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ABSTRACT

Tin-containing Group IV alloys show great promise for a number of next-generation CMOS-compatible devices. Not least of those are optoelectronic devices such as lasers and light-emitting diodes. To obtain reliable operation, a high control over the doping in such materials is needed at all stages of device processing. In this paper, we report tin-based donors in silicon, which appear after heat treatment of a silicon-tin alloy at temperatures between 650 °C and 900 °C. Two stages of the donor are observed, called SD I and SD II, which are formed subsequently. A broad long-lifetime infrared photoluminescence is also observed during the first stages of donor formation. We discuss evolving tin clusters as the origin of both the observed donors and the photoluminescence, in analogy to the oxygen-based thermal donors in silicon and germanium.

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I. INTRODUCTION

Group IV alloys containing tin (Sn) have in recent years become promising candidates for optoelectronic devices with the possibility of direct integration into silicon-based integrated circuits.^{1–15} This is due to the opening of a direct bandgap upon sufficient Sn alloying.^{1,2} Especially for GeSn and SiGeSn alloys, important milestones such as optically pumped lasers^{4–8} and electrically pumped light sources^{9–10} have been reported. In parallel to the work on Group IV light sources, SiGeSn and GeSn are also investigated for use in other electronic devices, such as photodiodes or tunneling field effect transistors.^{11–15}

For any electrical device, the control of doping densities is crucial for its reliable operation. Some studies have investigated extrinsic doping of Sn-containing alloys.^{16–20} However, in general it is tacitly assumed that Sn itself is electrically inactive, as it is an iso-valent species to Si and Ge. Indeed, the only Sn-related electrically active defect detected in early studies of Sn-doped Si was Sn-vacancy (SnV) pairs after irradiation.^{21–24} For the use in devices, however, large Sn concentrations well above the solubility limit are used. Under such circumstances, even electrically inactive species might form complexes, which act as donors. A well-known example of such a case is oxygen in Si and Ge, which at sufficiently high concentrations forms so-called thermal donors (TDs) (chains of threefold coordinated oxygen atoms) and new donors (NDs) (oxygen clusters forming around both carbon-containing and carbon-free nucleation centers) during annealing.^{25–35}

In this paper, we present evidence for Sn-based donors in SiSn alloys. Samples containing a thin layer of SiSn with $\sim 1.4\%$ Sn show donor concentrations in the order of 10^{17} cm^{-3} in this layer after heat treatment. We propose evolving Sn clusters as the origin of these donors, similar to the oxygen-based thermal and new donors.

As impurities in Si and Ge behave similarly, taking as an example again the formation of thermal donors in both Si^{27–29} and Ge,^{25,26} we argue that a similar donor behavior of high Sn concentrations should also be present in GeSn alloys.

II. TIN AS A DONOR IN SILICON

For our study, we used molecular beam epitaxy (MBE) to grow SiSn layers on highly doped n-type Si substrates. The nominally undoped SiSn layer contains $\sim 1.4\%$ Sn and is 10 nm thick. It is sandwiched between moderately n-type doped ($\sim 5 \times 10^{15} \text{ cm}^{-3}$) Si buffer and capping layers. For reference purposes, a sample with identical geometries, doping, and growth temperatures, but without the addition of Sn, was also grown.

A very simple and effective way to determine the effective donor concentration in a semiconducting sample is capacitance-voltage (CV) profiling. Therefore, we deposited gold Schottky diodes on the samples and measured their depletion capacitance. The results of these measurements are presented in Fig. 1, where Fig. 1(a) shows the results with a SiSn layer and Fig. 1(b) those of the reference sample. One can clearly see the layer structure of our samples, with the highly doped substrate beginning at a depth of

1.6 μm , followed by the lower doped Si buffer layer, and finally the SiSn/low-T grown layer at 0.6 μm .

