Lattice sites of implanted Fe in Si

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The angular distribution of $\beta^-$ particles emitted by the radioactive isotope $^{59}$Fe was monitored following implantation into Si single crystals at fluences from $1.4 \times 10^{12}$ cm$^{-2}$ to $1 \times 10^{14}$ cm$^{-2}$. We identified Fe on three distinct sites: ideal substitutional, displaced substitutional and displaced tetrahedral interstitial. Whereas displaced substitutional Fe was dominating for annealing temperatures below 500 °C, annealing between 500–700 °C caused the majority of Fe to occupy displaced tetrahedral interstitial sites. Ideal substitutional positions were increasingly populated following annealing at 800 °C and above. A comparison of the emission channeling results to Mössbauer and electron paramagnetic resonance experiments is given.

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I. INTRODUCTION

Due to the richness of the electrical and optical phenomena associated with Fe in silicon, it represents one of the most fascinating impurities and has been studied for decades, as is reviewed in Refs. 1–3. The importance of understanding the properties of Fe in Si is further underlined by its role in Si processing, where it acts, together with other transition metals such as Cu, Ni or Co, as one of the most dangerous contaminants. As a consequence, detailed and costly gettering schemes have to be applied in order to remove the trans-

imitters from substitutional Fe; 17,20–27

From these studies is that Fe in Si

is attributed to Fe on interstitial sites paired with a va-

which results from Fe in a damaged environment17,20–25 and is sometimes also termed the “amorphous” site; 26

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and references therein), but, with the exception of Fe-

acceptor pairs,15 never in a configuration of symmetry lower

than $T_d$.

with $\delta=+0.20–0.33$ mm/s and

$E_Q=0.83–1.0$ mm/s (at 300 K) which results from Fe in a damaged environment17,20–25

and references therein) with $\delta=+(0.08–0.03)$ mm/s (extrapolated to 0 K) which originates from substi-

by 300 K which is without doubt due to tetrahedral Fe;17,20–27

c a second doublet with $\delta=+(0.08–0.03)$ mm/s (extrapolated to 0 K) which is

which has been termed the “unknown”23 or “new” line22,24 and is attributed to Fe on interstitial sites paired with a vacancy.

However, with respect to direct lattice location methods, not much is actually known on Fe in Si. This is due to the fact that most structural techniques lack sensitivity at lower Fe concentrations and at higher concentrations Fe forms silicides. Bunker28 studied Si implanted with $10^{16}$ cm$^{-2}$ of Fe at 100 keV and annealed between 600 °C and 800 °C, using the method of extended x-ray absorption fine structure (EXAFS). It was concluded that the EXAFS results are consistent with Fe being located at a distorted interstitial site. Vartanyantz et al.29 investigated Si implanted with $5 \times 10^{15}$ cm$^{-2}$ of Fe at 80 keV and annealed at 750 °C using Rutherford backscattering spectroscopy and channeling (RBS/C). They found that the RBS signal from Fe was reduced by 30% for (111) channeling incidence, from which they concluded that 30% of Fe would be located on substi-

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they concluded that 30% of Fe would be located on substi-

proposed, resulting in Fe near a substitutional site from which it is shifted along a (111) direction.

The most convincing evidence for substitutional Fe in Si so far comes from Mössbauer experiments. The general picture which has emerged from these studies is that Fe in Si produces four characteristic Mössbauer signals: (a) a quadrupole-split doublet with $\delta=+0.20–0.33$ mm/s and

$E_Q=0.83–1.0$ mm/s (at 300 K) which results from Fe in a damaged environment17,20–25

tutional sites. However, this conclusion is ambiguous since reductions in the backscattering yield for (111) channeling may result not only from substitutional but also from a large variety of interstitial sites in Si.

We present here direct lattice location experiments of implanted Fe in Si. We were able to clearly identify Fe on at least 3 distinct sites: ideal substitutional sites (S), displaced substitutional sites (near-S), and displaced tetrahedral interstitial sites (near-T). We used the $\beta^-$ emission channeling technique,\(^{30}\) which makes use of the fact that charged particles emitted from radioactive isotopes in single crystals experience channeling or blocking effects along low-index crystal directions. This leads to an anisotropic emission yield from the crystal surface which depends in a characteristic way on the lattice sites occupied by the emitter atoms.

