Influence of n^+ and p^+ doping on the lattice sites of implanted Fe in Si

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We report on the lattice location of implanted ^{59}Fe in n^+ - and p^+ -type Si by means of emission channeling. We found clear evidence that the preferred lattice location of Fe changes with the doping of the material. While in n^+ -type Si Fe prefers displaced bond-centered (BC) sites for annealing temperatures up to 600°C , changing to ideal substitutional sites above 700°C , in p^+ -type Si Fe prefers to be in displaced tetrahedral interstitial positions after all annealing steps. The dominant lattice sites of Fe in n^+ -type Si therefore seem to be well characterized for all annealing temperatures by the incorporation of Fe into vacancy-related complexes, either into single vacancies which leads to Fe on ideal substitutional sites, or multiple vacancies, which leads to its incorporation near BC sites. In contrast, in p^+ -type Si the major fraction of Fe is clearly interstitial (near-T or ideal T) for all annealing temperatures. The formation and possible lattice sites of Fe in FeB pairs in p^+ -Si are discussed. We also address the relevance of our findings for the understanding of the gettering effects caused by radiation damage or P-diffusion, the latter involving n^+ -doped regions.

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I. INTRODUCTION

For decades, 3d-transition metals in Si have been in the focus of silicon research due to their unwanted presence as contaminants¹⁻⁵. Depending on the complexes that the transition metals (TMs) form, and thus on their lattice sites, deep levels can be created, forming recombination centers and, therefore, acting as lifetime killers for minority carriers^{2,5}. The electric passivation of TMs is required to prevent, e.g., the malfunctioning of electronic circuits based on silicon or the efficiency degradation of solar cells. To reduce the harmful effects of such deep levels a number of gettering techniques were developed in order to either trap TMs into inactive areas or to transform them into electrically inactive forms^{3,4,6}. Some of the gettering techniques rely on deliberately creating highly doped regions in the Si wafer, e.g. through p^+ -doping with boron, or by diffusing the n -type dopant P in from the surface, others on creating vacancies through irradiation. More recently TM-doped silicon has also attracted attention as a possible magnetic semiconductor system. The magnetic properties of TMs in Si are expected to depend on whether the TMs are incorporated substitutionally or interstitially and based on first principle calculations it was proposed that the position of the Fermi level (which depends on n - or p -doping) and the availability of vacancies are of crucial importance in controlling the lattice site⁷⁻¹². Most of the theoretical work on this subject concerned Mn in Si, but also Fe was addressed^{9,12}.

Regarding the gettering processes for TM contami-

nants in Si, Fe remains the best-studied species. While the macroscopic behavior of Fe during gettering can now be predicted to some extent, see e.g. Ref. 13, many fundamental questions on the basic underlying microscopic mechanisms are still poorly understood, among them the detailed knowledge of Fe lattice sites in different types of silicon, or when forming complexes with other impurities, such as dopants, or implantation defects, such as vacancies. For instance, the P-diffusion gettering process, which is nowadays widely used in the fabrication of n - p -junction Si solar cells¹³⁻²⁰ is known to create on top of a low p -doped multi-crystalline Si wafer highly-doped n^+ -regions, in which Fe is trapped. It has been recently suggested²⁰ that the high concentration of vacancies created during P-diffusion is a key ingredient in the gettering process; at the same time it is expected from theoretical grounds that Fe becomes less electrically active when it is trapped by Si vacancies²¹. Consequently, providing microscopic information what actually happens to Fe when it encounters Si vacancies in an n^+ -type environment, as is achieved in this paper, will be crucial to understand the fundamental principles underlying this gettering process. In p^+ -type Si, on the other hand, the formation of FeB pairs between the acceptor B and interstitial Fe is a well-known phenomenon studied by electrical and optical techniques^{1-3,22-24}, but so far no detailed information on the lattice sites of Fe in such pairs has been available, which is why we have also devoted special attention to this subject.

Emission Channeling (EC) is a unique technique which can investigate the lattice sites of low concentrations of impurities in single crystals. EC relies on implanting radioactive probe atoms that decay by the emission of β^- particles, which, on their way out of the crystal, experience channeling effects along some crystal directions,

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depending on the lattice site occupied by the probe atom.

EC has already been applied to study the lattice sites of ^{59}Fe in low and moderately doped n - and p -type Si^{25,26}. The results showed ^{59}Fe in three different positions: ideal substitutional (S), displaced substitutional (near-S) and displaced tetrahedral interstitial (near-T) sites. Iron on near-S sites was the dominating fraction for annealing temperatures below 500°C, while annealing between 500°C and 800°C moved the majority of ^{59}Fe to near-T sites, and ideal S sites dominated, along with near-T sites, the channeling patterns of 800-900°C annealed samples. Similar to other EC studies involving the transition metals Cu²⁷⁻²⁹ and Ag³⁰, it was suggested that the observed sites, in particular near-S sites, could be related not only to Fe interacting with single vacancies but also to vacancy clusters, such as divacancies³¹, where the TM prefers to sit between the two vacancies (bond-centered sites). Furthermore, ab initio calculations have recently confirmed the stability of fourfold vacancy clusters based on hexavacancy rings^{32,33}. It was theoretically predicted that interstitial Cu atoms can be trapped inside such vacancy clusters and their positions seem to be close to a displaced bond-centered site in an undisturbed crystal^{34,35}.

