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Donor complex formation due to a high-dose Ge implant into Si

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To investigate boron deactivation and/or donor complex formation due to a high-dose Ge and C implantation and the subsequent solid phase epitaxy, SiGe and SiGeC layers were fabricated and characterized. Cross-sectional transmission electron microscopy indicated that the SiGe layer with a peak Ge concentration of 5 at. % was strained; whereas, for higher concentrations, stacking faults were observed from the surface to the projected range of the Ge as a result of strain relaxation. Photoluminescence (PL) results were found to be consistent with dopant deactivation due to Ge implantation and the subsequent solid phase epitaxial growth of the amorphous layer. Furthermore, for unstrained SiGe layers (Ge peak concentration $\geqslant$7 at. %), the PL results support our previously proposed donor complex formation. These findings were confirmed by spreading resistance profiling. A model for donor complex formation is proposed.

Alloys of silicon and germanium are promising materials for use in the fabrication of high-performance devices in the future. Fabrication of Si-based heterojunction bipolar transistors (HBTs) and *p*-channel metal-oxide-semiconductor field-effect transistors (MOSFETs) using ultrahigh vacuum chemical vapor deposition (UHV-CVD) and molecular beam epitaxy (MBE) for the epitaxially grown SiGe layer have been reported.[1] SiGe devices have also been fabricated in layers formed by high-dose Ge implantation followed by solid phase epitaxy.[2] The potential advantage of implantation over UHV-CVD, MBE, and other epitaxial growth processes lies in its compatibility with standard silicon fabrication procedures and its convenience in selective area growth. However, formation of SiGe layers by high-dose Ge implantation presents some problems. With this process, extrinsic dislocation loops are formed during implantation due to excess recoiled Si interstitials. Additionally, a high Ge dose induces a lattice strain in the regrown SiGe layer, resulting in the formation of surface defects (stacking faults).[2,3] These defects degrade the performance of the devices formed in this layer. Compared to room-temperature implantation, Ge implantation performed at low temperature is reported to result in a reduction of the dislocation loops. Also, sequential implantation of C following Ge results in a reduction of stacking faults due to strain compensation.[2,3] In a previous study, we reported boron deactivation and/or donor complex formation due to high-dose Ge implantation.[2] In this communication, we report further characterization of Ge-implanted SiGe and Ge and C-implanted SiGeC layers by photoluminescence (PL), cross-sectional transmission electron microscopy (XTEM), and spreading resistance profiling (SRP) methods. The results are found to be consistent with previously reported electrical characteristics of SiGe devices.[2]

SiGe and SiGeC layers were fabricated by performing high-dose Ge and C implantation into 10 Ω cm *n*-type Si ⟨100⟩ substrates. The Ge implantation was performed at liquid-nitrogen temperature. A range of Ge dose from 2×10^{16} to 5×10^{16} cm^{-2} was used. An ion beam energy of 120 keV was used to obtain a 170-nm-thick amorphous layer with a peak Ge concentration ranging from 5 to 12 at. %. Carbon implantation was subsequently performed in one sample at room temperature with a dose of 2×10^{15} cm^{-2} and an energy of 20 keV to obtain a peak concentration of 0.5 at. % and a projected range (R_P) of about 65 nm. Rutherford backscattering spectrometry (RBS) results indicate that the R_P for Ge is about 70 nm. All samples were annealed at 800 °C for 1 h in nitrogen ambient to regrow the amorphous layer. Table I shows the implant conditions for the samples used in this study. Sample 1 is the Si control.

In a previous study, we had suggested boron deactivation and/or donor complex formation due to Ge implantation into Si was a cause.[2] In an effort to further investigate these findings which were based on capacitance-voltage (*C-V*) characteristics of n^{++}-p^{+} diodes formed in the SiGe layer, all five samples were characterized. Cross-sectional transmission electron microscopy was performed on all samples except the Si control (sample 1).[3] The XTEM results of samples 2 and 3 indicated that there are no surface defects for sample 2, whereas the strained SiGe layer in sample 3 relaxes to produce stacking faults from the surface to R_P. The diffraction pattern and the image along the [110] zone axis for sample 4 are shown in Fig. 1. Since the Ge dose is higher for this sample than for sample 3, the density of surface defects is expected to be larger, which is confirmed by XTEM images.[3] Due to strain compensation by the carbon, the image from sample 5 indicated a reduction in surface defects compared to sample 4.[3]

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TABLE I. Implant conditions for samples.

