PHYSICAL REVIEW B **73**, 165209 (2006)

Vacancy-impurity pairs in relaxed $Si_{1-x}Ge_x$ layers studied by positron annihilation spectroscopy

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(Received 25 January 2006; published 14 April 2006)

Positron annihilation spectroscopy was applied to study relaxed P-doped *n*-type and undoped $Si_{1-x}Ge_x$ layers with x up to 0.30. The as-grown SiGe layers were found to be defect free and annihilation parameters in a random SiGe alloy could be represented as superpositions of annihilations in bulk Si and Ge. A 2 MeV proton irradiation with a 1.6×10^{15} cm^{-2} fluence was used to produce saturated positron trapping in monovacancy related defects in the *n*-type layers. The defects were identified as V-P pairs, the *E* center. The distribution of Si and Ge atoms surrounding the *E* center was the same as in the host lattice. The process leading to the formation of V-P pairs therefore does not seem to have a significant preference for either Si or Ge atoms. In undoped $Si_{1-x}Ge_x$ we find that a similar irradiation produces a low concentration of divacancies or larger vacancy defects and found no evidence of monovacancies surrounded by several Ge atoms.

DOI: 10.1103/PhysRevB.73.165209 PACS number(s): 61.80.Lj, 78.70.Bj, 61.72.Ji

I. INTRODUCTION

Silicon germanium (SiGe) has attracted much attention for its potential uses in the semiconductor industry. The complete solubility of Si and Ge allows band-gap engineering between Si and Ge. Significant increase in the performance of transistors can be achieved using strained SiGe/Si heterostructures.[1,2] Strain is used to enhance the electron and hole mobilities.[3] The ability to incorporate SiGe into existing silicon based manufacturing processes is a further advantage of the material.[4]

Point defects exist even in high quality materials and they have an influence on the electric properties. Several authors have studied point defect related electric levels in SiGe. Mamor *et al.* have shown that the activation enthalpies of various deep-level defects decrease when the Ge concentration of a $Si_{1-x}Ge_x$ material is increased.[5] Monakhov, Kuznetsov, and Svensson have reported energy levels of defects induced by proton irradiation in strained $Si_{1-x}Ge_x$ using deep-level transient spectroscopy.[6,7] Both experimental and theoretical studies of energetics of vacancy formation in $Si_{1-x}Ge_x$ materials have shown a net energy gain of around 0.2 eV when a Ge atom replaces a Si atom next to a vacancy.[8,9] This suggests that there could be vacancy complexes surrounded by many more Ge atoms than predicted by the atomic abundances in the material. However, few direct observations of vacancies in $Si_{1-x}Ge_x$ have been reported[8,10] and most previous studies have been done on strained $Si_{1-x}Ge_x$ layers.

In this work we have used Doppler broadening positron annihilation spectroscopy (PAS) to study both undoped and phosphorus doped relaxed $Si_{1-x}Ge_x$ epitaxial layers with $x \leq 0.30$. We show that the annihilation parameters in as-grown SiGe layers can be constructed as superpositions of parameters in bulk Si and Ge lattices. We also show that proton irradiation produces monovacancy donor pairs, so-called *E* centers, in P-doped relaxed $Si_{1-x}Ge_x$ regardless of Ge concentration, as found in earlier studies on strained SiGe. The distribution of Si and Ge atoms around the *E* center is the same as in the surrounding lattice. The process leading to the formation of V-P pairs therefore does not seem to have a preference for either Si or Ge atoms. In undoped $Si_{1-x}Ge_x$ we show that irradiation produces a low concentration of divacancies or larger vacancies and found no evidence of monovacancy complexes surrounded by several Ge atoms.

II. EXPERIMENTAL METHOD

A. Positron measurements

Positron annihilation spectroscopy (PAS) has been shown to be a versatile tool for studying vacancy-type defects.[11,12] The annihilation radiation can provide atomic resolution into defects and atoms surrounding them. Studies of defect distributions in thin layers or even defect profiling with the Doppler broadening technique are possible by controlling the implantation energy of the positrons.

We used a monoenergetic positron beam to study defects and bulk properties of relaxed $Si_{1-x}Ge_x$ layers. Positrons were extracted from a ^{22}Na source and moderated with a 1 μm *W* foil. Positrons were then accelerated and implanted into the sample at selected energies between 0.1 and 25 keV. After implantation a positron thermalizes within a few picoseconds and typically diffuses for 100–250 ps until it annihilates with an electron. The positron diffusion length before annihilation varies from hundreds of nanometers to less than ten nanometers depending on the types of defects and their concentration in the material.[11,13] Diffusing positrons can be trapped by neutral and negatively charged defects. In particular, PAS is sensitive to open volume defects, which extend the positron lifetime and where the momentum distribution of electrons is narrower.