The SiSn layer in the as-grown samples has already been subjected to an *in situ* thermal budget of 500 $^{\circ}\text{C}$ during the growth of the capping layer. Further annealing steps for 20 min in the argon atmosphere critically impact the concentration of donors in the SiSn layer, as one can see in Fig. 1(a). The sample annealed at 725 $^{\circ}\text{C}$ contains $\sim 10^{17} \text{ cm}^{-3}$ donors in the Sn layer, whereas the concentration at the other temperatures shown is below $4 \times 10^{16} \text{ cm}^{-3}$, at which point the space charge region of the diode without applied bias extends beyond the SiSn layer. This detection limit depends on the effective donor concentration in the capping layer and can be different for other samples.

In contrast, the reference sample, shown in Fig. 1(b), shows a significantly lower donor concentration of $\sim 10^{16} \text{ cm}^{-3}$ in the low-T grown layer, which remains roughly constant for all annealing temperatures. The differences observed between the reference sample and the Sn-containing sample strongly indicate that the high donor concentration observed in the SiSn layer after 725 $^{\circ}\text{C}$ annealing is due to the presence of Sn.

To further confirm the different origins of the observed donors and thus the involvement of Sn, we performed admittance spectroscopy on both samples. The results are summarized in Fig. 2. The top images show the doping profiles from room-temperature CV measurements for both the Sn-containing and the reference sample annealed at 725 $^{\circ}\text{C}$. The second row shows the admittance

spectroscopy spectra in the temperature regions where peaks were observed. It is easily seen that peak A, which corresponds to the freeze-out of the main donor in the SiSn sample, and peak B, which corresponds to the donor in the reference sample, appear at very different temperatures. In the bottom part of the figure, the Arrhenius plots of the observed peaks are shown. One should note that the geometry of the samples, with abrupt changes of the donor concentration over several orders of magnitude, is not well suited for admittance spectroscopic measurements. Therefore, activation energy ranges are supplied instead of exact values. The peak labeled C was only observed in some samples, and its concentration is about 100 times less than that of the peak labeled A. We, therefore, conclude that its role in defining the donor concentration in the SiSn layer is minor and will focus our attention on the peak labeled A.

The strongly different peak temperatures and activation energies for peaks A and B confirm again the different origin of the

FIG. 1. Carrier concentration profiles obtained from CV measurements at room temperature for (a) the sample containing Sn and (b) the reference sample. The samples were annealed for 20 min at the indicated temperatures.

FIG. 2. Top: Carrier concentration profiles obtained from CV measurements for the Sn-containing sample (left) and the reference sample (right) annealed at 725 $^{\circ}\text{C}$. The color code is maintained throughout the figure. Middle: Admittance spectroscopy data for 1 MHz and 0 V from the same samples. Left: Low-temperature region, the data for the Sn-containing sample were multiplied by a factor of 100 to enable a comparison of the peak position with the reference sample. Right: High-temperature region. The peaks are labeled as in the top part. Bottom: Arrhenius plot from the admittance spectroscopy data shown in the middle graph. The determined activation energies are given in the figure. Peak B gives the same activation energy within experimental uncertainty for both the reference sample and the one containing Sn.

donors in the SiSn and the reference samples. The donor observed in the SiSn layer clearly depends on the presence of Sn. On the origin of the donor in the reference sample, we can only speculate.

We know from secondary ion mass spectrometry (SIMS) measurements that the sample contains $(1.0 \pm 0.3) \times 10^{17} \text{ cm}^{-3}$ of oxygen and $\sim 2 \times 10^{17} \text{ cm}^{-3}$ of carbon. When looking at these impurities as potential origin of the observed donor B, these values can be considered moderate in the case of oxygen and high in the case of carbon.³¹ In our previous study, DLTS measurements showed a high concentration of deep levels in the reference sample, which most likely belong to metallic impurities.³⁶ Furthermore, the low growth temperature of the layer at $0.6 \mu\text{m}$ is expected to create many vacancies and nucleation centers for cluster defects. Since donor B is located exclusively in this layer, this appears to be a crucial condition for the donor formation in the reference sample.