### II. EXPERIMENT

In order to dope with long-lived $^{59}$Fe ($t_{1/2}=44.6$ d) we implanted the precursor isotope $^{58}$Mn ($t_{1/2}=4.6$ s) at the ISOLDE on-line isotope separator facility at CERN. ISOLDE provides clean, mass-separated beams of radioactive Mn isotopes, which are produced by means of 1.4-GeV proton-induced nuclear fission from UC\(_2\) targets and chemically selective laser ion sources.\(^{31}\) During the $\beta^-$ decay of the $^{58}$Mn nucleus the resulting $^{59}$Fe atom receives a recoil around 200 eV, which assures that it is reimplemented and hence that its lattice position is not influenced by the previous site of $^{59}$Mn.

Fourteen Si single crystals were investigated. Table I gives their doping type, resistivity, growth method, surface orientation, and the implanted fluences. All implantations were done at room temperature under an angle of 7° to the surface normal in order to avoid channeled implantation and produce a well-defined depth profile. The depth profiles for these implantation conditions, as estimated by means of the SRIM 2003 (Ref. 32) or MARLOWE (Ref. 33) codes, are approximately Gaussian, centered at 532 Å with a straggling of 192 Å and peak concentrations of $2.0 \times 10^{13}$ atoms/cm\(^2\).

Following the implantation the crystals were mounted on a goniometer using sample holders entirely made of Ta and Mo. Annealing up to 900 °C in steps of 100 K was done in situ under vacuum better than $10^{-7}$ mbar. While the setpoint temperature was reached after 1–2 min, the cool down to room temperature lasted up to 30 min since the samples could not be quenched under vacuum. After each annealing step, the $\beta^-$ emission yield in the energy window 50–461 keV was measured at room temperature using the position-sensitive detector systems described in Refs. 34 and 35 as a function of angle from (100), (111), (110), and (211) directions.

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Type</th>
<th>Resistivity (Ω cm)</th>
<th>Growth method</th>
<th>Surface</th>
<th>Implanted fluence (cm(^{-2}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$P$</td>
<td>10 000</td>
<td>FZ</td>
<td>(111)</td>
<td>$1.4 \times 10^{12}$</td>
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<td>2</td>
<td>$P$</td>
<td>10–20</td>
<td>FZ</td>
<td>(100)</td>
<td>$5.3 \times 10^{12}$</td>
</tr>
<tr>
<td>3</td>
<td>$P$</td>
<td>10 000</td>
<td>FZ</td>
<td>(111)</td>
<td>$5.4 \times 10^{12}$</td>
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<tr>
<td>4</td>
<td>$P$</td>
<td>12–16</td>
<td>epi(^a)</td>
<td>(100)</td>
<td>$1.2 \times 10^{13}$</td>
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<td>10–20</td>
<td>FZ</td>
<td>(100)</td>
<td>$1.6 \times 10^{13}$</td>
</tr>
<tr>
<td>6</td>
<td>$P$</td>
<td>10 000</td>
<td>FZ</td>
<td>(111)</td>
<td>$2.0 \times 10^{13}$</td>
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<tr>
<td>7</td>
<td>$P$</td>
<td>10–20</td>
<td>FZ</td>
<td>(100)</td>
<td>$4.8 \times 10^{13}$</td>
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<tr>
<td>8</td>
<td>$P$</td>
<td>10 000</td>
<td>FZ</td>
<td>(111)</td>
<td>$1.0 \times 10^{14}$</td>
</tr>
<tr>
<td>9</td>
<td>$N$</td>
<td>700–1300</td>
<td>FZ</td>
<td>(111)</td>
<td>$4.0 \times 10^{12}$</td>
</tr>
<tr>
<td>10</td>
<td>$N$</td>
<td>7.3–12</td>
<td>CZ(^b)</td>
<td>(111)</td>
<td>$4.9 \times 10^{12}$</td>
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<tr>
<td>11</td>
<td>$N$</td>
<td>0.03</td>
<td>CZ</td>
<td>(100)</td>
<td>$8.0 \times 10^{12}$</td>
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<td>700–1300</td>
<td>FZ</td>
<td>(111)</td>
<td>$8.5 \times 10^{12}$</td>
</tr>
<tr>
<td>13</td>
<td>$N$</td>
<td>7.3–12</td>
<td>CZ(^b)</td>
<td>(111)</td>
<td>$1.0 \times 10^{13}$</td>
</tr>
<tr>
<td>14</td>
<td>$N$</td>
<td>700–1300</td>
<td>FZ</td>
<td>(111)</td>
<td>$4.0 \times 10^{13}$</td>
</tr>
</tbody>
</table>

