Bond-center hydrogen in dilute Si$_{1-x}$Ge$_x$ alloys: Laplace deep-level transient spectroscopy

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We apply Laplace deep-level transient spectroscopy *in situ* after low-temperature proton implantation into dilute Si$_{1-x}$Ge$_x$ alloys and identify the deep donor state of hydrogen occupying a strained Si-Si bond-center site next to Ge. The activation energy of the electron emission from the donor is ~158 meV when extrapolated to zero electrical field. We construct a configuration diagram of the Ge-strained site from formation and annealing data and deduce that alloying with ~1% Ge does not significantly influence the low-temperature migration of hydrogen as compared to elemental Si. We observe two bond-center-type carbon-hydrogen centers and conclude that carbon impurities act as much stronger traps for hydrogen than the alloy Ge atoms.

I. INTRODUCTION

A particular class of electrical active hydrogen centers in crystalline silicon can be associated with interstitial hydrogen occupying either the bond-center site (BC) or a position near the open tetrahedral site (T) in the silicon lattice.[1] Although these centers are unstable at room temperature, they play an important role as stepping stones for the migration of atomic hydrogen.[2,3] It has been shown[3–5] that slightly modified and thermally stabilized versions of the BC and T centers can form in the vicinity of impurities such as oxygen and carbon. This tendency of hydrogen to become trapped in a crystal strain field with only minor changes in the electrical properties appears to be a rather general feature. The strain causes elongation of some Si–Si bonds (and compression of others) with the consequence that hydrogen atoms are most easily incorporated in the elongated bonds. It should be noticed in this connection that the presence of elongated bonds has been suggested also to be responsible for trapping of impurities in amorphous or polycrystalline material.[6,7] The trapping influences the migration of hydrogen in crystalline silicon and can be an intermediate step in the formation of secondary defects, e.g., the formation of dopant-hydrogen pairs causing neutralization of shallow donors or acceptors. These pairs are similar to the strain-type defects in the sense that hydrogen binds to a Si atom next to the dopant[1] with comparable binding energies. Hence, technologically important compensation processes may be affected such as the surface hydrogenation of wafer material caused by a wet chemical etching at room temperature. We emphasize that the interstitial-type hydrogen strain-field defects are fundamentally different from most secondary defects formed in irradiated material as a result of hydrogen migration, e.g.,

those where hydrogen becomes trapped at one or more vacancies and forms a class of hydrogen decorated vacancy (V) centers such as VH or V$_2$H.[8] In these centers hydrogen breaks the distorted Si–Si bonds and saturates one of the dangling bonds with the consequence that another bond is left unsaturated and the remaining bonds are reconstructed. Such dangling-bond defects are generally electrically active with similar acceptor states in the upper half of the band gap. This qualitative picture also applies to dangling bond structures where a third agent is present such as the VOH center.[9]

A dilute Si$_{1-x}$Ge$_x$ alloy forms a system in which randomly distributed internal strain is imposed on the Si lattice in order to accommodate the incorporation of Ge atoms. This strain can play a role similar to that of the local strain in elemental silicon introduced by a carbon or an oxygen impurity. A specific question relates to bond-center hydrogen. Does this center become more stable or less stable in the vicinity of Ge and what is the effect on the electronic properties? The results for elemental Si indicate that the elongation of some of the Si-Si bonds in the neighborhood of interstitial oxygen aids the outward relaxation that hydrogen needs to enter the BC site and therefore promotes the incorporation of hydrogen into these strained bonds. A similar promotion effect has recently been ascribed to carbon at the substitution site next to an otherwise regular Si–Si bond.[5] Both these strained BC structures form during hydrogen implantation at low-temperature. In their positive charge states they anneal in the range 200–250 K and the carbon-related center converts to a Si-H-C structure where the hydrogen atom has swung from the carbon-strained BC site into a position between Si and C.

In this article we examine the influence of Ge on the formation and stability of bond-center hydrogen in a dilute

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$Si_{1-x}Ge_x$ alloy. We identify and characterize a Ge-strained bond-center defect, which is geometrically analogous to the C-strained bond-center defect described above.