Donor creation by cluster formation is especially known from oxygen in silicon, which forms thermal donors (TDs) at lower temperatures^{27–29} and new donors (NDs) after long-time annealing at temperatures above 600°C .^{30–35,37} The observed admittance spectroscopy peak with an activation energy of 55–70 meV is in agreement with the known energy levels for both TDs (50–150 meV)^{38,39} and NDs (30–120 meV).³⁵ TDs, however, are only stable for annealing temperatures below 600°C ,^{37–40} and NDs need very long annealing times in the order of 10 h or more.^{30,31,33,37} Furthermore, usually much higher oxygen concentrations than those present here are reported for both TD and ND formation.^{26,28–31,33,37} How strongly these requirements could be diluted by the presence of growth-related nucleation centers is at the moment a matter of speculation.

In the Sn-containing sample, only a small signal belonging to the donor observed in the reference sample can be observed in the admittance spectroscopy data (see Fig. 2) and not in all samples. Instead, another type of donor is observed, which is clearly Sn related. Previous studies of Sn-doped Si have not reported any

signs of this donor.^{21–24} The difference in the samples used in the previous studies and in our investigation is (i) the higher Sn concentration used in our samples, above the solubility limit of Sn in Si, and (ii) the growth via low-temperature MBE of the samples used in the present study. These two conditions point toward a complex microscopic structure as an origin of the donor state, which involves multiple Sn atoms and may be dependent on the presence of nucleation centers, as is also the case for the oxygen clusters creating TDs and NDs.

That a high concentration of Sn is critical to the donor formation is further underlined by the data shown in Fig. 3. While a sample with lower Sn content (0.3%) shows no measurable donor concentration after 20 min annealing at 725°C , a sample with a high Sn content of 5.0% contains $(1.40 \pm 0.05) \times 10^{18} \text{ cm}^{-3}$ donors. It should be noted that in the sample containing a large amount of Sn a high donor concentration was already observed after annealing at 600°C .

For the sake of completeness, it should be noted that segregation of Sb in the SiSn layer can be excluded as the origin of the increased donor concentration. It has been reported that Sb segregates away from compressive-strained layers,⁴¹ and both the high activation energy of 300–500 meV and the changes of the donor concentration with annealing temperature do not match those of the Sb shallow donor.

III. PROPERTIES AND FORMATION OF THE TIN DONOR

To gain further insight into the formation and the origin of the observed donor, the impact of annealing on the donor formation was studied in more detail. Figure 4 shows the impact of the annealing temperature. In Fig. 4(a), room-temperature CV profiles after 20 min annealing at different temperatures are displayed, shifted for clarity with a shift proportional to the annealing temperature. The flat part of the CV curves at larger reverse biases corresponds to the highly doped substrate. The CV curves annealed at temperatures between 650°C and 900°C show a plateau with varying extension. This plateau corresponds to the SiSn layer, with its length correlated to the donor concentration. The beginning of this plateau is marked as a guide to the eye.

Figure 4(b) shows the calculated donor concentration in the SiSn layer vs annealing temperature. The donor concentration was determined by fitting a simulated CV curve to the data, using the method described in Ref. 42, assuming a 10 nm wide SiSn layer. A detailed description of this process can be found in Sec. VI E. An example of a measured CV curve together with the fitted simulation is shown in the inset in Fig. 4(b). On each sample, several diodes were measured, and the statistical spread between those diodes is displayed as error bars.

The donor concentration in the SiSn layer shows a broad peak centered around 725°C , with a spike at 765°C . This shape hints toward a two-component process. To better resolve these components, isothermal annealing series at both 725°C and 765°C were performed. This shifts the thermal evolution times from the exponential into the linear regime. The results are shown in Fig. 5. The donor concentration shows two peaks, which we chose to label as SD I and SD II. The data taken at 765°C show a much faster change in donor concentration than that taken at 725°C . For a

FIG. 3. Donor concentration in the SiSn layer for different Sn concentrations after 20 min annealing at 725°C . The red dashed line marks the detection limit of the CV measurements.