A change of doping type can have profound implications on the preferred lattice sites of impurities by several active mechanisms. Generally speaking, if the impurity is electrically active, the formation energies and solid solubilities of its various configurations are directly coupled to the electron-hole charge equilibrium in the semiconductor. Hence, a change of the Fermi level can lead to a particular form of impurity defect becoming more or less energetically favorable. In the simplest case, a change of the Fermi level will directly change the prevailing charge state of the impurity itself. For instance, interstitial iron has a well-known deep donor level at $E_V + 0.40$ eV, i.e. close to the valence band^{1,2}. While in intrinsic and n -type Si interstitial iron is neutral, it will prevail in a +1 charge state in p -type Si, and, in principle, Fe might prefer a different interstitial site. Another example is the increase in the solubility of donors in case of counter-doping with acceptors. If, e.g., an interstitial impurity acts as a donor while the substitutional form is an acceptor, counter doping with acceptors will clearly increase the solubility of donors. A particular case is the situation when certain charge states of an impurity enable it to form pairs with other impurities. The most common such example are the formation of donor-acceptor pairs, e.g. $\text{FeB}^{1-3,22,23}$. The binding energy, which is gained when the pairs are formed, can cause the impurity within the pair to be much more stable and hence prevail over other configurations in the lattice. On the other hand, the position of the Fermi level also changes the preferred charge states and concentrations of other defects that can interact and form complexes with Fe. For instance, the single vacancy in Si has been reported to exist in various charge states, ranging from -2 in highly n -type to +1 or +2 in highly p -type Si³⁶. Neutral or pos-

itively charged interstitial Fe_i^+ will obviously much easier combine with negatively charged vacancies in n -type Si than with positively charged ones in p -type Si.

In our previous EC study²⁵, no significant changes were observed in the ^{59}Fe lattice position when using different types of Si for resistivities above ~ 0.01 Ωcm . However, this was attributed to the possibility that the Fermi level, following implantation into low or moderately doped Si, is most likely close to the mid-gap position, due to the fact that the concentration of implantation defects is, by several orders of magnitude, larger than those of n - or p -type dopants. Therefore, in this work, we have applied the EC technique to study the lattice sites of ^{59}Fe implanted into highly doped n^+ - and p^+ -type Si. Our results confirm the presence of ^{59}Fe in three different lattice sites: displaced bond-centered (near-BC), displaced tetrahedral interstitial (near-T) and ideal substitutional (S) sites. We show that the stability of ^{59}Fe on near-BC sites changes with the doping of the material. By comparing with other experimental techniques from literature, we also show evidence of FeB pairs in p^+ -type Si, with ^{59}Fe on near-T sites. Although FeB pairs dissociate easily during a low temperature annealing, they should also form again during cooling down, while defects produced during implantation tend to disappear upon annealing.

II. EXPERIMENT

Czochralski grown silicon samples were doped with the long-lived isotope ^{59}Fe ($t_{1/2} = 44.6$ d) by implanting the precursor isotope ^{59}Mn ($t_{1/2} = 4.6$ s) at the on-line isotope mass separator facility ISOLDE at CERN, with 60 keV. Upon decay of ^{59}Mn , the ^{59}Fe atoms receive a mean recoil of 200 eV, assuring their re-implantation and thus avoiding any influence from the previous site of ^{59}Mn .

The samples used were n^+ -type Si (n^+ -Si) with a $\langle 111 \rangle$ surface, doped with arsenic, and p^+ -type Si (p^+ -Si) with a $\langle 100 \rangle$ surface, doped with boron. The resistivity and arsenic concentration of the n^+ -Si sample were < 0.001 Ωcm and $[\text{As}] > 1.2 \times 10^{20}$ cm^{-3} , while the resistivity and boron concentration of the p^+ -Si sample were < 0.002 Ωcm and $[\text{B}] > 6.5 \times 10^{19}$ cm^{-3} .

^{59}Fe was implanted in both types of Si during approximately 2 h to obtain a fluence of 6×10^{12} cm^{-2} , with each sample mounted in such a way that the surface normal was off beam by 10° to avoid channeled implantation. In our previous studies of ^{59}Fe in low-doped Si^{25,26}, 14 samples were studied of which 9 were $\langle 111 \rangle$ and 5 $\langle 100 \rangle$ oriented, but no significant difference was found in the lattice location of Fe. We hence believe that the different surface type of the two Si samples will have no particular influence on the outcome of the studies presented here. The depth profile of the implanted ^{59}Fe was obtained using the SRIM code³⁷. The implanted ^{59}Fe profile is approximated by a Gaussian distribution centered at 545 Å from the surface, with a straggling of 207 Å and a peak

concentration of $1.1 \times 10^{18} \text{ cm}^{-3}$. SRIM simulations also show that about 1000 vacancies per implanted Fe ion are generated at 0 K and that their distribution profile peaks at about half way from the surface to the maximum implanted ^{59}Fe concentration. The concentration peak of the vacancy profile was approximately $1 \times 10^{21} \text{ cm}^{-3}$.