II. TECHNICAL DETAILS

A. Sample preparation

The data presented in this work were obtained with Schottky diodes prepared on samples cut and polished from a float-zone (FZ) and annealed $Si_{1-x}Ge_x$ phosphorus-doped bulk crystal[10] with the Ge fraction $x=0.008$ measured by secondary-ion mass spectroscopy (SIMS). The concentrations of oxygen and carbon were obtained as $\leqslant 1 \times 10^{16}$ cm^{-3} and $\sim 3 \times 10^{16}$ cm^{-3} by infrared absorption, respectively. The donor concentration was measured to $\sim 4 \times 10^{13}$ cm^{-3} corresponding to an alloy resistivity of about 100 Ω cm. In addition we used a sample prepared from as-grown[11] Czochralski $Si_{1-x}Ge_x$ with $x=0.013$. The sample material was preannealed at 650 °C to remove thermal donors. The interstitial oxygen concentration $[O_i]$ was measured as 8×10^{17} cm^{-3} and the carbon concentration $[C_s]$ as $\sim 3 \times 10^{16}$ cm^{-3}. As reference samples we used Schottky diodes made on 100-Ω cm FZ 50-Ω cm Czochralski grown (Cz), and carbon-rich 20-Ω cm FZ silicon (C-FZ). The concentrations of oxygen and carbon in the Cz silicon were measured to 1×10^{18} and 1×10^{16} cm^{-3}, respectively. The corresponding figures for the C-FZ material were obtained as 1×10^{16} and 1×10^{17} cm^{-3}.

B. Experimental procedure

Two $Si_{1-x}Ge_x$ alloy samples (or one alloy sample together with a reference sample) were mounted on the cold finger of a cryocooler and implanted with protons (or helium ions to provide control samples) at a temperature of 60 K. The implantation energy was chosen for the individual samples so that the peak of the implants would match the depletion width of the diode under suitable reverse bias. For the $Si_{1-x}Ge_x$ sample this energy was 750 keV corresponding to a reverse bias of ~ 3 V. In this way we could perform subsequent *in situ* deep-level transient spectroscopy (DLTS) utilizing the Laplace method[12] to deconvolute composite capacitance transients into emission-rate spectra. *In situ* measurements are essential so that the sample can be held at low temperature during the period between irradiation and measurement to avoid uncontrolled migration of the implanted hydrogen. The sample bias was chosen to place the implantation profile close to the edge of the reverse-bias depletion layer in order to minimize the electric field at the depth of the implants and at the same time maximize the amplitude of the DLTS signals. The implantation doses were monited *in situ* by capacitance-voltage profiling. All samples with $\leqslant 35\%$ compensation at the peak of the implants could be utilized maintaining an exponential shape of the individual capacitance transients. Besides the improved resolution, a special feature of the Laplace method is that isothermal spectra are recorded, which makes the method particularly suitable for annealing studies. In the present work we first recorded ''as-implanted spectra'' in the temperature range from
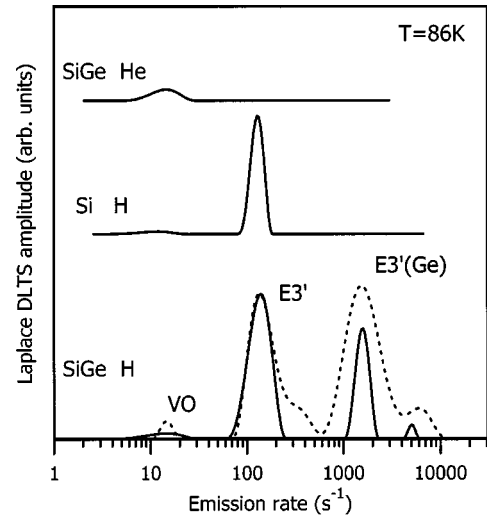

FIG. 1. Laplace DLTS spectrum measured *in situ* after implantation of hydrogen at 60 K into short-circuited Schottky diodes made on FZ *n*-type $Si_{1-x}Ge_x$ alloy (0.8% Ge) reveals two donor signals $E3'$ and $E3'$(Ge). Comparison with analogously H-implanted Si and He-implanted $Si_{1-x}Ge_x$ establish that $E3'$(Ge) originates from a hydrogen defect associated with germanium. The overlaid $Si_{1-x}Ge_x$ spectrum is obtained with Cz material (1.3% Ge) and has been normalized to the $E3'$ signal of the FZ material. The small satellites of the main peaks can be ascribed to the presence of oxygen in the Cz sample.