\(^{a}\)The thickness of the epitaxial layer of the epi-Si sample #4 was 6–7 μm on a 0.01–0.02 Ω cm $p^+$-substrate.

\(^{b}\)The oxygen concentration of samples #10 and #13 was characterized as 6.5–6.7 × 10\(^{18}\) cm\(^{-3}\) by the manufacturer.
The lattice sites of implanted Fe in Si

changed while the maximum anisotropy along these two axes and also along the [110] directions has more than doubled [Figs. 2(a) and 2(b)]. On the other hand, the [110], [211], and [111] effects are now characterized by minima instead of maxima, as is clearly visible in Figs. 2(c) and 2(d). The situation with channeling maxima along [100], [111], and [110] and minima along [100], [211], and [111] is typical for emitter atoms on or close to tetrahedral interstitial (T) positions since the T sites are located within [100] and [111] atomic rows and [110] planes but interstitial with respect to [110], [211], and [111]. Finally, the patterns following 900 °C annealing [Figs. 3(a)–3(d)] are clear proof that the dominant lattice sites of Fe are substitutional again, showing very pronounced channeling along all crystal directions including [110], [211], and [111].

While the experimental results presented in Figs. 1–3 clearly illustrate changes in the preferred lattice sites of Fe in a qualitative way, quantitative information is obtained from fitting the experimental data by the results of simulations of $\beta^-$ emission yields for a variety of sites. The general theory for the simulation of emission channeling, the so-called "many beam" approach, is described in Ref. 30 and some computational details on its implementation for Si can be found in Ref. 34. To approximate the continuous $\beta^-$ energy spectrum of $^{59}$Fe, simulations were done for electron energies from 50 keV to 450 keV in steps of 25 keV, and the results averaged according to the theoretical spectral $\beta^-$ distribution. As one-dimensionally projected root mean square (rms) displacement of Si atoms we used $u_r(Si)=0.0803 \, \text{Å}$, corresponding to a Debye-temperature of 504 K. We calculated characteristic two-dimensional patterns of electron emission probability within a range of $\pm 3^\circ$ around the [100], [110], [111], and [211] directions in steps of $\Delta x=\Delta y=0.05^\circ$ for S, T, hexagonal interstitial (H), bond center (BC), antibonding (AB), split [100] (SP) and the so-called Y and C sites, as well as [111] and [100] displacements between all of these positions. The location of these sites in the diamond lattice can be found in Refs. 38 and 39. The fit procedures used in order to compare theoretical yields and experimental patterns take into account the angle resolution of the detection setup and have been described in detail previously.\textsuperscript{34,35} Note that as a general rule in fitting any emission channeling

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FIG. 1. (a)–(d) Normalized $\beta^-$ emission yield from sample #8 in the vicinity of [111], [110], and [211] directions following annealing at 300 °C. (e)–(h) Best fit results, corresponding to (e) 5% ($S+T$), 54% near-($S+T$), and 41% $R$, (f) 12% ($S+T$), 61% near-($S+T$), and 27% $R$, (g) 3% $S$, 41% near-$S$, 22% near-$T$, and 34% $R$, (h) 0% $S$, 39% near-$S$, 21% near-$T$, and 40% $R$.

FIG. 2. (a)–(d) Experimental emission channeling patterns from sample #8 following annealing at 600 °C. (e)–(h) Best fit results, corresponding to (e) 30% ($S+T$), 113% near-($S+T$), and $-34\%$ $R$, (f) 30% ($S+T$), 104% near-($S+T$), and $-34\%$ $R$, (g) 11% $S$, 14% near-$S$, 75% near-$T$, and 0% $R$, (h) 3% $S$, 34% near-$S$, 99% near-$T$, and $-36\%$ $R$. 