A few days after the implantation, the samples were mounted on a goniometer made of Ta and Mo and annealed in situ up to 900°C in steps of 100°C , during 10 min, under vacuum better than 10^{-5} mbar. During annealing, the time it took to heat up the sample was quite fast (a few minutes at most). On the other hand, the cool down was slow, lasting up to 30 min to reach room temperature for the highest annealing temperatures. After each annealing step, the β -emission yield in the energy window 50-461 keV was measured at room temperature using a position-sensitive detector. The electron intensity patterns were taken as a function of angle ($\pm 2.5^\circ$) near the $\langle 110 \rangle$, $\langle 100 \rangle$ and $\langle 111 \rangle$ axis in n^+ -Si and near the $\langle 211 \rangle$, $\langle 100 \rangle$ and $\langle 111 \rangle$ axis in p^+ -Si. For each experimental EC pattern, electrons that are scattered into the detector by the chamber walls were taken into account by subtracting a flat background pattern, obtained with Monte Carlo electron scattering simulations³⁸, from every pattern. Each measurement took about 1-2 days depending on the necessary statistics for each orientation.

III. RESULTS

The two-dimensional experimental data were fitted using calculated emission channeling patterns, obtained with the so-called *many beam* approach²⁵. The calculated emission channeling patterns include the emission probability of the substitutional (S), hexagonal (H), tetrahedral (T), bond-centered (BC), anti-bonding (AB), split (SP) and the so-called Y and C sites, as well as $\langle 111 \rangle$, $\langle 100 \rangle$ and $\langle 110 \rangle$ displacements between these positions. The location of these sites can be found in Ref. 27. To understand the results and data analysis, one should first discuss the fitting procedure adopted in this study. First, each experimental pattern was fitted by considering one fraction only. Depending on the annealing temperature and whether it was n^+ - or p^+ -Si we obtained three types of sites: ideal substitutional sites (S), sites displaced from bond-centered towards substitutional sites (near-BC) and sites displaced from ideal tetrahedral interstitial towards AB sites (near-T). We then fitted each pattern again by considering these three fractions in the proportion that best decreased the χ^2 of fit. We note that the near-BC sites from this study can be interpreted as near-S sites observed in previous studies on Fe in Si^{25,26}. In fact, new simulations that include more displacements from S towards BC sites (step width $0.0588 \text{ \AA}$ vs. $0.1470 \text{ \AA}$ in Refs. 25 and 26) were here used which enabled us to conclude that these displacements are such that the sites are closer to BC than

FIG. 1. (color online) Comparison of the two-dimensional experimental and calculated emission channeling patterns from ^{59}Fe in n^+ -Si in the vicinity of $\langle 110 \rangle$, $\langle 100 \rangle$ and $\langle 111 \rangle$, following (a) room temperature implantation and (b) annealing at 600°C . The reduction of the channeling effect of the $\{111\}$ planes after the 600°C anneal proves the increase of the near-T fraction. In fact, in (a) only 23% of ^{59}Fe is on near-T sites (21% on ideal S sites and 50% on near-BC sites), while in (b) 40% of ^{59}Fe is on near-T sites (16% on ideal S sites and 44% on near-BC sites).

to S sites. We would like to point out that we can only assess the quality of fit for those lattice sites that we have calculated the emission yield. It thus can never be excluded with absolute certainty that there exist lattice sites which would provide a better fit but which were not calculated. However, the fact that we considered ~ 250 different lattice sites displaced along the major directions $\langle 111 \rangle$, $\langle 100 \rangle$ and $\langle 110 \rangle$ in the unit cell in steps of less than $0.06 \text{ \AA}$, gives us some confidence that we probably did not miss the actual sites by a large amount. On the

other hand, sites that are of very low structural symmetry as a rule lead to very small anisotropy in emission channeling patterns, and the possible fraction of emitter atoms on such sites can be estimated from the random fraction in our experiments, which amounts to the deviation of the sum of all fractions from 100%. It is also important to understand that the use of 3 fit fractions only does not necessarily mean that not more than 3 different lattice sites of Fe are present in our samples. For instance, likely candidates for additional sites of Fe would be ideal BC and ideal T sites. However, if one performs 4-site fits where these sites are allowed in addition, no significant decrease of χ^2 is found, and possible Fe fractions on these sites are small. Therefore, for instance ^{59}Fe on ideal BC sites was not further considered in the following discussion.

Figure 1 shows the experimental and best fit patterns of ^{59}Fe in $n^+\text{-Si}$, obtained after room temperature implantation (a) and after annealing at 600°C (b), in the vicinity of $\langle 110 \rangle$, $\langle 100 \rangle$ and $\langle 111 \rangle$. After room temperature implantation ^{59}Fe prefers to stay on near-BC positions, but a smaller fraction is also present on ideal S and near-T sites. These fractions do not change much while annealing up to 500°C . However, after annealing at 600°C [Fig. 1 (b)] one can observe a less pronounced channeling effect in the $\{111\}$ planes of the $\langle 110 \rangle$ pattern, which corresponds to an increase of the near-T fraction. Although this behavior is similar when compared to the previous study on low and moderately doped n - and p -type Si, in the present case of $n^+\text{-Si}$ the near-T sites never became the dominant fraction and have their highest population following annealing in a narrow temperature range, around 600°C (*cf.* the discussion of Fig. 3 below). The displacements of the fitted near-BC and near-T sites in $n^+\text{-Si}$ were both $\sim 0.8 \text{ \AA}$ (corresponding to 70% from S to BC and from T to AB sites, respectively), except after annealing at 600°C where the displacement of the near-T sites was $\sim 0.2 \text{ \AA}$. This means that for most annealing temperatures the interstitial fraction of Fe in $n^+\text{-Si}$ was actually found somewhat closer to the AB than to the T site.