60 to 87 K where no significant annealing occurred. Then isochronal annealing sequences were carried out and ''as-annealed spectra'' were obtained choosing suitable temperatures for data recording below 87 K. Because of the relatively low temperature needed, the peaks of the Laplace spectra occur at low emission rates. This makes it essential that the samples are shielded against the thermal radiation inside the implantation chamber during measurements.[13]

III. RESULTS AND ANALYSIS

A. Identification of bond-center signals

Figure 1 depicts the Laplace DLTS spectra obtained at 86 K after implanting hydrogen at 60 K into short-circuited diodes at a dose of $\sim 10^9$ cm^{-2}. Prior to the implantation no signal is present in the displayed emission-rate range and only very small and insignificant process-induced signals were revealed (by conventional DLTS) during cooling of the sample from room temperature. The spectrum for the FZ $Si_{1-x}Ge_x$ alloy is compared to a spectrum obtained for a reference diode made from 100-Ω cm commercial FZ wafer material implanted at the same temperature and measured so that the electric field at the implantation range is about the same in the two cases. No significant peaks other than those shown appear in the emission rate range $0.05-5 \times 10^3$ s^{-1} between 60 and 87 K. The reference spectra from the silicon samples reveal the center known as $E3'$ in the literature,[14] which has been ascribed previously to hydrogen at the regular bond-center site[3,15] corresponding to the transition $H^0(BC) \rightarrow H^+(BC) + e_C$. Apart from a shift in emission rate due to field dependence, an identical reference spectrum was

taken with 20-Ω cm elemental Si grown in the same reactor as the alloy sample. As depicted, the $E3'$ signal is present also in the spectra from the proton-implanted $Si_{1-x}Ge_x$ together with a satellite signal. We shall denote this satellite signal $E3'(Ge)$ anticipating our final assignment, namely, that it originates from a strained bond-center site next to an alloy Ge atom.

To demonstrate that both $Si_{1-x}Ge_x$ signals are indeed hydrogen-related, Fig. 1 includes a reference spectrum obtained with a $Si_{1-x}Ge_x$ sample implanted with helium to the same depth. As can be seen this spectrum shows no trace of the $E3'$ signals but does reveal the A-center signal (VO), also seen in the hydrogen-implanted samples. From their strengths we infer that the two $E3'$ signals together account for the majority ($\geqslant 70\%$) of the implanted protons. In accordance with previous results for pure silicon,[3] we assume that the remaining implants are most likely hidden in the form of negatively charged hydrogen at T sites. The $E3'(Ge)$ signal is about a factor of 12.5 stronger than expected for a pure statistical population of Si-H-Si bond-center sites next to the Ge atoms of the alloy. The same overpopulation factor is obtained with the Cz sample containing 1.3% Ge (see the dashed overlay in Fig. 1). The overpopulation factors have been determined from statistical simulations, which take into account the various ways that hydrogen can be introduced into the bonds of an alloy of given composition. The sizable overpopulation (in conjunction with the fact the two $E3'$ signals together account for most of the implanted hydrogen) demonstrates that ultrafast migration of the implants to reach Ge sites occurs in the final stage of thermalization. This is fully in accordance with previous results for pure silicon,[3,5] where it was found that considerable direct trapping occurs at interstitial oxygen in oxygen-rich material and at carbon in carbon-rich material, respectively. Similarly, the direct trapping at carbon is observed also in the present work for the case of the oxygen-lean, carbon-rich $Si_{1-x}Ge_x$ sample. See Fig. 2 and next section for further discussion.