In Doppler broadening spectroscopy the momentum of the annihilating electron-positron pair is detected as broadening of the 511 keV annihilation peak. We used a Ge detector with an energy resolution of 1.3 eV at 511 keV for measuring the annihilation spectra. In the annihilation event two photons are emitted in almost opposite direction at the same time. The intensity of the background radiation can be reduced significantly, at the expense of a slower count rate, by requiring both photons to be detected in co-incidence. For co-incidence measurements we added a bismuth germanium oxide (BGO) scintillation detector opposite to the Ge detector to the system. This improves the peak-to-background ratio by a factor of 100 to about $1:10^4$. Using the co-incidence technique the measurement of core-electron momenta up to $p \approx 40 \times 10^{-3}$ m_0c is possible allowing a direct comparison of measurements and theoretical electron momentum distribution.

In the single detector measurements the changes in the annihilation spectrum were described using the conventional S and W line parameters.[12] The S parameter is defined as the fraction of counts in the central part of the annihilation peak where the annihilating electron-positron pair momentum is low. These annihilations correspond mainly to valence electrons. The W parameter describes the fraction of annihilations in the wing regions on both sides of the annihilation spectrum. These annihilations are mostly with core electrons. The energy windows are selected so that the parameters are maximally sensitive to changes in the annihilation environment. The S parameter energy window is normally chosen symmetrically around the peak and in this work we required the energy of the annihilation photon E_γ to lie in the range $|E_\gamma - 511\text{ keV}| < 0.83$ keV. The W parameter windows were selected as $3.00\text{ keV} < |E_\gamma - 511\text{ keV}| < 7.60$ keV. Typically open volume defects are detected as an increase (decrease) of the S (W) parameter.

The measured S and W parameters are superpositions of S and W parameters corresponding to different positron annihilation states in the lattice. In the simplest case there are only such two states, e.g., the bulk and the surface or the bulk and a single defect state. In this case the measured parameters are given by

$$S = \eta_1 S_1 + \eta_2 S_2, \tag{1}$$

$$W = \eta_1 W_1 + \eta_2 W_2, \tag{2}$$

where S_i (W_i) is the S (W) parameter of state i, η_i the annihilation fraction in state i. The above equations are parametrized equations of a straight line in the (S,W) plane. Therefore the slope of the line the S and W parameters form in the (S,W) plane can be used to identify defects on an S-W plot. Also, a nonlinear behavior in an S-W plot is caused by at least three positron annihilation states in the lattice.

The annihilation parameters can be used to calculate the vacancy concentration in the lattice if the defects, where annihilations take place, are known. The positron annihilation rate κ_V into a defect is given by

$$\kappa_V = \frac{1}{\tau_B} \frac{S - S_B}{S_V - S}, \tag{3}$$

where τ_B is the positron lifetime in defect free lattice, S is the measured parameter, S_B is the defect free lattice parameter and S_V the S parameter of the defect. The total concentration of vacancy defects is related to the annihilation rate through the trapping coefficient μ_V via

$$c_V = \kappa_V \mu_V, \tag{4}$$

where a value $\mu_V = 10^{15}$ s^{-1} is typical for negatively charged vacancies.[12]

TABLE I. Properties of the $Si_{1-x}Ge_x$ samples.

Sample	[Ge] (%)	Sample type	Doping [P] (cm^{-3})	Irradiation p^+ (cm^{-2})
1	10	Undoped		
2	10	n-type	10^{18}	
3	20	Undoped		
4	20	n-type	10^{18}	
5	20	n-type	10^{19}	
6	30	Undoped		
7	30	n-type	10^{18}	
8	10	n-type	10^{18}	1.6×10^{15}
9	20	n-type	10^{18}	1.6×10^{15}
10	30	n-type	10^{18}	1.6×10^{15}
11	20	Undoped		1.6×10^{15}

B. Samples

We studied relaxed $Si_{1-x}Ge_x$ grown by chemical vapor deposition on Czochralski grown Si(100) substrates. Relaxation of the samples was achieved by growing a buffer layer with a gradually increasing Ge concentration. The buffer layer Ge concentration increased at a rate of 10%/μm. The final Ge concentration in the epitaxial layer varied between 10% and 30% and the relaxed top layer thickness was 1 μm. For reference purposes we used p-type Si and Ge bulk samples. The reference samples had only one lifetime component in their positron lifetime spectra and thus their vacancy concentration is below detection limit.