Emission channeling patterns from ^{59}Fe in $p^+\text{-Si}$ are shown in Fig. 2, after room temperature implantation (a) and after annealing at 400°C (b). As is quite obvious from the $\langle 211 \rangle$ patterns, the $\{111\}$ planes present visible blocking effects after room temperature implantation [Fig. 2 (a)], which become even more intense by increasing the annealing temperature up to 400°C [Fig. 2 (b)]. This blocking effect is also a consequence of the occupation of near-T sites. From Fig. 3 (c) we can see that this near-T fraction increases by annealing up to 500°C , where it starts to reduce until ^{59}Fe diffuses through the bulk or to the surface, at the annealing temperature of 900°C . The near-BC sites in $p^+\text{-Si}$ were displaced $\sim 0.6 \text{ \AA}$ from ideal S sites, for all annealing temperatures. However, in contrast to $n^+\text{-Si}$, different displacements for the near-T sites are here observed (Fig. 4), suggesting the existence of different ^{59}Fe complexes.

FIG. 2. (color online) Comparison of the two-dimensional experimental and calculated emission channeling patterns from ^{59}Fe in $p^+\text{-Si}$ in the vicinity of $\langle 211 \rangle$, $\langle 100 \rangle$ and $\langle 111 \rangle$, following (a) room temperature implantation and (b) annealing at 400°C . With annealing temperatures up to 400°C , the channeling effect of the $\{111\}$ plane in the as-implanted state is converted to a blocking effect, showing a considerable increase of the near-T fraction. In fact, in (a) 48% of ^{59}Fe is on near-T sites (18% on ideal S sites and 21% on near-BC sites), while in (b) 91% of ^{59}Fe is on near-T sites (no ideal S nor near-BC fractions were detected).

Note that the sum of all fitted fractions, which is also shown in Fig. 3, may deviate from 100%. While small deviations can be explained by statistical errors in the analysis, there are also some systematic effects: (1) After the implantation, a small fraction of ^{59}Fe is located in heavily damaged surroundings or sites of very low crystal symmetry (random sites), so that the sum of all regular and identified site fractions becomes smaller than 100%; (2) When some of the ^{59}Fe moves towards the surface

FIG. 3. (color online) Annealing temperature dependence of the fractions of ^{59}Fe in n^+ -Si (a) and p^+ -Si (c), in comparison to the average results of low doped Si (i -Si) from Ref. 26 (b).

compared with the assumed implantation depth profile, the intensity of the channeling effects is increased as well as the corresponding fitted fractions. This explains why the sum may reach values above 100% at intermediate annealing temperatures²⁵; if diffusing, ^{59}Fe accumulates at the surface (out-diffusion) or escapes to the bulk of the wafer (in-diffusion), channeling effects are lost, the random fraction increases, and the sum drops to values below 100%²⁵. This is what supposedly happens at the highest annealing temperatures.

IV. DISCUSSION

As we have seen, the lattice site preference of Fe changes with the doping type of the Si material. The observed lattice sites of ^{59}Fe can be either related to its isolated form or complexes with other defects. Because isolated interstitial iron is a very fast diffuser, even at room temperature, it is quite unlikely that the majority of ^{59}Fe prevails in the implanted region in the form of isolated

interstitial Fe. In contrast, the formation of complexes with other defects seems to be a more plausible explanation for the observed lattice sites. These complexes can be a result of aggregation of ^{59}Fe with damage defects or pairing with other impurities. A considerable fraction of ^{59}Fe in complexes with other defects can only be present if the defect concentration has at least the same order of magnitude as the implanted ^{59}Fe concentration. Therefore, observation of complexes of ^{59}Fe and C can be excluded since typical concentrations of C in Si are of the order of 10^{16} cm^{-3} that when compared to the iron peak concentration is two orders of magnitude smaller. What is not obvious to rule out is for instance the pairing of ^{59}Fe with O or H whose typical concentrations may be comparable to the implanted iron peak concentration (10^{18} cm^{-3}). However, no significant difference was observed between low doped Czochralski and Float Zone Si in the previous EC study^{25,26} and, therefore, O and ^{59}Fe seem not to have paired in considerable quantities on the reported experiments. Regarding the formation of complexes between Fe and H, deep level transient spectroscopy (DLTS) has observed the existence of new levels when H is intentionally introduced in n -type Si doped with Fe³⁹. However, the levels disappeared again after annealing at 175°C. Although the lattice location of ^{59}Fe in hydrogenated Si samples has not yet been investigated by means of EC, the fact that pronounced changes in the lattice locations of Fe are absent up to an annealing temperature of 200°C, suggests that such Fe-H complexes are probably not a characteristic feature in our experiments. In order to investigate this issue, we are planning to study the lattice location of ^{59}Fe also in hydrogenated Si samples. Another possibility that cannot be ruled out is the presence of clusters of ^{59}Fe such as dimers. In fact, Fe precipitates easily in Si. Yet, previous EC experiments which used implanted Fe fluences that varied up to a factor of 50 and hence covered a wide range of ^{59}Fe concentrations, have not given any hints that would allow to confirm the presence of such clusters²⁵. Regarding possible Fe traps, from the viewpoint of concentration the most likely interaction of Fe is hence not with C, O or H, neither by forming clusters of ^{59}Fe such as dimers, but with self interstitials, vacancies or dopants (As or B). For ionized dopants, the Coulomb interaction can act as a decisive force which drives the formation of pairs. For instance, while there are no indications that interstitial Fe, either neutral Fe^0 or positively charged Fe^+ , should pair with positively charged donors such as As^{+40} , the formation of pairs between positively charged interstitial Fe_i^+ and negatively charged acceptors, e.g. B^- , is a well-known phenomenon^{1-3,22,23,40}. In the next subsections we discuss each type of observed lattice site that we unambiguously identified, comparing with ab initio calculations^{21,40,41} and Mössbauer spectroscopy⁴²⁻⁴⁵ studies from literature.