Sample	Ge dose ($\times 10^{16}$ cm^{-2})	Peak Ge (at. %)	Peak C (at. %)
1	0	0	0
2	2	5	0
3	3	7	0
4	5	12	0
5	5	12	0.5

Preliminary results of photoluminescence measurements performed on the samples are shown in Fig. 2. The excitation was provided by an argon ion laser with a wavelength of 514.5 nm. The laser beam diameter was 2 mm, and the incident power was kept constant at 500 mW. The temperature was maintained at $\sim$10 K. The results seem to indicate that Ge implantation results in phosphorus deactivation as well as dopant complex formation. It has been reported that boron and phosphorus concentrations in silicon can be estimated by computing the ratio of the dopant peak intensity to the intrinsic peak intensity for the bound and for the free excitons, respectively.[4] The emission lines for boron and phosphorus, as well as for intrinsic silicon, are banded together around 1.09–1.10 eV. Due to the higher temperature ($\sim$10 K) as well as a larger photon energy step (0.62 meV) used in this study compared to that of Tajima's study,[4] the individual peaks could not be resolved. Thus, we were unable to estimate the phosphorus concentration from our PL results, even for the Si control sample. However, as indicated by Tajima and other authors,[5,6] the dopant peak intensity far exceeds the intrinsic peak intensity for doping concentrations greater than $\sim 10^{14}$ cm^3. The PL peak heights shown in our study may not precisely quantify dopant concentration, but it is reasonable to assume that these heights vary directly with dopant concentration. Thus, assuming that the emission line due to the dopant complexes also lies in the same energy range (shallow dopant complex), the maximum peak intensities of our samples were compared. The peak height of sample 2 is less than that of the Si control (sample 1). This may be attributed to dopant deactivation due to Ge implantation. One expects that the extent of dopant deactivation would somewhat depend on the Ge dose, and an increase in the Ge dose would result in an increase in the deactivation. Contrary to this reasoning, and as can be seen for sample 3, the efficiency of the PL response increases, as shown by the increase in the peak intensity. We believe that the degradation of the quality of the material due to ion implantation is not the primary cause for the reduction of the PL peaks in samples 2 and 3, otherwise, the PL response of sample 3 would have been weaker compared to that of sample 2, which has better crystalline quality than sample 3, as verified by XTEM.[3] This increase may be attributed to a compensation of phosphorus deactivation by the formation of dopant complexes resulting from strain relaxation. For samples 4 and 5, the peak intensity increases by about two orders of magnitude, supporting the fact that once the critical Ge dose for strain relaxation is exceeded ($\sim 3\times 10^{16}$ cm^{-2}), any further increase in the Ge dose results in a significant increase in net dopant concentration.

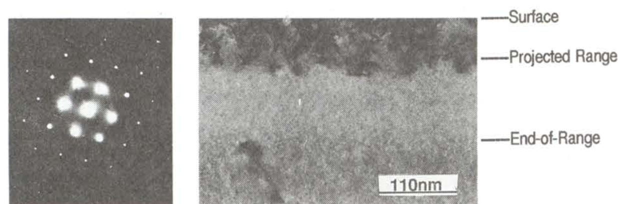

FIG. 1. Diffraction pattern and image along the [110] zone axis for sample 4.

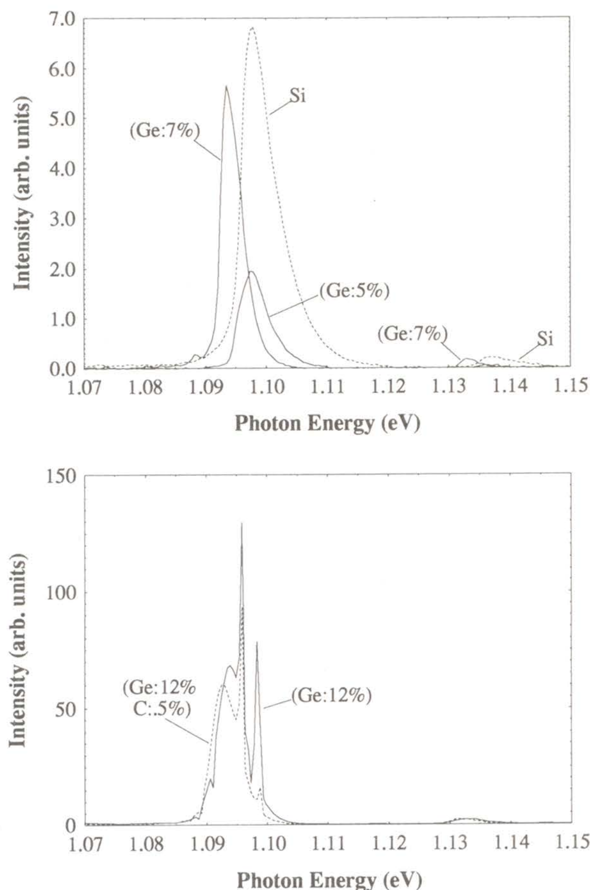

FIG. 2. PL spectra for Si, SiGe, and SiGeC samples.