In this work we studied both undoped and n-type material. The n-type conductivity was achieved by doping with P to concentrations $[P]=10^{18}$ cm^{-3} and $[P]=10^{19}$ cm^{-3}. In order to produce a homogenous defect distribution in the $Si_{1-x}Ge_x$ layer, some samples were irradiated with 2 MeV protons with a fluence of 1.6×10^{15} cm^{-2}. The range of these protons far exceeds the range of positrons (maximum average positron implantation depth $\lesssim 3$ μm) used in the experiment and the fluence was chosen high enough to produce saturated positron trapping, as determined by Sihto *et al.*[8] Properties of the studied materials are shown in Table I.

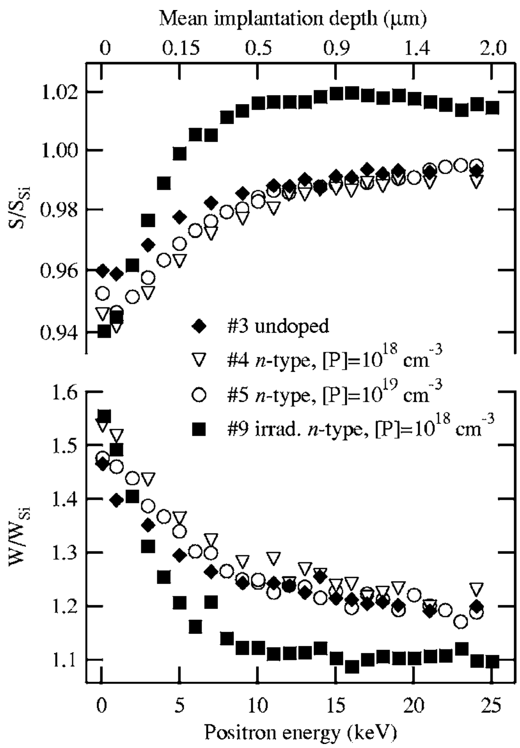

FIG. 1. Low momentum parameter S and high momentum parameter W as a function of positron energy in samples containing 20% germanium. The mean positron implantation depth is shown for clarity.

C. Theoretical momentum distribution

We used theoretical calculations of the positron annihilation spectrum to predict and analyze the results. Review of the methods and the interpretation of the spectra can be found in Ref. 14. For calculations we used the atomic superposition method in a 216 atom supercell using SiGe lattice constants determined earlier by Dismukes, Ekstrom, and Pfaff.[15] Positrons in the lattice were treated using the conventional scheme, i.e., positron density in the material is vanishingly small. The annihilation rates with different electron states were obtained in the local density approximation using the Boronski-Nieminen enhancement factor to calculate the effect of positron on the electron density.[16] The momentum distribution of the electron positron pairs was obtained by summing the contribution of annihilations in different electron states. For more details on the method, see Ref. 17 and references therein.

III. RESULTS

A. Doppler broadening spectroscopy

Annihilation spectra for all the studied samples were measured as a function of positron implantation energy. The S and W parameters as a function of implantation energy relative to the Si lattice for layers containing 20% germanium are shown in Fig. 1. The mean positron implantation depth corresponding to the used acceleration energies is marked on the top axis. For all Ge concentrations the curve consists of three regions: the surface, the SiGe layer and the substrate. At small energies ($E<3$ keV) most positrons annihilate at the surface. Surface annihilations produce a low S and a high W parameter that is almost the same in all samples due to annihilations in the native oxide. Increasing the implantation energy, the S parameter values gradually increase and the W values decrease as more positrons annihilate in the SiGe layer. At higher energies, $E>15$ keV, a large fraction of positrons already reaches the buffer layer or the substrate.

The as-grown and the irradiated samples show a distinctly different behavior. In the as-grown layers the transition from the surface to the SiGe layer to the substrate is smooth. In the irradiated sample both the S and W parameters increase with increasing energy up to about 10 keV and above 10 keV form a plateau. The plateau corresponds to a region where positrons are unable to diffuse to the surface or the substrate and annihilation parameters correspond to annihilations solely in the SiGe layer. Also, in the irradiated piece the S parameter is always higher than in the as-grown ones, a clear signal that vacancies were formed in the irradiation process. At the same time the W parameter decreases, which is consistent with vacancies in the lattice.

The S and W parameter curves of differently doped as-grown samples are very similar for any fixed Ge concentration. In all the undoped samples the parameters change slightly faster from the surface value to the values in the $Si_{1-x}Ge_x$ layers than in the n-$Si_{1-x}Ge_x$. This shows that the positron diffusion length in undoped layers is shorter, possibly due to an electric field close to the surface in the n-type layers. However, because the surface and the buffer layers are similar in all the samples, comparison between different samples is possible.