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patterns always an isotropic component has to be included, which is given by 1 minus the sum of all other fitted fractions.\(^{30,34,38}\) Provided that the scattering background and the depth profile of emitter atoms is accurately known and there is no enhanced dechanneling due to defects in the crystal, the isotropic component reflects the fraction of emitter atoms on so-called random (R) sites, which are sites in heavily damaged surroundings or sites of very low crystal symmetry. Consequently, inaccurate knowledge of the scattering background or emitter depth profile will lead to inaccuracies in assessing the fraction of emitter atoms on R sites.

It turned out that our experimental results can only be satisfactorily described by, apart from Fe on random sites, considering Fe on at least three distinct lattice sites: ideal substitutional sites, displaced substitutional sites, and displaced tetrahedral interstitial sites. While the samples always contain a mixture of Fe on these three lattice sites and random sites, Fe on near-S sites dominates the patterns in the as-implanted state and following annealing up to 300 °C (Fig. 1). On the other hand, Fe on near-tetrahedral interstitial sites is best visible following annealing at 600 °C (Fig. 2), and Fe on ideal S sites following annealing at 800–900 °C (Fig. 3). By ideal substitutional sites we mean Fe on substitutional sites showing isotropic Gaussian displacements with \( \mu = 0.079 \) Å due to thermal vibrations only. The value of 0.079 Å is a best guess assuming that Fe acts as a simple mass defect in the Si lattice. The displaced substitutional sites are sites exhibiting static displacements around 0.4–0.7 Å from the ideal S position, and the displaced tetrahedral interstitial sites are located 0.3–0.8 Å from the ideal T position. Both in case of the near-S and near-T sites all possible displacements from the ideal S and T sites along (111) and (100) directions were tried in the fits. However, similar chi square values were obtained and the direction of the static displacement could therefore not be pinpointed. The values of 0.4–0.7 Å and 0.3–0.8 Å for the displacements thus represent the statistical uncertainty, taking into account displacements along different crystal directions that lead to a similar quality of fit. The best fit results to the experimental patterns obtained are shown in Figs. 1–3 panels (e)–(h). Note that we cannot exclude that additional lattice sites play a certain minor role, especially ideal T sites could be occupied to some smaller extent as well.

Figures 4 and 5 show the best fit fractions for the three considered sites as a function of annealing temperature for the \( p \)-type and \( n \)-type samples, respectively. We first note that all samples showed the general feature of site changes from near-S to near-T and then to S with increasing annealing temperature. Second, within the range of doping types studied (all samples were relatively moderately doped), there are no significant differences visible between \( n \)- and \( p \)-type Si. Also no clear trend distinguishes the results obtained with oxygen-lean float-zone (FZ) or oxygen-rich Czochralski (CZ) material, and even the implanted fluence, which ranged from \( 1.4 \times 10^{12} \, \text{cm}^{-2} \) to \( 1.0 \times 10^{14} \, \text{cm}^{-2} \), seems to have no pronounced effect on the lattice location of Fe. Third, we note that for annealing temperatures at 600 °C and above the...
sum of the three fitted fractions generally becomes larger than 100% and the random fraction (not shown) reaches negative values. An explanation for this apparently unphysical result will be given below.