FIG. 4. (a) CV curves at room temperature after 20 min annealing at different temperatures between 500 °C and 900 °C. The curves are shifted for clarity, with the shift proportional to the increase in annealing temperature. The kinks in the CV curves, which correspond to the end of the SiSn layer, are also marked by black dots. (b) Normalized donor concentration vs annealing temperature in the SiSn layer, calculated after Ref. 42. The red dashed line marks the detection limit of the CV measurements. The inset shows an example CV curve with the fitted simulation.

better comparison with Fig. 4(b), the vertical dotted line highlights the annealing time of 20 min used in the isochronal study. One can see that the initial part of the peak in Fig. 4(b) is due to SD I, whereas the sudden spike and the subsequent reduction in donor concentration stem from SD II.

These findings agree with the model proposed above, namely, the formation of Sn clusters which create donor levels in silicon. Other known Sn-related defects, i.e., the SnV pair^{21–24} and Sn nanocrystals,^{36,43,44} do not match the observed behavior. SnV pairs anneal out at temperatures below 600 °C^{21–24} and cannot explain the two-component evolution seen in the isothermal studies. The nanocrystals appear after annealing at 600 °C, but undergo no significant changes up to annealing temperatures of 900 °C,^{36,44} whereas a strong dependence on the annealing temperature is observed for the Sn donor.

The SiSn layer is under compressive strain due to the presence of the large Sn atoms. At the same time, the layer can be assumed

FIG. 5. Donor concentration in the SiSn layer for samples annealed at 725 °C and 765 °C vs annealing time.

to be rich in vacancies due to the low growth temperature. Since Sn diffusion is enhanced by the presence of vacancies⁴⁵, the annealing steps will lead to significant movement of the Sn atoms in the SiSn layer. As mentioned above, Sn aggregates into Sn nanocrystals at temperatures above 600 °C to relieve the strain.

The exact mechanism of the formation and geometry of the clusters proposed for the donor activity is at this point mostly speculation. Drawing inspiration from TDs and NDs,^{25–35} Sn atoms could form chainlike structures, assisted by SnV pairs, or form loose precipitates, which act as donors. Since the donor activity cannot be directly correlated to the presence of the Sn nanocrystals with ~1000 atoms inside each nanocrystal, the former hypothesis seems more likely.

The double-peak shape of the donor concentration vs annealing time indicates either the formation of two distinct donor complexes or the evolution of one into another. The latter hypothesis agrees well with the Sn cluster model, where evolving clusters first form the first donor (or donor group) SD I and then SD II with an electrically inactive intermediate stage. Similar effects are known from oxygen-related thermal donors, where up to 17 different types of donors are formed through the evolution of oxygen clusters.^{26,28,29}

IV. CORRELATION OF THE TIN DONOR TO PHOTOLUMINESCENCE RESULTS

The dependence of the donor concentration on the annealing temperature bears some similarity with that of the long-lifetime infrared emission observed from Si containing Sn precipitates reported previously.⁴⁴ Therefore, we investigated time-resolved emission spectra (TRES) vs annealing temperature and time to compare the light emission to the donor concentration. For this comparison, samples from the same wafer as for the electrical characterization were used. The results are shown in Fig. 6.

Figure 6(a) shows the long-lifetime part, from 4000 to 9000 ns, of the spectra of the samples annealed at 765 °C for the indicated times. The spectra are normalized to the intensity of the 1148 nm Si peak at short lifetimes, to account for differences in intensity due to slightly different collection adjustments. The lifetimes of the 1148 nm lines are nearly identical, confirming that different intensities do not stem from differences in crystalline quality created during the annealing. The spectra show a broad IR luminescence signal, similar to the one reported in Ref. 44. Comparing the different spectra, it seems that the maximum of the peak shifts to higher energies with increasing annealing time.