B. Varying Ge concentration

The effect of the lattice Ge atoms on the annihilation parameters can be seen by plotting the S parameter as a function of the W parameter. Changes in the sample Ge concentration will produce correlated changes of both annihilation parameters in the (S,W) plane. An (S,W) plot of $Si_{1-x}Ge_x$ for varying x is shown in Fig. 2. Different concentrations fall into distinct regions in the plot, separated by the dotted lines. For positron energies between 0.1 and 15 keV the (S,W) pairs fall on a line joining the surface and a state corresponding to the $Si_{1-x}Ge_x$ layer. At similar energies the measured W parameter clearly increases for higher sample Ge concentration. Also the S parameters are slightly lower. The annihilation spectrum from Ge atoms is therefore broader and flatter, and we attribute the changes in S and W parameters to show increased annihilations with Ge electrons. Our calculations show that Ge $3d$ electrons should increase the annihilation intensity in the selected W parameter window, in agreement with the measurements.

If the energy were further increased, and positrons penetrated deeper into the sample, the parameters would turn towards those of the Si substrate ($S=W=1$). A slight turning can be seen at the highest energies in the layer with 10% Ge concentration as it has a lower density and thus positrons penetrate deeper into the sample at maximum energy. The

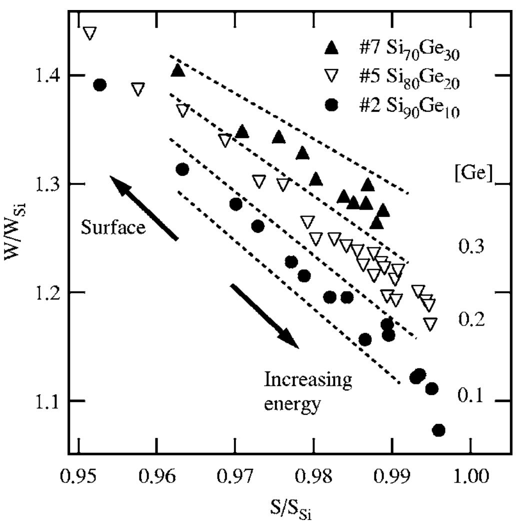

FIG. 2. The S and W parameter pairs in as-grown samples relative to parameters in Si. Increasing the positron implantation energy the parameters change from their values at the surface to those characteristic to SiGe and finally the substrate.

turning point is not sharp because the Ge concentration in the buffer layer decreases only gradually and the width of the positron implantation profile is broad, comparable to the mean implantation depth.

We collected the SiGe layer-specific S and W parameters from all the samples minimizing the effects of the surface and the substrate. For reference we included the parameters of defect-free p-type Si and of high purity Ge. Also included are previous results on strained P-doped $Si_{0.96}Ge_{0.04}$ studied by Sihto *et al.*[8] The results are shown in Fig. 3. All the as-grown samples are in an increasing order of the Ge concentration and fit well on a line joining Si and Ge, except the undoped $Si_{0.70}Ge_{0.30}$ sample. This shows that the annihilation parameters of SiGe layers can be explained as superpositions

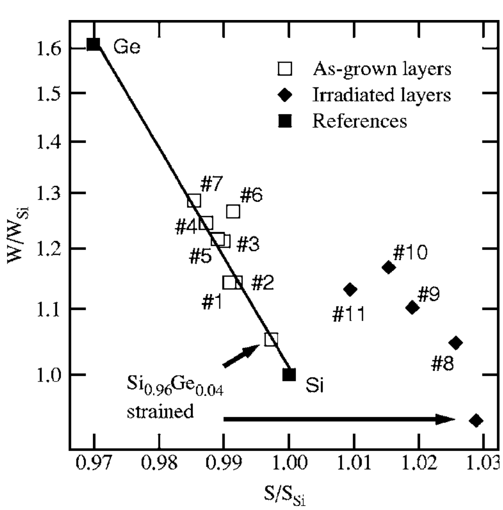

FIG. 3. The S-W parameters of all the studied SiGe layers and Ge relative to parameters of defect-free Si. All as-grown samples, except sample 6, fall on a line joining Si and Ge. Irradiated samples have a higher S and a lower W parameter indicating vacancy formation.

of annihilations in Si and Ge lattices. Interestingly, the change of annihilations parameters with Ge concentration seems to be larger than the Ge concentration of the lattice. The 30% SiGe alloy leads to about 50% effect in the S and W parameters (Fig. 3), showing that positron annihilation prefers Ge atoms instead of Si. Similar phenomena have been observed earlier in metals alloys, where it was proposed that different atom types would have different relative positron affinities.[18–20] Unlike binary alloys studied by Stott, Kubica *et al.*,[18,19] Si and Ge have very similar electronic structures and electron affinities. Puska *et al.* have also shown that positron affinities to Si and Ge are almost identical, slightly favoring Si[14]. The increased Ge annihilations are therefore likely due to lattice relaxation induced by the larger Ge atoms.