During the implantation stage we may assume that hydrogen migrates as H^0 through the open areas of the lattice where only moderate lattice relaxation is needed to accommodate the process. Eventually, this migration stage leads to trapping of H^0 into the bond-center site, or capturing of an additional electron and trapping of H^- at the T site. Only a minor part of the implant becomes $H^-(T)$ because the main part overcomes the barrier to form either the $E3'$ or the $E3'(Ge)$ center. Under the condition that both types of bond-center sites can be treated as sinks at 60 K we find the $E3'(Ge)$ barrier lowered by ~ 13 meV as compared to the $E3'$ barrier. This calculation is based on the assumption that during the final stage of thermalization, the implants possess an average kinetic energy somewhat lower than both barriers and move over distances much larger than the average distance between Ge atoms. The treatment of both bond-center sites as sinks and thereby the ascription of the overpopulation phenomenon to a lowering of the barrier for capture of hydrogen at a bond-center site next to Ge are substantiated by annealing measurements, which we discuss in detail in the next section.
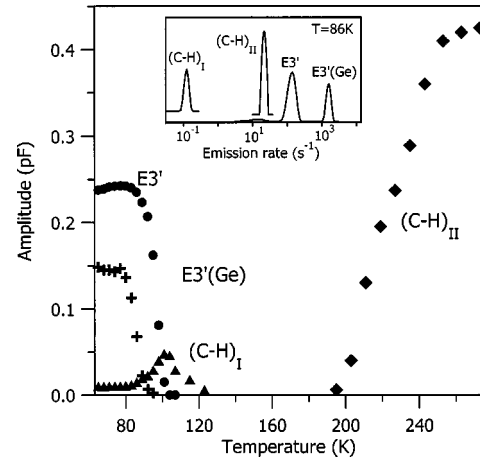

FIG. 2. Annealing of the alloy $E3'$ and $E3'(Ge)$ centers shown in Fig. 1 carried out in 5-min isochronal steps and with an unbiased diode. The emission rate spectra are taken at low temperature after each annealing step choosing suitable rate windows as shown by the inset. The center $(C\text{-}H)_I$ that appears transiently is carbon-related (cf. Fig. 3) and analogous to $E3'(Ge)$ as discussed in the text. The annealing process $H^0(BC) + e^- \rightarrow H^-(T)$ at ~ 100 K hides the implanted hydrogen at T sites, and all implanted hydrogen is recovered in another carbon-related center, which causes the $(C\text{-}H)_{II}$ emission.

B. Isochronal annealing

In n-type silicon the neutral bond-center defect $H^0(BC)$ becomes unstable at ~ 100 K. At this temperature the interstitial hydrogen overcomes the barrier towards the T site[3] and captures an electron to form $H^-(T)$. This is the lowest-energy configuration for interstitial hydrogen in n-type material.[1] Figure 2 depicts results of an isochronal annealing series that compare the annealing of $E3'$ and $E3'(Ge)$. As can be seen, both signals disappear at almost the same temperature with the $E3'(Ge)$ center being slightly less stable than the $E3'$ center. Taking the two prefactors to be the same and using the activation energy of the $E3'$ annealing ~ 0.295 eV determined previously,[15] we estimate the barrier for the annealing of $E3'(Ge)$ to be ~ 0.26 eV. As shown in Fig. 2 a center denoted $(C\text{-}H)_I$ grows in and disappears again, correlated with the disappearance of $E3'$ and $E3'(Ge)$. This center is somewhat deeper than both $E3'$ centers and the corresponding Laplace DLTS signal is outside the rate window of Fig. 1. We include as an inset in Fig. 2 a part of the emission-rate spectrum in the pertinent rate window to show how the $(C\text{-}H)_I$ signal appears in the Laplace spectrum as a clear and well-separated peak. We emphasize that the transient appearance of $(C\text{-}H)_I$ at the zero-bias annealing stage of the $E3'$ signals is just another manifestation of the swift migration of $H^0(T)$ as already discussed in connection with the formation of $E3'(Ge)$ in the implantation process. Here, the H^0 migration occurs during the conversion $H^0(BC) \rightarrow H^0(T) \rightarrow H^-(T)$.

