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# Positron annihilation spectroscopy of vacancy complexes in SiGe

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## Abstract

The aim of this contribution is to present a review of the results related to vacancy complexes in SiGe obtained in the positron group at Helsinki University of Technology. We have studied proton irradiated undoped and P doped SiGe layers with Ge concentration from 4% to 30%. The dominating defect after irradiation in the n-type layers is found to be the E-center, i.e. the vacancy phosphorus complex, no preferred association with either Ge or Si is found for the vacancy after irradiation. The E-center is observed to be mobile in the temperature interval 150–200 °C and to migrate until it encounters a Ge atom and forms the V–P–Ge complex. This complex anneals out in temperatures above 200 °C. We estimate that the binding energy increases by approximately 0.1–0.2 eV when a Ge atom neighbours an E-center. For the undoped irradiated samples, we find no indication of vacancies surrounded by one or several Ge atoms, i.e. the presence of Ge around a vacancy is not enough to make the defect stable at room temperature. The dominating defect in undoped irradiated samples is most likely the divacancy.

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## 1. Introduction

During recent years we have seen an escalating interest in SiGe and Ge research and SiGe has already been implemented into existing Si technology. Strained SiGe layers have been shown to produce high electron mobility transistors where the achievable electron mobilities can be an order of magnitude higher than in relaxed materials [1].

In this review we present how positron annihilation spectroscopy (PAS) have been used to identify vacancy complexes in SiGe in the positron group at Helsinki University of Technology [2–4]. The work has focused on the E-center in P doped strained and relaxed SiGe. Here we present the main results obtained by Doppler broadening spectroscopy. In the references cited above also core electron momentum measurements (coincidence Doppler broadening) have been performed, which support these results.

## 2. Positron annihilation spectroscopy

For the investigation of irradiation induced vacancy defects in thin layers we use PAS in Doppler broadening mode. PAS has since the mid 1980s been used as a versatile tool in the study of vacancy defects in semiconductors [5,6]. The technique is especially useful for the investigation on the thermal stability, formation and annealing of vacancy defects since measurements over a wide range of temperatures is possible.

Positrons can either be taken directly from a $\beta^+$ source, as is done in the conventional lifetime and Doppler broadening measurements, or as in the case of thin layers be moderated and then accelerated to a desired energy and implanted in the sample. This enables the study of defect distributions in thin layers and even defect profiling with the Doppler broadening technique. After implantation the positrons thermalize within a few picoseconds and thereafter diffuse in the sample until they annihilate with electrons. Neutral and negative vacancy type defects in the lattice can

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act as positron traps. When a positron is trapped by a vacancy its lifetime increases and the momentum distribution of the annihilating electron-positron pair narrows, because of the reduced electron density.

The momentum of the annihilating positron-electron pair can be detected as Doppler broadening of the 511 keV annihilation line. For the measurement of the Doppler broadening we used a Ge detector with an energy resolution of 1.3 keV at 511 keV. For the presentation of Doppler broadening measurements it is customary to use the parameters $S$ and $W$ to describe the shape of the annihilation line. The low momentum parameter $S$ is the fraction of counts in the central part of the annihilation line and thus it describes mainly annihilation with low momentum valence electrons. Correspondingly $W$ is the high momentum parameter obtained as the fraction of counts in the wing region of the annihilation line describing annihilation mainly with core electrons. Consequently an increase (decrease) in $S$ ($W$) parameter indicates the presence of vacancy type defects.

The measured $S$ ($W$) parameter is a superposition of the $S$ ($W$) parameter of the bulk and the parameters of the different defects in the sample. Near the surface, the annihilation of the positron at the surface also has to be accounted for. In the simplest case where the positrons only annihilate in two different states the measured $S$ and $W$ 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 $\eta_1$ and $\eta_2$ are the fraction of positrons annihilating in states 1 and 2, respectively. Consequently $\eta_2 = 1 - \eta_1$. From the equations above it is evident that, in this case, the measured parameters form the segment of a line in the $(S, W)$ plane between the two annihilation states $(S_1, W_1)$ and $(S_2, W_2)$. This fact can be useful for the identification of trapping centers.

For the high momentum region of the annihilation line, the contribution of the momentum of the thermalized positron is negligible and the spectrum is dominated by the core electrons. This part of the annihilation line can therefore be used to identify the surroundings of the vacancy.

## 3. Samples

The studied samples were epitaxial $Si_{1-x}Ge_x$ layers on Czochralski grown Si(100) substrates. The silicon substrate was weakly n-type (P doped $\sim 10^{14}$ cm$^{-3}$). In order to obtain a clean deposition surface, the substrate was subjected to a $H_2$ atmosphere for 2 min prior to the deposition of the SiGe layer. The SiGe layer was grown with chemical vapor deposition (CVD) and the layer thickness for the strained SiGe samples was 1 μm. Two germanium concentrations were used for the strained samples, 4% and 7%. The layers were grown n-type with a P concentration of approximately $10^{18}$ cm$^{-3}$. The samples for the study of relaxed SiGe were also CVD grown on similar substrates, with a gradually increasing Ge concentration in the buffer layer. The rate of increase was 10 %/μm.

Table 1
The characteristics of the strained samples used in the study

| Ge content (%) | $p^+$ fluence (cm$^{-2}$) |
|---|---|
| 4 | – |
| 4 | $3 \times 10^{14}$ |
| 4 | $6 \times 10^{14}$ |
| 4 | $1.6 \times 10^{15}$ |
| 7 | – |
| 7 | $3 \times 10^{14}$ |
| 7 | $6 \times 10^{14}$ |

Table 2
Properties of the relaxed $Si_{1-x}Ge_x$ samples used in the study

| | [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 | $10^{18}$ | $1.6 \times 10^{15}$ |
| #9 | 20 | n-type | $10^{18}$ | $1.6 \times 10^{15}$ |
| #10 | 30 | n-type | $10^{18}$ | $1.6 \times 10^{15}$ |
| #11 | 20 | undoped | – | $1.6 \times 10^{15}$ |

In order to produce a homogeneous defect distribution within the SiGe layer, some of the samples were irradiated with 2 MeV protons. The proton fluence varied between $3 \times 10^{14}$ cm$^{-2}$ and $1.6 \times 10^{15}$ cm$^{-2}$ for the strained samples. The highest irradiation fluence produced saturated positron trapping into vacancy defects, hence this fluence was chosen for the relaxed samples. A summary of the samples used in this study can be found in Tables 1 and 2.

## 4. The identification of the E-center (V–P) in strained SiGe

### 4.1. Introduction of vacancies vs. fluence and positron annihilation states

In Fig. 1 we show the Doppler parameters $S$ and $W$ as a function of positron implantation energy for as-grown and as-irradiated samples normalized to the respective values in bulk Si. Also indicated in the figure is the mean positron implantation depth. As can be noted, the results for the as-grown samples (Ge content 4% and 7%) are almost identical and the SiGe layer cannot be clearly distinguished since the $S$ and $W$ parameters continuously approach the silicon substrate values with increasing positron implantation energy.

For the samples implanted with a proton fluence of $6 \times 10^{14}$ cm$^{-2}$ the $S$ and $W$ parameters clearly differ from the non-irradiated samples. A hint of a plateau in the $S$ parameter can be distinguished for this sample. When the