A. ideal S sites

Substitutional iron has already been observed in Si by means of Mössbauer spectroscopy and emission channeling techniques. A natural explanation for the formation of substitutional Fe is the presence of high concentrations of vacancies created during implantation^{25,45,46}. In fact, as previously noted, the implanted ^{59}Fe produced a large amount of vacancies and thus the condition for the trapping of ^{59}Fe by single vacancies was probably satisfied. In particular, a fraction of Fe on ideal S sites is present in n^+ -Si and i -Si following all annealing steps up to 900°C (Fig. 3), showing its considerable thermal stability and thus its high dissociation energy from the ideal S site, which was estimated in the previous study to be $E_D(\text{Fe}_S) = \sim 2.6 - 3.5 \text{ eV}$ ²⁶. In comparison, the calculated binding energy of substitutional Fe to a vacancy, from Refs. 40 and 41, is 2.93 - 3.20 eV, which, after adding the migration energy of interstitial Fe of $\sim 0.7 \text{ eV}$, would result in an activation energy for dissociation around 3.6 - 3.9 eV. In p^+ -Si the stability of the ideal S sites seems to be much lower. It has been suggested that substitutional iron acts as a deep acceptor in Si, being negatively charged in n -Si, but neutral in p -Si²¹. This fact, together with the fact that positively charged interstitial Fe_i^+ should not easily combine with positively charged Si vacancies in p -Si (as was outlined in the introduction), may explain the larger fractions of ideal substitutional Fe observed in i - and n^+ -Si since the solubility of substitutional Fe should be higher in n -Si (where it acts as counter-dopant to the donors). We also note that only a small fraction of substitutional ^{59}Fe is present at low annealing temperatures in both types of highly doped Si. This can be explained by the fact that the quantity of vacancies is so large that most of the single vacancies aggregate into complexes of multivacancies.

B. near-BC sites

Iron on near-BC sites has also been observed previously using EC, as a near-S fraction^{25,26}, being assigned to complexes of ^{59}Fe with multivacancies. From Fig. 3 one can see that ^{59}Fe is stable on near-BC positions up to 500°C in n^+ -Si, while in p^+ -Si it starts to dissociate from these sites already at 300°C. We also note that ^{59}Fe is stable in these sites up to 400°C when using low and

moderately doped n - and p -type Si²⁶. We can estimate values for the dissociation energy E_D of ^{59}Fe from near-BC sites, using^{26,47}:

$$E_D = k_B T \log \left[\frac{\nu_0 \Delta t}{N} \frac{1}{\log \left(\frac{f_{n-1}}{f_n} \right)} \right], \quad (1)$$

where ν_0 is the attempt frequency, Δt the annealing time, T the annealing temperature, f_n the fraction after annealing at T , f_{n-1} the fraction following the previous annealing step, i.e. before the anneal at T , and N the required number of steps for ^{59}Fe to go to another type of trap or to diffuse through the bulk or to the surface so that channeling is not observed. We consider two limits for N : an upper limit for the dissociation energy is obtained for $N = 1$, i.e. when one successful attempt is enough to move ^{59}Fe to a more stable type of trap or to initiate diffusion through the bulk or to the surface; the other case occurs when ^{59}Fe is freed from near-BC sites but is retrapped again by the same type of trap multiple times, until it diffuses through the bulk or to the surface²⁶. For this last case, and supposing that ^{59}Fe on near-BC sites is due to vacancies, we take $N = 3\pi R^2 \phi$, where R is the capture radius of the multivacancy trap, while ϕ is the fluence of the implanted ^{59}Fe times the number of created vacancies by each ^{59}Fe . By using $R = 1 \text{ nm}$ and $\phi \sim 6 \times 10^{15} \text{ cm}^{-2}$ one obtains the estimate of $N \sim 550$. Table I shows the E_D values for ^{59}Fe on near-BC sites by using $T = 600^\circ\text{C}$ in n^+ -Si and $T = 300^\circ\text{C}$ in p^+ -Si. It also shows estimated values in low-doped Si from Ref. 26. From this table and from Fig. 3, supposing that the complex that this fraction is associated with is the same in all samples, since the displacements are in accordance with each other ($\sim 0.6 - 0.8 \text{ \AA}$), we can conclude that the stability of ^{59}Fe on near-BC sites increases from p^+ - to n^+ -Si. Also, one can deduce that if these sites would be related to impurity defects, these impurities would have to be present in both p^+ - and n^+ -Si, which obviously excludes the main dopants. Summarizing, our data show that the stability of the near-BC fraction clearly increases from p^+ - to n^+ -doped material, but rather than concluding that this effect is due to the direct interaction of Fe with the dopants in higher concentrations, it seems to be a consequence of an upward shift in the Fermi-level and, consequently, on the charge states of Fe and the multi-vacancy traps involved. We should now discuss the origin of the near-BC sites. From theoretical calculations it was proposed that a divacancy in Si should trap an Fe atom in a position that is centered between the two vacant Si sites, which corresponds to a BC site⁴¹. Based on emission channeling data and ab initio calculations, similar configurations were previously also proposed by us for a number of transition metals (Fe, Cu and Ag⁴⁸, Sn⁴⁹, Mn⁵⁰) inside a divacancy in Ge. The theoretically predicted energy to completely dissociate the Fe atom from the divacancy in Si is $\sim 3.5 \text{ eV}$ ⁴¹, which is $\sim 0.8 - 1.8 \text{ eV}$ larger than our estimated values for ^{59}Fe dissociation from near-BC sites. What is

TABLE I. Estimated activation energies E_D for dissociation of ^{59}Fe from near-BC sites (displaced $\sim 0.6\text{-}0.8 \text{ \AA}$ from ideal S towards BC sites), and from near-T sites (displaced $\sim 0.2 \text{ \AA}$ from ideal T).