All P-doped layers lying on a line between pure Si and pure Ge suggest that there are no positron trapping defects such as vacancies in the measured layers. Thus the concentration of vacancies is below the detection limit, $\lesssim 10^{15}$ cm^{-3}. In Fig. 3 the i-$Si_{0.70}Ge_{0.30}$ layer 6 has a higher S and lower W parameter than the P-doped layer 7 showing that vacancies were formed during the growth of the undoped layer. Using typical values for mono- and divacancies with $S_V/S_b = 1.03-1.1$, a rough estimate, $[c_V] \approx 1-5\times 10^{16}$ cm^{-3} for the vacancy concentration can be given. It is possible that P doping slows down the growth rate and thereby the rate of vacancy generation implying P-doped samples being of higher quality. Also sample 4 differs from the other layers with $[\mathrm{Ge}]=0.20$; though it is located on the line between Si and Ge in Fig. 3, it has a higher W and a lower S parameter than other samples where Ge concentration was 20%. This suggests that the actual Ge concentration is higher than intended.

C. Irradiated $Si_{1-x}Ge_x$ layers

In order to study native point defects in the $Si_{1-x}Ge_x$ layers, the layers were irradiated using 2 MeV protons, as explained in Sec. II. Proton irradiation is expected to generate a high concentration of Frenkel pairs. In both Si and Ge monovacancies have been shown to be mobile at room temperature, while divacancies are stable.[21,22] After irradiation only vacancies that encounter impurity atoms or other vacancies during migration remain in the samples. Ge atoms in Si increase the stability of simple vacancies so that in Ge-doped Si vacancies are stable up to 200 K[23] and in $Si_{0.95}Ge_{0.05}$ up to 295 K.[24] Also, the stability of vacancy donor pairs increases so that the temperature, where they anneal out, is 60 K higher in $Si_{0.75}Ge_{0.25}$ than in Si.[25] However, increasing the layer Ge concentration above $x \geqslant 0.83$ electron irradiation does not produce vacancy-type defects.[10]

Figures 1 and 3 show the behavior of S and W parameters as a function of implantation energy in the irradiated samples. The irradiated samples have a much higher S and a lower W parameter than the corresponding as-grown samples. The n-type layers 8–10 fall on a line in the (S,W) plot while the only undoped irradiated sample (11) is separate from all others. This shows that all the irradiated layers contain vacancies and the surroundings of the vacancies may

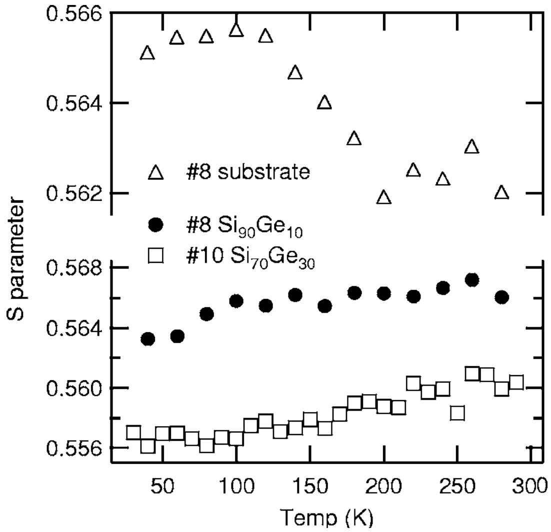

FIG. 4. The slightly decreasing S parameter in the $Si_{1-x}Ge_x$ layers with decreasing temperature indicates saturated positron trapping, while the increasing S parameter in the substrate indicates that vacancies are in a negative charge state.

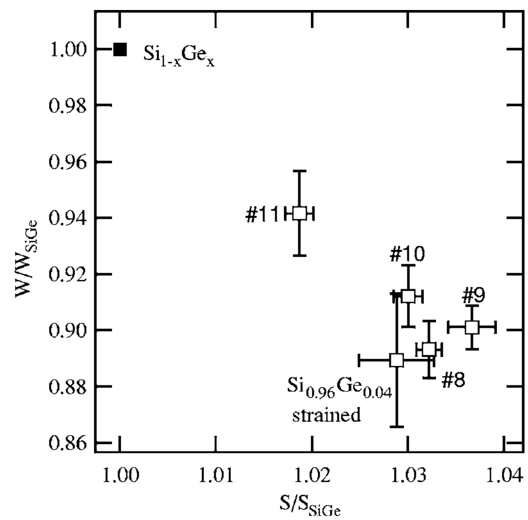

FIG. 5. The S and W parameters in the irradiated samples relative to the as-grown ones show that in all the n-type samples the irradiation induced defects have a similar structure.

be different in the P-doped and undoped layers.