IV. DISCUSSION

In interpreting the results of our lattice location experiments one has to consider the damage created during the ion implantation process. It is estimated from SRIM (Ref. 32) or MARLOWE simulations that around 800–1300 vacancies and interstitials are created for every implanted Fe atom. The simulations indicate that the initial vacancy distribution is approximately a Gaussian of 330 Å, i.e., centered at somewhat more than half of the projected range of the implants. However, it is clear that annealing considerably changes the concentration and nature of the vacancy-like defects, with simple vacancies annihilating with interstitials or clustering into multiple vacancies. Fe obviously reacts with some of the vacancy-like defects, which leads to its incorporation on or near substitutional sites, similar to the case of Cu in Si, which we investigated previously. However, while there exist some parallels between our current results on Fe in Si and our previous findings on the lattice location of implanted Cu in Si, there are also significant differences. Both of the implanted transition metals were found mostly on near-substitutional sites in the room-temperature as-implanted state. In the case of Cu, annealing above 200 °C resulted in Cu progressively disappearing from near-substitutional sites and being incorporated on random sites. Assuming a simple one-step model for this process, we estimated an activation energy around 2.2 eV for the dissociation of near-substitutional Cu, and if retrapping at vacancies from the implantation process was included in the model, the estimate was somewhat lower, around 1.8 eV. Fe also starts to disappear from near-substitutional sites at similar annealing temperatures, and its stability at near-substitutional sites can therefore be estimated to be also around 2.0 eV. However, instead of escaping to random sites it is increasingly found on displaced-tetrahedral interstitial sites following annealing at temperatures between 400 °C and 700 °C. Cu is an ultrafast diffuser in Si, which means it easily reacts with other defects even at room temperature and its interstitial state is hence extremely difficult to observe. On the other hand, it is well known that Fe can be quenched in the interstitial state following high-temperature annealing. Although all our samples were cooled slowly it might therefore be that the pronounced interstitial fraction of Fe simply represents quenched interstitial Fe which remains after the near-substitutional Fe complexes have broken up, interstitial Fe has been diffusing a short distance in the sample and the sample is cooled to room temperature again. What is not in favor of this interpretation, however, is the fact that the interstitial Fe is clearly displaced around 0.3–0.8 Å from the ideal T position. As will be discussed below in conjunction with Mössbauer results from the literature, it seems possible that the near-T Fe is due to Fe-V complexes, i.e. interstitial Fe bound to a neighboring vacancy.

With respect to transition metals on ideal substitutional sites, we have previously observed the incorporation of Cu on ideal S sites, however, only in highly n-type Si and following annealing between 500 °C and 700 °C. Fe on ideal S sites is clearly observed in moderately doped n- and p-Type Si and its stability is significant since it is still present in considerable amounts in many samples even following annealing at 900 °C.

We should note here that the damage created during implantation exceeds the n- or p-doping level of all our samples by orders of magnitude. For instance, the electrically active P concentration in the sample with lowest resistivity (sample #11) corresponds to roughly $1.7 \times 10^{17}$ cm$^{-3}$. Even in the sample implanted with lowest fluence (sample 1 with $1.4 \times 10^{13}$ cm$^{-2}$) the concentration of Fe reaches $1.4 \times 10^{13}$ cm$^{-3}$ in the peak of the implantation profile, and the initial defect concentration is even around three orders of magnitude higher. It is hence likely that the Fermi level is in midgap position in the implanted region, which would explain why we did not observe major differences between moderately doped n- and p-type Si. Samples with much higher doping levels (n$^+$ or p$^+$ material) have to be used in order to investigate a possible influence of the Fermi level on the lattice location of Fe. Such measurements are currently under way, and preliminary results show that the interstitial fraction of Fe is dominant in p$^+$-Si while it is considerably reduced in n$^+$-Si.

We will now discuss the fact that the fitted fractions of Fe reaches values above 100%. Since dechanneling due to the thermal motion of the Si atoms causes an approximately exponential damping of the wave function of channelled electrons, the intensity of the channeling effects depends on the depth profile of the emitter atoms. In our analysis we have assumed Gaussian $^{59}$Fe depth profiles of 532(192) Å resulting from 60 keV implantation. However, it has been reported that Fe implanted to a fluence of $1 \times 10^{15}$ cm$^{-2}$ in Si is pushed towards the surface during solid phase epitaxial
regrowth. Following implantation of Si samples with various heavy ions it was also observed that Fe and other transition metals such as Cu preferentially decorate two regions in the implanted sample: the end of range of the implanted ions, the so-called Rp-region, and midway between the projected range and the surface, the so-called Rp/2-region. It has been suggested that vacancy-type defects at half of the projected range act as effective gettering sites for Fe in the Rp/2 region. We have therefore also undertaken simulations for shallower depth profiles of Fe, centered at half of the 60 keV implantation depth. Under these assumptions the sum of the regular Fe fractions would be around 80%. Redistribution of the Fe towards the crystal surface and the resulting badly defined emitter depth profiles could thus well explain the apparent fractions larger than 100% and also the considerable differences in fractions between various samples.