Fe-site	p^+ -Si	i -Si	n^+ -Si
near-BC	1.37-1.68 eV	1.91-2.37 eV	2.15-2.63 eV
near-T	-	2.57-3.20 eV	2.28-2.80 eV

particularly difficult to reconcile with theoretical predictions is the displacement of Fe from the ideal BC site towards S sites, which is indicated by our results. In that respect, however, it is worth while to point out the following. Based on ab-initio calculations, so-called four-fold configurations have been proposed to be particularly stable for 3-6 vacancy clusters in Si^{32,33}. The fourfold configuration is based on a hexavacancy ring where extra Si atoms have been inserted in interstitial sites near BC positions, where they satisfy the dangling bonds of four Si atoms. Similar geometries were already proposed if a hexavacancy is filled up by Cu atoms instead of Si host atoms^{34,35} and it appears possible that this may be the case also for other transition metals such as Fe. It seems hence feasible that the near-BC fraction, which we observe in our experiments, represents a mixture of Fe not only inside double vacancies (where it should occupy ideal BC sites) but also inside more complicated multi-vacancies (where it should sit off the BC site). Such a mixture of sites in close vicinity would be quite impossible to resolve with the emission channeling technique and could result in the near-S or near-BC fractions that we have identified in the case of Fe^{25,26} and this work²⁷⁻²⁹, Cu²⁷⁻²⁹ and Ag³⁰.

C. near-T sites

First we note that Fe on interstitial near-T sites is never dominant in n^+ -Si. We attribute this to the high thermal stability of the near-BC fraction in n^+ -Si, which keeps Fe gettered and prevents interstitial Fe from becoming prominent. In the case of i-Si^{25,26}, we proposed the near-T fraction not to be free interstitial Fe, but probably also bound to vacancy-related defects. This point of view was considerably strengthened in the meantime by the theoretical study⁴¹ published by Estreicher et al. in 2008. They predicted that interstitial Fe_i assumes metastable positions next to a vacancy or double vacancy, and that around 3 eV are needed for Fe to completely escape from this trap, while the positions of Fe in these Fe_i-V and Fe_i-V₂ complexes were predicted also somewhat shifted (~ 0.2 - 0.3 Å) from the ideal T towards the AB sites. Both the displacements and expected activation energies for dissociation are similar to our data (*cf.* Tab. I).

The observed near-T sites in p^+ -Si deserve a more careful analysis due to the possible formation of FeB pairs, which is driven by the Coulomb interaction between positively charged interstitial Fe_i⁺ and negatively charged substitutional B⁻ acceptors. The diffusion of Fe and the kinetics of the formation and dissociation of FeB pairs are quite well studied, *cf.* Refs. 1–4, 22–24. Note that we have also discussed the mathematical formulae used in the following in more detail in Ref. 51, where they were applied to a similar case, the pairing of interstitial Li⁺ with substitutional B⁻. The time constant τ until a freely diffusing interstitial Fe⁺ is captured at a B⁻ ac-

ceptor can be calculated by the well-known formula^{2,22,23}

$$\tau = [4\pi RC_B D]^{-1}, \quad (2)$$

where R is the Coulomb capture radius, C_B the ionized B concentration, and D the diffusion coefficient of interstitial Fe_i⁺ at temperature T . Using $R = 47$ Å, $D = 1 \times 10^{-3} \exp(-0.67 \text{ eV}/k_B T) \text{ cm}^2/\text{s}$ as in Refs. 2 and 22 and $C_B = 6.5 \times 10^{19} \text{ cm}^{-3}$ (the acceptor concentration in our p^+ sample) we obtain for instance $\tau = 0.38 \text{ s}$ at 20°C, $2 \times 10^{-5} \text{ s}$ at 200°C, $2 \times 10^{-8} \text{ s}$ at 600°C, and $4 \times 10^{-9} \text{ s}$ at 800°C. On the other hand, the breakup rate Λ of FeB pairs can be estimated using the formula^{2,51}