The annealing results lend further support to our interpretation that swift hydrogen migration in conjunction with barrier lowering is responsible for the overpopulation rather than increased stability of the Ge-perturbed center. The ob-
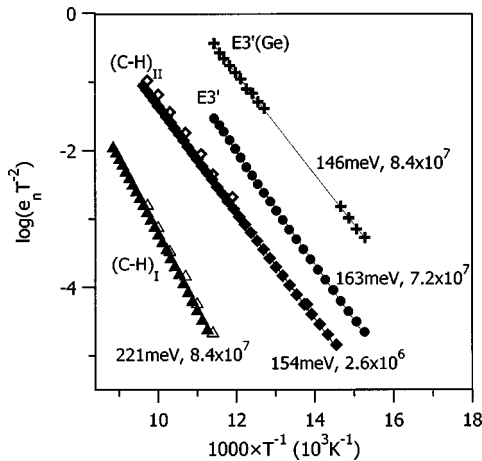
FIG. 3. Arrhenius analysis of $E3'$ and (C-H) centers in the $Si_{1-x}Ge_x$ alloy. The identity of $(C-H)_I$ and $(C-H)_{II}$ plots (filled symbols) with the analogous plots of data obtained with a C-FZ reference sample [open symbols (Ref. 5)] is demonstrated. The emission activation energies and preexponential factors (in $s^{-1} K^{-2}$ units) are given for each plot.

FIG. 4. Schematic diagrams of (a) $(C-H)_I$, (b) $E3'(Ge)$, and (c) $(C-H)_{II}$ centers.

servation that $E3'(Ge)$ is less stable than $E3'$ and that both centers convert into globally stable H^- configurations exclude the possibility that the two centers could have reached a state of thermal equilibrium during implantation. If this had been the case one would expect the Ge-perturbed center to be *underpopulated*. Furthermore, as a consequence of the implied exchange of hydrogen between the two centers, it would be expected that a considerable fraction of the implanted hydrogen would be hidden as migrating $H^0(T)$. In consequence, it would be expected that a continuous migration of H^0 away from the BC sites [to subsequently form $H^-(T)$ by electron capture] would occur at the implantation temperature. It is clear from our results that this leakage from the BC configurations through $H^0(T)$ does not happen.

From the Arrhenius analysis presented in Fig. 3 we conclude that $(C-H)_I$ is identical to a carbon-hydrogen center previously identified in carbon-rich float-zone silicon[5] under experimental conditions similar to those of the present study. The $(C-H)_I$ defect has also been observed by infrared absorption,[16] and interpreted[5,16] as a carbon-perturbed form of bond-center hydrogen. As mentioned in the Introduction it consists of a carbon atom at a substitution site of the silicon lattice next to a Si-H-Si three-center bond [see Fig. 4(a)]. The initial concentrations of the $E3'$ and $E3'(Ge)$ centers account for the main part of the hydrogen. In accordance with the previous results for pure silicon,[3] we assume that the disappearance (Fig. 2) of both $E3'$ signals results from hydrogen jumping away from the bond-center site. However, the figure also reveals that the entire strength of the original signals can be recovered at ~ 225 K. At this annealing temperature a new signal appears that is identical to the carbon-hydrogen center denoted $(C-H)_{II}$ observed under similar annealing conditions in carbon-rich silicon and ascribed to the acceptor state of the three-center Si-H-C defect.[5] This identification follows from the Arrhenius plots (Fig. 3) and annealing behavior.
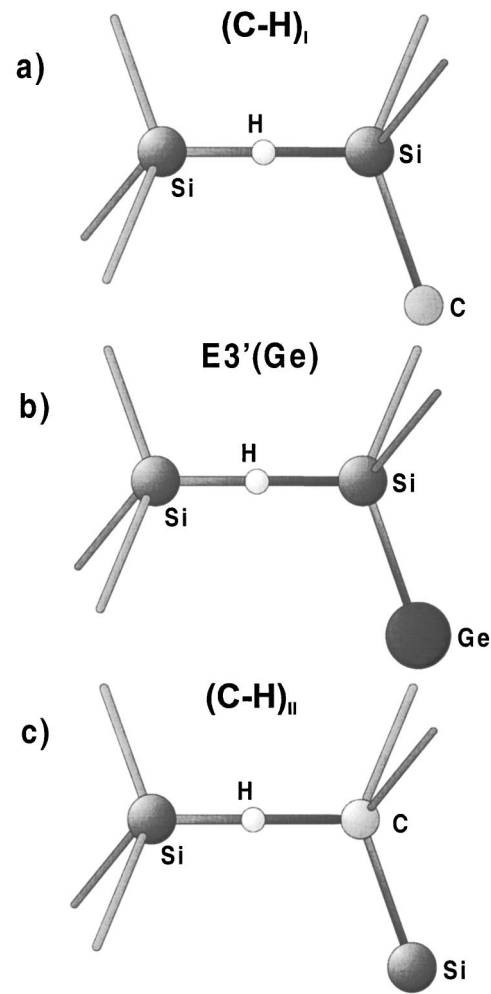
C. Arrhenius analysis