The charge state of a vacancy defect can be studied by measuring the positron annihilation spectra as a function of temperature. For negatively charged defects positron trapping increases when the temperature decreases, while for neutral defects trapping is temperature independent.[11,12] Higher positron trapping rate into vacancies leads to a higher measured S and a lower measured W parameter. However, if all positrons already annihilate in negatively charged vacancies, the annihilation parameters remain constant. In all cases the thermal expansion of the lattice, which increases the S parameter, has to be considered.

Figure 4 shows the S parameter as a function of measurement temperature in the proton irradiated Si substrate and the $Si_{1-x}Ge_x$ layers with $x=0.1$ and $x=0.3$. In the Si substrate the S parameter increases strongly when temperature decreases until below approximately 100 K the change stops and the S parameter remains constant. In the $Si_{1-x}Ge_x$ layers, on the other hand, the parameters slightly but steadily decrease as the temperature goes down during the whole temperature range. In the P-doped $Si_{1-x}Ge_x$ layers the S_V/S_B values are what is expected for monovacancies and, accounting for the thermal expansion, the S parameter is constant. The vacancies formed in similar P-doped $Si_{1-x}Ge_x$ samples under proton irradiation have been shown to be negatively charged.[8] Therefore the constant S parameter indicates saturated positron trapping, i.e., very high vacancy concentration. The results agree with previous studies where a similar irradiation fluence generated a vacancy concentration over 10^{18} cm^{-3}.[8] In P-doped layers the PAS spectrum is therefore purely from defects in the lattice, not the surrounding $Si_{1-x}Ge_x$ lattice.

To better identify the defects in different irradiated layers, we calculated the changes in the S and W parameters relative to their corresponding $Si_{1-x}Ge_x$ bulk values, as shown in Fig. 5. The change in the annihilation parameters is similar when either the Ge concentration of the bulk SiGe lattice changes or when the average Ge concentration around a defect changes. Therefore, this removes the effects of varying Ge concentration in the host lattice, better revealing changes that are not related to the sample Ge concentration. We have included results from strained $Si_{0.96}Ge_{0.04}$ reported by Sihto *et al.* in Ref. 8. Sihto's measurements were made both before and after the natural oxide layer at the sample surface has been etched off. We use here the data with the native oxide as in the samples of this work.

In all P-doped layers the changes in the S and W parameters are almost equal. The increase in the S parameter is about 3% and the decrease in the W parameter 10% from the as-grown values for all Ge concentrations. This shows that the defects are the same in all the samples and the changes observed relative to Si are due to the changes in the Ge concentration of the alloy. The 3% increase in the S parameter is typical for monovacancies, while in Si divacancies or larger vacancy clusters have been shown to increase the S parameter by at least 5%.[26,27] This shows that the same defect is dominant in all n-type layers and the concentration of Si and Ge atoms surrounding it is similar as in the host lattice. We attribute the defect to the vacancy phosphorus pair (E center) as (i) it has the size of a monovacancy, (ii) it exists in P-doped material and (iii) the clean monovacancy is unstable at room temperature. The E center has also been identified in electrical experiments in P-doped strained SiGe with $[Ge]<0.13$ after proton irradiation.[7]

The irradiated undoped $Si_{0.80}Ge_{0.20}$ 11 is separate from all other layers. In the S-W plot it is located half way between the as-grown and the P-doped irradiated layers. The increase in the S parameter from the as-grown parameters is 1.9% and decrease in the W parameter 6%. The increase in the S parameter is too small to be caused by saturation trapping into simple vacancies or vacancy impurity pairs. The vacancy concentration can be estimated to be $\leqslant 5\times10^{17}$ cm^{-3} using reasonable S parameter estimates for monovacancies or larger vacancy-type defects ($S_V/S_B\geqslant 1.03$). In Si rich $Si_{1-x}Ge_x$, proton irradiation therefore generates a low concentration of either monovacancies surrounded by several Ge

TABLE II. W parameters from theoretical calculations for simple vacancies and vacancy phosphorus pairs in different $Si_{1-x}Ge_x$ materials in the momentum range $11.5-29.5\times10^{-3}$ m_0c.