$$\Lambda = \nu_0 \exp(-E_A/k_B T), \quad (3)$$

where ν_0 is the attempt frequency, and the activation energy E_A for dissociation of the pairs is the sum of the binding energy E_B plus the migration energy E_M of interstitial Fe⁺ in Si, $E_A = E_B + E_M$. Using an attempt frequency of the order of the lattice vibrations^{2,51}, $\nu_0 \sim 1 \times 10^{12} \text{ s}^{-1}$, and using $E_B = 0.65 \text{ eV}$ and $E_M = 0.67 \text{ eV}$ (from Refs. 2, 22 and 23), one estimates that the average lifetime $1/\Lambda$ of a FeB pair is $5 \times 10^{10} \text{ s}$ at 20°C, 120 s at 200°C, $4 \times 10^{-5} \text{ s}$ at 600°C, and $2 \times 10^{-6} \text{ s}$ at 800°C. Hence, for the high B concentration of $6.5 \times 10^{19} \text{ cm}^{-3}$ the capture of diffusing Fe_i⁺ into FeB pairs should always be faster than the average rate of breakup of the pairs for practical annealing temperatures. Considering that a typical ⁵⁹Fe channeling pattern takes a day or so to be measured, it is clear that, in the absence of any other traps, at room temperature we would always measure Fe in FeB pairs, since, even if no pairs were existing during annealing, they would form again at 20°C within a few seconds. The rms width of diffusion d during time t at temperature T is generally given by the well-known Einstein relation $d = [6D(T)t]^{1/2}$. As outlined in Ref. 2, the diffusion coefficient D of Fe is reduced in the presence of FeB pairs, so that

$$d = [6f_i D(T)t]^{1/2}, \quad (4)$$

should be used, where f_i is the fraction of free interstitial Fe (in contrast to the paired fraction). If f_i is calculated using, e.g., the formulae in Refs. 2, 22 and 23, one estimates for $t = 10 \text{ min}$ at 20°C $d = 0.04 \text{ Å}$, but already 600 Å at 200°C, and 580000 Å at 600°C. It is hence clear that the fact that FeB pairs are easily formed does not mean that long-range diffusion of Fe is completely suppressed, it is only slowed down somewhat since at elevated temperatures pairs are dynamically formed and break up again. Fe has thus ample possibility to react with other defects in the sample, e.g. vacancy-type defects resulting from the implantation. What will thus determine in which complexes Fe is actually found in p^+ -Si, is the stability of the FeB pairs vs the stability of Fe in other defect complexes, the relative concentrations of the trapping centers and, last but not least, their charge states. In that respect, Fe⁺ and B⁻ are oppositely

FIG. 4. (color online) Displacements of the near-BC and near-T sites, occupied by ^{59}Fe , from S towards BC sites and from T towards AB sites, respectively, in p^+ -Si.

charged, so that Coulomb interaction certainly would allow the formation of FeB pairs already at room temperature. On the other hand, since the stability of Fe within vacancy defects is, in general, much higher than the stability of FeB pairs, already moderate annealing should break up FeB pairs and favor the trapping of Fe within vacancy-type complexes. Finally, if the concentration of vacancies is reduced during high temperature annealing, FeB pairs might be dominating again after cool down to room temperature.

The displacements of interstitial Fe from the ideal T sites as a function of annealing temperature (Fig. 4) show both abrupt and gradual changes. In the as-implanted state, Fe is found displaced from ideal T sites ~ 0.43 Å towards the AB position. However, annealing at 100°C already changes the position to the ideal T site, while increasing the annealing temperature further the displacement gradually reaches around 0.5 Å again, comparable to the value in the as-implanted state. Hence, if FeB pairs are present in considerable quantities in our sample, it is quite likely that the Fe atom may be displaced from T sites within the pairs. If one assumes simple electrostatic binding in the pair, the distance a between Fe^+ and B^- would be fully determined by the pair binding energy E_B according to 2 and 22 and 51

$$a = q^2 / (4\pi\epsilon\epsilon_0 E_B), \quad (5)$$

where $q = 1$ are the charges within the pair and $\epsilon = 11.9$ the dielectric constant of Si. Using $E_B = 0.65$ eV^{2,22} one arrives at $a = 1.86$ Å, which means that under these assumptions Fe^+ would be displaced 0.49 Å from the ideal T site towards the AB site within the pair. However, the microscopic structure of trigonal FeB pairs predicted by ab-initio calculations⁴⁰ points towards Fe and B occupying ideal tetrahedral interstitial and substitutional sites, respectively, but with the four Si nearest neighbors around the B uniformly displaced inward by 0.27 Å. How such a breathing mode relaxation of the Si atoms around the B would influence the emission channeling effects from the neighboring ^{59}Fe is currently not feasible to predict quantitatively, however, it seems possible

it might have a similar effect as a small displacement of the ^{59}Fe itself. Summarizing, there are good reasons that suggest that ^{59}Fe within FeB pairs might result in emission channeling patterns that exhibit a displacement from ideal T site patterns.