It is well known that Fe in Si tends to form thermodynamically stable silicide precipitates. Hence one might expect that the lattice sites following high-temperature annealing represent Fe within small silicide precipitates and the formation of the precipitates to depend on the Fe concentration of the samples. It is therefore very surprising that no correlation of the various Fe lattice sites with the implanted fluence was observed. This puzzling behavior will need to be investigated in further experiments using higher implanted doses of Fe.

V. COMPARISON WITH MÖSSBAUER AND EPR DATA

Our observation of Fe on ideal S, near-S, and near-T sites also gives valuable information for the interpretation of Mössbauer spectroscopy (MS) and EPR experiments. We generally confirm the existence of interstitial Fe and substitutional Fe as inferred from MS, however, a 1:1 correspondence between channeling and MS results is complicated by the fact that most of the available Mössbauer data rely on completely different annealing time scales than emission channeling and many other techniques. Basically all MS results at low Fe concentrations were observed in source experiments either following Coulomb excitation of $^{57}$Fe (Ref. 17, 20, and 26) or following the implantation and decay of $^{57}$Mn ($t_{1/2}=1.7$ min). In Coulomb excitation experiments (which we will abbreviate as $^{57}$Fe$^*$) a large recoil always accompanies the heavy ion bombardment excitation process, and in $^{57}$Mn → $^{57}$Fe decay experiments a $\sim 40$ eV recoil results from the nuclear decay of $^{57}$Mn. Therefore, in both cases the MS level probes the situation in a narrow time window ($\sim 140$ ns) immediately after recoil implantation. While any reaction of Fe itself can only be studied on this time scale, the overall damage accumulation and damage annealing in the sample is dominated by the fact that the experiments are done on-line, i.e., the measurement temperature is also the implantation temperature. Due to dynamic annealing, implantations at elevated temperatures result in considerably reduced concentrations of primary defects while secondary defect complexes become more prominent. In addition, the outcome of the experiment may depend on the thermal history of the sample, e.g., if the experiment is started at low temperatures, initially defects are accumulat-
TABLE II. Proposed correspondence between the Fe lattice sites found in emission channeling experiments, the lines identified in Mössbauer studies, and major EPR centers.

<table>
<thead>
<tr>
<th>Emission channeling</th>
<th>Mössbauer</th>
<th>EPR</th>
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</thead>
<tbody>
<tr>
<td>Random</td>
<td>(a) damage doublet</td>
<td></td>
</tr>
<tr>
<td>Ideal $T$ interstitial (not seen)</td>
<td>(b) interstitial singlet</td>
<td>Fe$^+$ and Fe$_0^-$</td>
</tr>
<tr>
<td>Near-$S$</td>
<td>(c) substitutional singlet</td>
<td>$NL19$</td>
</tr>
<tr>
<td>Near-$T$ interstitial</td>
<td>(d) interstitial “new line” doublet</td>
<td>$NL19^?$</td>
</tr>
<tr>
<td>Ideal $S$</td>
<td>either not yet seen or (c) substitutional singlet</td>
<td>not seen</td>
</tr>
</tbody>
</table>

center, which scatter from 160 °C (Ref. 18) to 500 °C (Ref. 19), rather point to Fe on near-$S$ sites. Our experiments show that the incorporation of large fractions of Fe on ideal substitutional sites requires annealing temperatures above 700 °C. Since these temperatures have not been reached in on-line Mössbauer experiments, it seems possible that they did not produce Fe on ideal $S$ sites in sufficient quantities to be detected.

VI. CONCLUDING REMARKS

Our study confirmed that Fe in Si exhibits a richness of structural properties, in particular that it is able to occupy at least three different lattice sites: near-tetrahedral interstitial sites, near-substitutional sites, and ideal substitutional sites. We provided the first direct evidence for Fe on or near-substitutional sites in Si, thus confirming the interpretation of Mössbauer data. The fact that at least three different Fe sites were clearly observed shows the demand for a more refined theoretical treatment of the structural properties of Fe-related defects in Si.

Finally, our results, which are consistent with implanted Fe being trapped by vacancy like defects at the end of its projected range and, following annealing above 600 °C, also around half of its implanted range, provided further insight in the nature of the defects responsible for the gettering behavior of radiation damage.

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