Material	Defect	W/W_{Ref}	Reference
$Si_{80}Ge_{20}$	V-Ge_1	0.85	$Si_{80}Ge_{20}$
$Si_{80}Ge_{20}$	V-Ge_2	1.02	$Si_{80}Ge_{20}$
$Si_{80}Ge_{20}$	V-Ge_3	1.11	$Si_{80}Ge_{20}$
$Si_{80}Ge_{20}$	V-Ge_4	1.26	$Si_{80}Ge_{20}$
$Si_{90}Ge_{10}$	V-P	0.94	Si
$Si_{90}Ge_{10}$	V-P-Ge	1.14	Si
$Si_{80}Ge_{20}$	V-P	1.03	Si
$Si_{80}Ge_{20}$	V-P-Ge	1.22	Si
$Si_{70}Ge_{30}$	V-P	1.07	Si
$Si_{70}Ge_{30}$	V-P-Ge	1.30	Si

atoms or vacancies at least the size of divacancies trapped in the material during irradiation.

Calculations show that the most abundant defect is a monovacancy surrounded by four Ge atoms, whose formation energy is 1 eV lower than that of V-Si_4.[9] Already at [Ge]=0.05 the amount of V-Ge_4 complexes is 20 times larger than of V-Si_4 though lattice sites surrounded by four Ge atoms are five orders of magnitude less likely. In $Si_{0.80}Ge_{0.20}$ the concentration of lattice sites where V-Ge_4 formation is possible is $\approx10^{20}$ cm^{-3}, i.e., higher than P doping in n-type layers leading to saturation trapping. Hence, if V-Ge_4 is stable the vacancy concentration would be expected to be as high as in the P-doped layers. Theoretical calculations on simple vacancy defects (see Table II) show that V-Ge_3 and V-Ge_4 complexes would produce W parameters that are much higher than the observed value 0.94. We therefore conclude that the undoped $Si_{1-x}Ge_x$ layers contain a low concentration of divacancies or larger defects.

D. Core-electron measurements

For getting detailed information on the surroundings of the annihilation site we performed coincidence measurements of selected as-grown and irradiated samples. Results for as-grown layers with $[P]=10^{18}$ cm^{-3} are shown in Fig. 6. Results are plotted relative to identical measurements of p-type Si. The annihilation intensity at small momenta in all the layers is very close to the values obtained in Si. At electron momenta $p>5\times10^{-3}$ m_0c the annihilation intensity starts to increase above Si and the increase is stronger in those layers where the Ge concentration is higher. At $p>10\times10^{-3}$ m_0c the intensity curve flattens in layers with [Ge]=0.1 and [Ge]=0.2, while in $Si_{0.70}Ge_{0.30}$ the intensity keeps increasing. The similarity at low momenta is expected as the properties of valence electrons in Si and Ge are very similar. At higher momenta, however, Ge $3d$ electrons increase the annihilation intensity considerably, as evidenced by the above unity intensity in Fig. 6.

Coincidence measurement results from the irradiated layers with $[P]=10^{18}$ cm^{-3} are shown in Fig. 7. The shape of the curve is very different from the as-grown layers showing

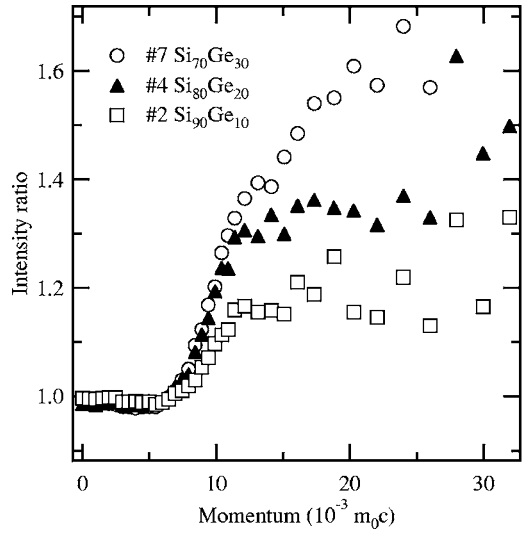

FIG. 6. Coincidence Doppler spectra of the as-grown n-type layers relative to the spectrum of bulk Si. Ge atoms increase the high momentum annihilations in the range $p>10\times10^{-3}$ m_0c.

oscillations. The oscillations are due to Si lattice crystal symmetries inducing anisotropy in the electron momentum density while randomly oriented vacancy defects have a more isotropic momentum distribution. In the figure at very low momenta the intensity has increased several per cent and a minimun well below unity has appeared at $p\approx6\times10^{-3}$ m_0c. The intensity then increases as in the as-grown layers but has another local minimum at $p\approx15\times10^{-3}$ m_0c. The high momentum intensity in irradiated layers remains much below what was observed in the as-grown samples for the whole high momentum region.