Figure 3 compares Arrhenius plots of the emission data obtained with the alloy sample and data obtained with a sample of carbon-rich FZ silicon. The plots labeled $(C-H)_I$ and $(C-H)_{II}$ and marked with full symbols relate to the centers with the same labels shown in Fig. 2 appearing during annealing. As can be seen, the Arrhenius plots are practically identical to those obtained with the carbon-rich sample (open symbols[5]). This result forms a solid basis for the interpretation of the annealing data given in Sec. III B. The activation energy and preexponential factor determined from the $E3'$ plot agree with results for pure silicon in accordance with identical positions of the emission peaks as shown in Fig. 1. Note that the preexponential factors of the $E3'$, $E3'(Ge)$, and $(C-H)_I$ emission rates listed in the figure are very similar (and large), supporting the conclusion that all three emission signals are from deep donors. This conclusion is consistent with the observation that all emissions also show electrical field dependence. Contrary to this, the lack of field dependence and the smaller prefactor of $(C-H)_{II}$ indicate emission from a deep acceptor. It should be noticed, however, that $(C-H)_{II}$ is identical to the carbon-hydrogen DLTS signal
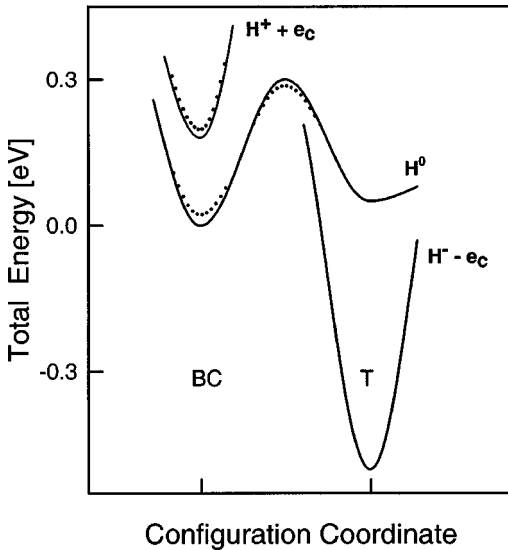
FIG. 5. Configuration diagrams of interstitial hydrogen in elemental Si and $Si_{1-x}Ge_x$ alloy. The dotted lines are modified potential curves indicating the role of strain imposed by an alloy Ge atom next to bond-center hydrogen (see Fig. 4).

known as $E3$ in the literature,[17–19] and previously assigned as a donor signal, an issue which is discussed in more detail elsewhere.[5] The field dependencies of $E3'$ and $E3'(Ge)$ measured for the alloy sample are practically equal, which means that the difference in activation energies obtained from the Arrhenius analysis of Fig. 3 should equal the zero-field value of this difference. The $E3'$ activation energy has been extrapolated to zero electrical field[3] with the result $\Delta H \sim 175$ meV, and combining this value with the difference $\delta = 17$ meV obtained form the Arrhenius plots of $E3'$ and $E3'(Ge)$ we get $\Delta H \sim 158$ meV as an estimate for the zero-field activation energy of $E3'(Ge)$.

IV. DISCUSSION

A sketch of the total-energy variations of the three charge states H^-, H^0, and H^+ along paths connecting neighboring BC and T sites in the configuration space of the silicon lattice has been presented previously.[3,4] In Fig. 5 we depict a similar sketch in order to show how these hydrogen configuration potentials are modified in the vicinity of the Ge atoms of the dilute alloy. The construction of the modified diagram is based on the assumption, already anticipated in the data analysis, that $E3'(Ge)$ originates from hydrogen occupying a strained bond-center site neighboring a Ge atom [see Fig. 4(b)]. The key data to quantify the diagram are the lowering of the formation barrier by ~ 13 meV estimated in Sec. III A, the decrease in thermal stability by ~ 35 meV derived in Sec. III B, and the decrease in activation energy by ~ 17 meV obtained in Sec. III C. As it can be seen the diagram indicates a slightly reduced stability of the strained bond-center site as compared to the regular site. According to the theoretical estimates[7] the lowering (increasing) of formation energy of the bond-centered Si-H-Si configuration is about 4 meV per 0.001 Å distortion of the Si–Si bond length. These figures