Figure 6(b) shows the integrated luminescence intensity from 0.775 eV to 1.0 eV as a function of the annealing time, compared with the donor concentration for the same annealing temperature. The maximum luminescence intensity is reached before SD I has reached its maximum concentration and drops very fast. The same effect can be seen when comparing luminescence intensity vs annealing temperature [see Fig. 6(c)], where the maximum luminescence intensity is reached for an annealing temperature of 700 °C.

FIG. 6. (a) TRES of SiSn samples annealed at 765 °C for the indicated times in minutes. Shown is the long-lifetime part of the spectrum, integrated from 4000 ns to 9000 ns after the excitation pulse. (b) and (c) Normalized integrated PL intensity from 4000 ns to 9000 ns between 0.775 eV and 1 eV (b) vs annealing time and (c) vs annealing temperature. For comparison, the normalized donor concentration is also shown.

From these results, we argue that the broad IR luminescence originates from early stages of Sn clusters, which will transform into the donors observed by capacitive measurements. The shift of the luminescence peak maximum also indicates an evolution of the underlying energy levels, in agreement with the model of evolving Sn clusters proposed above for the Sn donors.

V. TIN AS A DONOR: THE RELEVANCE TO THE FIELD OF GROUP IV ALLOYS

The results presented here show the formation of Sn-related donors in Si. Most of the work currently reported on the application of Sn-containing Group IV alloys though focuses on GeSn.^{1,3–15} However, Ge and Si respond similarly to impurities and defects. As an example, oxygen clusters form TDs both in Si^{27–29} and in Ge.^{25,26} Therefore, it seems reasonable to assume that similar Sn donors can also be found in GeSn.

The reported temperatures of above 600 °C for the donor formation are quite high, considering that due to Sn precipitation, the thermal budget for Sn-containing devices is relatively low. However, with increasing Sn content, even heat treatments at lower temperatures could create significant amounts of Sn donors. It is known that Sn diffusion happens via vacancy-assisted diffusion⁴⁵ and that compressive strain enhances vacancy-assisted diffusion of dopants.⁴⁶ From this, an enhanced Sn diffusion and, therefore, enhanced formation of Sn cluster donors can be assumed in alloys with higher Sn content. Indeed, the test sample containing 5.0% Sn showed high donor concentration already at lower annealing temperatures.

The effects of unintentional donor creation in device structures can be detrimental. For instance, the donors may arise in nominally intrinsic layers during processing. Such layers are typically used in the active region of lasers, light-emitting diodes (LEDs),^{9,10,47} and photodiodes.^{11,12} These devices employ p-i-n diodes to enhance carrier collection in/from the active region. A transformation of these layers into moderately to highly doped n-type would drastically change the band alignments across the diode, reducing the efficiency of light emission and detection.

Likewise, the donors could cause (over-)compensation of p-type doping. Basically all devices are based on variations of pn junctions. The worst case scenario here would be the transformation of the p-type region into n-type, removing the diode structure and rendering the device useless.

In conclusion, the unexpected role of Sn as a donor in Si is not only a fascinating insight into complex defect physics in semiconductors, but the transformation of an isovalent alloy component into a donor species through clustering also has wide-ranging consequences for device design and processing.

VI. METHODS

A. Materials

Wafers were grown using molecular beam epitaxy (MBE) on highly doped n-type Si substrates. A thin undoped SiSn layer (10 nm) with a Sn concentration of ~1.4% was grown at low temperature (200 °C) to enable Sn incorporation into the Si lattice. It is separated from the substrate by an Sb-doped buffer layer of 1000 nm thickness and overgrown with an Sb-doped capping layer

of either 600 nm or 1200 nm thickness, with a nominal doping density of $5 \times 10^{15} \text{ cm}^{-3}$. Both buffer and capping layer were grown at 500 °C. The reference sample was prepared with the same dimensions and growth temperatures, but without the addition of Sn into the low-temperature grown layer.