The curves of the irradiated samples n-$Si_{0.80}Ge_{0.20}$ 9 and n-$Si_{0.70}Ge_{0.30}$ 10 are very similar up to 10×10^{-3} m_0c where the higher Ge concentration in sample 10 increases the annihilation intensity above what was observed in 9. Sample 8,

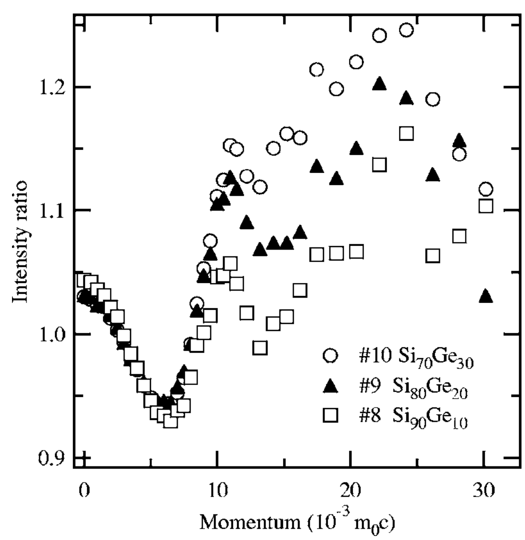

FIG. 7. Coincidence Doppler spectra of the irradiated samples relative to bulk Si. Oscillations are due to crystal symmetries of the reference Si lattice.

with 0.1 Ge fraction, has a slightly higher intensity at 0×10^{-3} m_0c and the minimum at 6×10^{-3} m_0c is lower than in the other layers. At high momenta layer 8 has a smaller intensity than the layers with more Ge. Calculated momentum distributions of V-P pairs with varying number of Si and Ge atoms around it produce similar shaped spectra as observed in the experiment. The theoretical W parameters of V-P pairs, where the vacancy is surrounded by 0 or 1 Ge atoms, are calculated in Table II. From calculated spectra the number of Ge atoms surrounding the E center can be deduced to be between zero and one in all the layers. On purely probabilistic grounds the expected number of Ge atoms in $Si_{1-x}Ge_x$ layers with 0.10, 0.20 and 0.30 Ge fraction is 0.3, 0.6 and 0.9, respectively. We thus conclude that the process, which leads to the formation of the E centers, has at most a very weak attraction to Ge atoms.

The results are in agreement with previous measurements about the abundance of Ge atoms surrounding the E centers by Sihto *et al.* Elkin and Watkins determined that the energy gain of pairing a vacancy and a dopant atom is roughly the same for all group V atoms, around 1 eV.[28] Recent calculations by Ramamoorthy and Pantelides show an energy gain of 1.3 eV for V-As pairs.[29] During migration negatively charged vacancies will experience a long range Coulomb attraction to the positive phosphorus atoms, while the potential due to lattice relaxation is very short range. Vacancies formed in the irradiation process are therefore likely to get trapped to the nearest P atoms and the distribution of Ge atoms around the E center then reflects the Ge concentration of the host lattice. To move to a site where there are more germanium atoms, the E center would have to overcome a migration barrier. In Si it has been shown that high temperature anneal will enable the V-As complexes to diffuse until it gets trapped by arsenic atoms to form V-As_2 or larger complexes.[30] Similar accumulation of Ge atoms near the E centers explains the results obtained by Sihto *et al.*[8]

IV. CONCLUSIONS

We have studied vacancy-type defects in relaxed $Si_{1-x}Ge_x$ layers with Ge concentrations up to 30% using positron annihilation spectroscopy. We studied both undoped and n-type P-doped layers. The n-type as-grown $Si_{1-x}Ge_x$ layers were defect free while the undoped layers contained vacancies in the 10^{16} cm^{-3} range. We show that in the as-grown $Si_{1-x}Ge_x$ alloys the annihilation parameters can be constructed as superpositions of positron annihilations in Si and Ge. The fraction of annihilations with Ge atoms is larger than the atomic abundances suggest. We attribute this to the larger size of Ge atoms.

A 2 MeV proton irradiation with 1.6×10^{15} cm^{-2} fluence was used to produce enough vacancies to get saturated positron trapping into the vacancies in the n-type layers. In irradiated undoped $Si_{1-x}Ge_x$ we found a small concentration of divacancies or larger vacancy-type defects. In the n-type samples we found the same defect is formed regardless of Ge concentration. The defect has the size of a monovacancy and our results agree with vacancy phosphorus pairs (the so-called E center) that have been observed earlier in strained $Si_{1-x}Ge_x$. We show that the germanium concentration surrounding the E centers is the same as in the host lattice. We can thus conclude that the structure—or the migration process leading to the formation—of V-P pairs does not have a preference for Si or Ge atoms.

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