O-H_2 center in silicon. All units are in Å.

H-H	Si-H	Si-O	Si^{H}-^{H}Si	Si_{O}-Si
1.50	1.49	1.65	4.15	3.24

TABLE II. Calculated LVM's for V-O-H_2 in silicon. All frequencies and isotopic shifts (IS) are in cm^{-1}. N.D. stands for not detected.

	Obs.	IS	Calc.	IS	Symm.
V-^{16}O-H_2	2151.5		2176		A_1
	2126.4		2173		B_1
	943.5		1076		B_2
	N.D.		774		B_1
	N.D.		771		A_1
V-^{16}O-D_2	1567.4	584.1	1564	612	A_1
	1549.1	577.3	1559	614	B_1
	943.2	0.3	1076	0	B_2
	N.D.		765	9	B_1
	N.D.		698	73	A_1
V-^{16}O-H-D	2140.6	10.9	2174	2	A'
	1557.3	569.1	1562	611	A'
	~943.5	~0	1076	0	A''
	N.D.		774	0	A'
	N.D.		706	65	A'
V-^{18}O-H_2			2176	0	A_1
			2173	0	B_1
			1021	55	B_2
			753	21	B_1
			770	1	A_1

1.25-eV higher in energy than the first where the hydrogen atoms lie inside the vacancy.

For the relaxed configuration, the Si-O bond lengths were 1.65 Å compared with 1.75 Å in the A center.[35] Clearly, the saturation of the Si dangling bonds has increased the strength of the Si-O bonds. The calculations indicate that the energy released when the hydrogen molecule interacts with the the A-center to form V-O-H_2 is 2.4 eV. This strongly supports the view that A centers are effective traps for mobile H_2 molecules.

The local vibrational modes (LVM's) for the defect along with their isotope shifts are given in Table. II. The calculated and observed frequencies and their isotopic shifts are in reasonable agreement. The two highest frequencies, at 2176 and 2173 cm^{-1}, are the symmetric and antisymmetric Si-H stretching modes, respectively. The 1076- and 774-cm^{-1} frequencies are the antisymmetric stretching and bending modes of the Si-O-Si unit, i.e., where the oxygen atoms vibrate in (110) and $(1\overline{1}0)$ symmetry planes perpendicular to the C_2 axis.

The calculated isotopic shifts (Table II) shows that the oxygen and hydrogen-related LVM's are completely decoupled: in either case, oxygen or hydrogen isotopic substitution does not affect the LVM's. For example, the 1076-cm^{-1} O-related mode is unaffected by deuteration in agreement with observations.

The two highest H-related LVM's are also almost independent. The highest LVM is an A_1 mode and lies 3 cm^{-1} above the antisymmetric B_1 mode. This is somewhat less than the observed splitting of about 25 cm^{-1} presumably due to an overestimate in the separation of the H atoms. The observed splitting is similar to the one found (22.5 cm^{-1}) for the VH_2 center.[4]

The calculated oxygen-related mode at 1076 cm^{-1} is about 100 cm^{-1} greater than the observed mode but both are much higher than that calculated for the A center at 787 cm^{-1}.[19] This increase in frequency demonstrates that the saturation of the Si reconstructed bond leads to stronger Si-O-Si bonds and mirrors what is seen experimentally: namely the neutral A center has a mode at 835 cm^{-1} while the O-related mode in VOH_2 lies at 943.5 cm^{-1}.

We also found two LVM's around 770 cm^{-1}. The lower frequency one at 771 cm^{-1} is a symmetric Si-H bending mode and the higher one at 774 cm^{-1} is a Si-O-Si bending mode. These modes have not been detected presumably because they possess small effective charges.

V. DISCUSSION

It is implied from our data and calculations that the lines at 943.5, 2126.4, and 2151.5 cm^{-1} are related to the V-O-H_2 complex. Moreover, all three lines and their associated isotopic shifts are well reproduced by a structure with a strong binding energy (2.4 eV) between the A center and a hydrogen molecule. The earlier assignment of the line at 891 cm^{-1} to V-O-H_2 (Ref. 15) is inconsistent with our study and leaves unresolved the assignment of this center. This line is, however, one of the most intense LVM bands found in proton-implanted Cz-Si,[15] as well as in electron-irradiated Si:O,H crystals, annealed at about 300 °C.

We found that the growth of the 891.5 cm^{-1} band occurs simultaneously with the disappearance of the V-O-H_2 complex but the band is unaffected by the substitution of hydrogen by deuterium, and could not be correlated with any other line. A tentative assignment for this band is to a V-O_2-H_2 complex. This defect consists of two oxygen atoms sharing a vacancy with a hydrogen molecule, possibly at a nearest tetrahedral interstitial site. The H_2 molecule would only slightly perturb the vibrations of oxygen atoms in VO_2 (895.3 cm^{-1}) in the same way as H_2 in the O_i-H_2 center.[17,18] If this is the case, then LVM's close to 3700 cm^{-1} are to be expected, but were not observed due to their small effective charges. The complexes would be formed from the capture of V-O-H_2 complexes by interstitial oxygen atoms. However, the high thermal stability of such a defect has to be accounted for, and further studies are required to determine its structure and formation mechanism.

VI. CONCLUSION

H_2 molecules, which are introduced into moderately doped silicon crystals by high-temperature indiffusion from a H_2 (D_2) gas ambient, with subsuequent quenching to room temperature, can interact strongly with defects produced by irradiation with fast electrons. In Cz-Si crystals, the interaction of mobile H_2 molecules with A centers leads to the creation of V-O-H_2 complexes. This complex gives rise to infrared-absorption lines at 943.5, 2126.4, and 2151.5 cm^{-1}. *Ab initio* calculations showed that the most stable configuration of V-O-H_2 consists of a C_{2v}-symmetry structure where an oxygen and two hydrogen atoms share a vacancy site. The calculated LVM's and their isotopic shifts reproduce well the experimental values. It is tentatively suggested that the interaction of the V-O-H_2 complexes with interstitial oxygen atoms results in the formation of V-O_2-H_2 complexes, which are responsible for the infrared-absorption line at 891.5 cm^{-1}.

ACKNOWLEDGMENTS

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