Finally we would like to compare the present interpretation of the emission channeling results on ^{59}Fe in p^+ -Si with those of on-line Mössbauer spectroscopy^{43,45} from $^{57}\text{Mn} \rightarrow ^{57}\text{Fe}$. In these experiments, the radioactive probe ^{57}Mn ($t_{1/2} = 1.45$ min) is implanted, which decays into the well-known 14.4 keV excited Mössbauer state $^{57\text{m}}\text{Fe}$ ($t_{1/2} = 98$ ns). Note that characteristic thermally activated interactions of Fe have to happen within the short time interval of the 140 ns lifetime of the $^{57\text{m}}\text{Fe}$ probe, which requires considerably higher temperatures than in conventional annealing experiments. In any case, due to the very short time window of the Mössbauer state, this type of experiments may not be sensitive to interactions that take place between Fe and defects present in relatively low concentrations in the samples. In p^+ -Si below 600°C the dominating fraction in the Mössbauer spectrum resulted from Fe in a quadrupole-split defect, which was interpreted as complexes of interstitial Fe with vacancies, $\text{Fe}_i\text{-V}$, and would correspond to Fe on near-T sites in our ^{59}Fe experiments. Around 600°C and above, this $\text{Fe}_i\text{-V}$ related fraction started to disappear, for which an activation energy of ~ 1.1 eV was estimated. The reduction in the $\text{Fe}_i\text{-V}$ related signal was accompanied by the appearance of a new quadrupole-split line in the Mössbauer spectrum, which was interpreted as resulting from the formation of ^{57}FeB pairs during the 140 ns lifetime of $^{57\text{m}}\text{Fe}$. Besides an isomer shift and quadrupole split that are characteristic for interstitial Fe, a major argument for the identification as ^{57}FeB pairs was the fact that the diffusion length of Fe is estimated to reach ~ 16 Å during the lifetime of the Mössbauer state^{43,45}, a value which is comparable to the average distance between B dopants. We can use eq. 3 in order to estimate, approximately, at which temperature such a transition of Fe from $\text{Fe}_i\text{-V}$ complexes to FeB pairs should be observable in emission channeling experiments. Assuming that only one successful attempt against an activation energy of 1.1 eV is needed on an annealing time scale of 10 min, one arrives at a temperature of 102°C . This would mean that our as-implanted measurements would be characterized mainly by Fe in $\text{Fe}_i\text{-V}$ complexes, which are broken at annealing temperatures higher than 100°C , leading to the increased formation of FeB complexes. As was discussed above and in Ref. 25, $\text{Fe}_i\text{-V}$ complexes are most likely responsible for at least a part of the near-T fraction in ^{59}Fe emission channeling experiments, so they should be difficult to distinguish from FeB pairs, in which Fe occupies a similar lattice site. However, as is illustrated in Fig. 4, an abrupt change of displacement from ideal T sites is observed for an annealing temperature of 100°C , and in light of the Mössbauer results it is tempting to interpret this as a transition from $\text{Fe}_i\text{-V}$ complexes to FeB pairs. Such an argument, though, may

be misleading. Since the p^+ sample was kept at room temperature for four days before the annealing step at 100°C took place, such transition may have happened, at least partially, already before the first annealing step.

In conclusion, by taking into account all three types of arguments presented, kinetic estimates regarding the formation and stability of FeB pairs, their likely geometrical structure, and the comparison to Mössbauer results in similar samples, one states that it is difficult to arrive at a coherent picture of the nature of the near-T sites observed in the p^+ -Si EC and Mössbauer experiments. While there are quite strong arguments that both FeB pairs and other interstitial Fe-related complexes, e.g. Fe_i-V, contribute to the measured patterns in varying fractions at all annealing temperatures, we tend to favor the view that FeB pairs may be particularly important in the as-implanted state and following the highest annealing temperatures, i.e. when the near-T sites are characterized by the relatively large displacements up to ~ 0.5 Å. This interpretation, however, would require a very efficient mechanism that favors pairing of Fe and B over the formation of Fe_i-V complexes already in the as-implanted state. It seems possible that Coulomb attraction might be such a powerful driving force, for instance if directly following the implantation in p^+ -Si Fe⁺ would preferentially interact with B⁻ and, to some extent, with neutral vacancies, but it would be repelled from positively charged vacancies.

V. CONCLUSION

We have given for the first time clear and direct evidence that the predominant lattice location of Fe in Si changes with the doping of the material. While in analogy to previous experiments, in low-doped Si, the same three types of lattice sites (ideal substitutional S, near-BC, and near-T) were identified with varying fractions depending on the annealing temperature, the near-T sites were clearly dominant in p^+ -Si, and near-BC or ideal S sites in n^+ -Si. We show evidence that the near-BC sites are due to the same type of complex after all annealing steps as a result of the similar displacement from BC towards S sites, independently of the type of silicon used. However, their thermal stability increases when the doping is changed from p^+ to i and further to n^+ . The dominant lattice sites of Fe in n^+ -Si seem to be well characterized for all annealing temperatures (except maybe $T_A=600^\circ\text{C}$) by the incorporation of Fe into vacancy-related complexes, either into single vacancies which leads to Fe on ideal substitutional sites, or multiple vacancies, which leads to its incorporation near BC sites. We point out that this strong interaction between Fe and vacancy-type defects in n^+ -Si and the high thermal stability of the formed complexes can provide an explanation for the P-diffusion gettering effect, where Fe is gettering in a less electrically active form in the n^+ -doped surface region created during the in-diffusion of

phosphorus.

In contrast, in p^+ -Si the major fraction of Fe is clearly interstitial (near-T or ideal T) for all annealing temperatures. The microscopic nature of the interstitial sites in p^+ -Si as function of annealing temperature is not clear at the moment, although the formation of FeB pairs is obviously expected to play a major role. Arguments have been presented that point towards the possibility that the lattice site of Fe within FeB pairs is considerably displaced (up to 0.5 Å) from the ideal T site towards the AB site. While this would be quite well in accordance with the lattice site estimated from the measured pair binding energy found in the literature, it is not obvious to reconcile it with the structure of the FeB pair predicted by ab-initio calculations, which consists of Fe on an ideal T site with only a breathing mode relaxation (0.27 Å inward) of the four Si atoms surrounding the B atom. In any case, a considerable displacement of Fe in FeB pairs would mean that its site is difficult to distinguish from the displaced T sites found in low-doped or n^+ -Si, which were attributed to interstitial Fe next to vacancy-type defects.

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