Samples cut from the same wafer were heat treated in an argon atmosphere either for 20 min at temperatures between 500 °C and 900 °C or for times varying from 45 s to 2 h at 725 °C and 765 °C. After the heat treatment, the native oxide layer was removed by an HF dip and Au Schottky contacts were thermally evaporated. The ohmic contact was formed by eutectic InGa on the backside of the samples. The diode quality was tested by room-temperature current-voltage measurements.

B. Compositional determination by SIMS

To determine the concentrations of C, O, and Sn in the MBE grown layers, secondary ion mass spectrometry (SIMS) was performed in an ION-TOF SIMS 5 instrument. To calibrate the system for carbon and oxygen measurements, reference samples were measured where the respective concentrations were beforehand determined by low-temperature FTIR. The Sn concentration was calibrated on reference samples with a Sn concentration known from Rutherford back-scattering spectrometry.

C. Capacitance-voltage measurements

The doping profiles were recorded by capacitance-voltage (CV) measurements. For the CV measurements shown in this study, the samples were measured at room temperature in one session to avoid temperature fluctuations. The CV measurements were performed on an Agilent 4284 A LCR meter at 100 kHz sampling frequency and with 100 mV test signal.

D. Admittance spectroscopy measurements

Admittance spectroscopy was performed on selected samples in a closed-cycle He cryostat at temperatures between 300 and 25 K. The capacitance and conductance of the samples were measured with an Agilent 4284 A LCR meter, and the frequency was varied between 10 kHz and 1 MHz. In admittance spectroscopy, the real part (the conductance G) of the complex admittance is measured as a function of temperature and frequency f . Deep defects contribute to the conductance if the test frequency is slower than their emission rate at this temperature. This leads to a peak of G/f when the frequency matches the emission rate.

E. Doping profile simulations

As the investigated samples contain a very small region of interest, which is thinner than the Debye length, and sharp changes in doping concentrations over several orders of magnitude, the doping profiles obtained by the standard method of analyzing the slope of $1/C^2$ will show broadened features with peak/valley values different from the actual doping densities. To obtain correct doping densities in the SiSn layer, a CV curve was simulated using the process outlined in Ref. 42, which will be briefly explained here.

The simulation algorithm analyses the propagation of the potential ψ and the electric field $E = -d\psi/dx$ from the interface

of the Schottky diode into the bulk of the sample. The starting value for ψ at the interface is given by the applied voltage plus the built-in potential (set to 0.8 V) of the diode. The starting value of the electric field $E(0)$ at the interface is guessed.

The electric field is then numerically calculated stepwise into the bulk according to

$$\frac{dE}{dx} = \frac{q}{\epsilon} [N(x) - N(\infty)e^{-q\psi/kT}], \quad (1)$$

with q being the elementary charge, ϵ being the semiconductor permittivity, k being the Boltzmann constant, T being temperature, and $N(x)$ being the net density of ionized donor ions. $N(x)$ is given as a series of rectangular doping distributions with the position of the steps known from the growth process and the initial concentrations estimated as $1 \times 10^{15} \text{ cm}^{-3}$ (capping layer), $2 \times 10^{17} \text{ cm}^{-3}$ (SiSn layer), and $1 \times 10^{14} \text{ cm}^{-3}$ (buffer layer) and the substrate concentration fixed at $2 \times 10^{18} \text{ cm}^{-3}$. From E the potential is calculated, and $E(0)$ varied so as to fulfill the boundary condition that ψ has to converge to 0 deep in the bulk. This process is repeated for a number of voltages so that an array of V, E pairs is generated. The capacitance C for each voltage point can then be calculated using the approximate differential

$$C = \epsilon \frac{\Delta E(0)}{\Delta V}. \quad (2)$$

The generated CV curve is then compared to the measured data, and the concentrations in the capping, SiSn, and buffer layers are varied until the best fit is obtained.

F. Photoluminescence measurements

The optical investigations were performed in a setup identical to the one used in Ref. 44. The samples were cooled down to 16 K and were excited by a short laser pulse with a wavelength of 400 nm and a pulse duration of ~ 35 fs. The light emitted from the sample was investigated using a monochromator and a photo-multiplier tube.

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