To verify the formation of dopant complexes and to determine if it was donor or acceptor, SRP measurements were performed. The results are shown in Fig. 3. A hot-point probe was used to ascertain that all samples remain n type after Ge and C implantation. The profile for sample 1 is not shown since it is the starting Si wafer and has a constant resistivity. For the SiGe and SiGeC samples, the majority electron concentration was estimated from the resistivity profile assuming that the free carrier mobility is the same as that in Si. In reality, the mobility of carriers in these strained layers will be somewhat lower than that in crystalline Si. However, resistivity changes amounting to approximately 2 orders of magnitude cannot be attributed

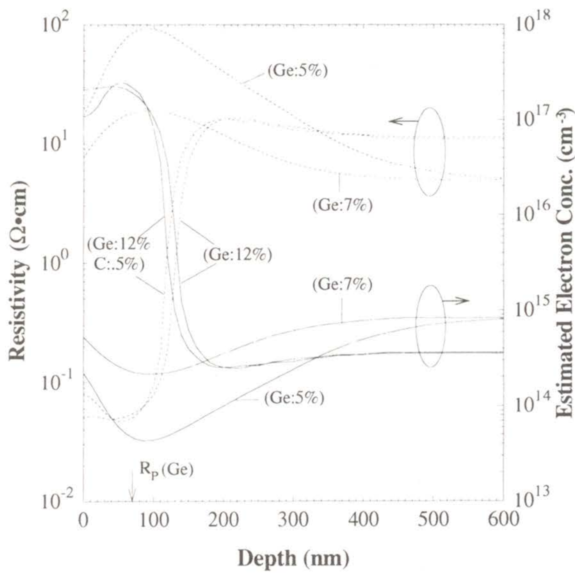

FIG. 3. Resistivity profiles obtained from SRP. Estimated electron concentration profiles calculated from the resistivity profiles, assuming free carrier mobility to be same as in Si.

to mobility changes alone since such a change would be far greater than any expected or reported change in mobility. The resistivity for sample 2 around the projected range of the Ge ions is higher than the bulk resistivity by about an order of magnitude. Since this change is larger than the expected change in mobility for this alloy,[1] it can once again be attributed to phosphorus deactivation due to the Ge implant into Si. The decrease in resistivity for samples 3, 4, and 5 correlates very well with the PL results, thus confirming the formation of donor complexes.

A model for donor complex formation is shown in Fig. 4. The correlation between XTEM and SRP/PL results indicates that donor complexes are formed via the strain relaxation associated with the formation of misfit dislocations. These defects then combine with the interstitial impurities present in silicon, e.g., oxygen, to result in a donor complex. Even though the defects themselves are expected to act as trap sites, the PL results seem to indicate that the donor complexes are shallow. This is illustrated in the energy band diagram in Fig. 4. XTEM results for sample 5 show a reduction in the defect density due to the strain compensation by C implantation. This should result in the reduction of donor complex formation. However, as seen by the SRP results, there is little change in the resistivity

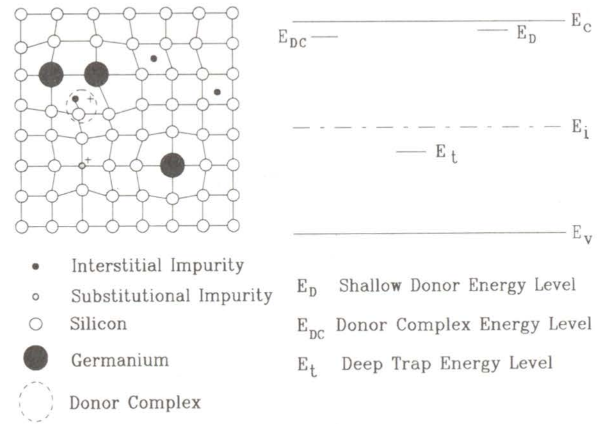

FIG. 4. Model for donor complex formation.

and, hence, the net donor concentration. This suggests that for high doses of Ge, the interstitial impurity concentration might be a limiting factor for donor complex formation.

Results of SRP and PL measurements performed on SiGe and SiGeC specimens support the earlier investigation using *C-V* measurements that suggested a dopant deactivation due to the high-dose Ge implantation into Si. Furthermore, once the critical Ge dose for strain relaxation is exceeded, shallow donor complexes seem to be formed in the SiGe layer from the surface to the projected range of the Ge. Any increase in the Ge dose beyond the critical dose appears to result in a significant increase in net donor concentration.

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