are consistent with the intuitive explanation that a Si–Si bond next to a longer Si–Ge bond should be compressed and thereby oppose the outward relaxation needed to accommodate a hydrogen atom. Hence, the diagram is fully consistent with the assumed structure of the $E3'(Ge)$ center. One may argue that moving the Ge atom one step further away from hydrogen could cause a strain that would tend to increase the Si–Si bond length and thereby aid the incorporation of hydrogen in the second nearest Si–Si bond to Ge. We do not rule out that this might happen. However, we shall assume the effect on the total-energy curves to be small so that this center cannot be discerned from undisturbed bond-center hydrogen. This is similar to the case when strain is caused by interstitial oxygen in elemental silicon. In this case the oxygen-strained center $E3''$ cannot be discerned from the regular bond center $E3'$ on the basis of emission rates alone,[3] only the stability is influenced. A small amount of $E3''$ is actually produced in the $Si_{1-x}Ge_x$ alloy during implantation. However, because it is unstable under zero-bias implantation it converts immediately to the corresponding T-site defect,[4] the presence of which is hidden in the increased amount of recovered hydrogen in the form of $(C-H)_{II}$ with an amplitude larger than the sum of the $E3'$ amplitudes (see Fig. 2).

The configuration scheme (Fig. 5) reflects the similarity of the experimental properties of $E3'$ and $E3'(Ge)$, a similarity that in our view also excludes that the $E3'(Ge)$ signal could originate from hydrogen bound directly to Ge. The analogy of $E3'(Ge)$ and $(C-H)_I$ supports this conclusion. A Si–Si bond next to a shorter Si–C bond should be elongated with the consequence that hydrogen at a carbon-strained bond-center hydrogen should be more stable than regular bond-center hydrogen, in agreement with the observation that $(C-H)_I$ is formed transiently in $E3'$ annealing. As indicated by the configuration diagram the bond-center configurations (strained or unstrained) are metastable in n-type material. The zero-bias annealing causes the formation of strained or unstrained $H^-(T)$. With carbon present in the sample, the subsequent emission $H^-(T) \rightarrow H^0(T)$ at ~ 225 K and fast migration of neutral hydrogen[20] then lead to the formation of the Si-H-C defect structure sketched in Fig. 4(c). Because the Fermi level is below the Si-H-C acceptor level at 225 K we may assume that the defect eventually forms in its occupied donor state,[5] whereas its presence is revealed upon cooling to low temperature by the acceptor emission $(C-H)_{II}$. We may assume that the less stable $(C-H)_I$ rather than the more stable $(C-H)_{II}$ forms directly during implantation at low temperature because the barrier for its formation is lower. At the higher annealing temperature a small difference in barrier height is less important and the neutral $(C-H)_I$ defect is unstable anyway. The fact that the Si-H-C defect and not the analog Si-H-Ge defect forms during annealing indicates that the latter defect is less stable or nonexistent.

V. CONCLUSION

We have compared the properties of bond-center hydrogen in dilute $Si_{1-x}Ge_x$ alloy and elemental silicon. In

$Si_{1-x}Ge_x$ we identified two donor levels. One is practically identical to the corresponding level of elemental Si, and one is slightly shallower and corresponds to a Si-H-Si bond-center defect next to a Ge atom. Both donor configurations form during low-temperature implantation but the strained configuration is overpopulated in comparison to a random distribution as a consequence of fast hydrogen migration in the implantation process. We determined configuration potentials of the Ge-strained structure that are remarkably close to those of isolated hydrogen in elemental silicon. This indicates that hydrogen migration is only moderately affected by dilute alloying with germanium, consistent with the additional result that hydrogen interacts with carbon impurities during migration in much the same way as in elemental silicon. During this migration at low temperature a carbon analog to the Ge-perturbed bond center hydrogen forms. We conclude that in the sequence Ge, Si, C the variation of the group-IV element at the neighbor site of the Si-H-Si bond center causes the donor level to deepen and the stability of the defect (in its neutral charge state) to increase.

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