CHARACTERIZATION OF GE OUTDIFFUSION AND SI CAP THICKNESS IN STRAINED SI/SIGE STRUCTURES BY SIMS

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Abstract. The outdiffusion of Ge from the SiGe underlayer into the thin Si cap layer in strained Si/SiGe material systems can affect the mobility of carriers in the channel, and in extreme cases the channel thickness or even the gate oxide integrity. This outdiffusion can be affected by epi growth temperature, rate and source gas, as well as by point defects at the Si/SiGe interface. The Si cap layer is very thin, on the order of 10 nm, such that the required depth resolution information of Ge outdiffusion is very challenging. This paper focuses on the SIMS measurement of the Ge outdiffusion and the Si cap thickness, and the accuracy and precision of the Ge measurement.

INTRODUCTION

Strained Si on relaxed SiGe is a promising candidate for mobility enhancement of carriers in the Si channel of CMOS devices [1]. The Si channel strain, defect density, interface roughness, dopant concentration, thickness and purity are all important parameters to measure and subsequently control. Ge outdiffusion from the relaxed SiGe underlayer into the top strained Si cap can affect both the effective thickness of the channel and the purity of the channel. In addition, the Ge mole fraction in the relaxed SiGe can affect the channel strain. Accurate and precise characterization of both the Ge outdiffusion profile and the Ge content of the relaxed SiGe layer is essential.

The Ge outdiffusion into the strained Si channel can be affected by the Si epi growth temperature, growth rate, and source gases, as well as post-epi processes that may subsequently enhance Ge diffusion. Examples of the latter are defect-creating processes such as implantations followed by thermal anneals, because Ge diffusion can be greatly affected by point defect densities.

For the semiconductor device manufacturing industry to adopt this strained Si technology widely, significant effort will be required to characterize the relationship between process variables and the resulting film characteristics. Optimal process design also requires manufacturers to focus on associated economic factors in addition to the film performance in the devices. For instance, parameters such as growth rate will have

significant effects upon the cost of the processing. The accurate characterization of the film as a function of growth conditions will help manufacturers obtain the highest degree of performance/cost ratio.

Secondary Ion Mass Spectrometry (SIMS) is a key characterization tool that can measure both the Ge outdiffusion into the strained Si channel and the Ge mole fraction in relaxed SiGe. SIMS is best known for measuring dopant and impurity distributions and concentrations in Si semiconductors. In these cases the elements to be measured are typically in the ppba to ppma concentration range. The use of SIMS to measure matrix level compositions is less well known, and requires different technology in terms of reference materials, protocols, and data processing in order to make the measurement accurate and with acceptable precision. In addition, with appropriate SIMS instrumentation and protocols it is possible to accurately measure the strained Si channel thickness on monitor wafers.

This paper focuses on the SIMS measurement of the Ge outdiffusion and Si cap thickness, and the accuracy and precision of the Ge measurement.

SIMS TECHNOLOGY

In SIMS a focused primary ion beam (e.g., O_2^+, Cs^+) sputter erodes the surface of a sample resulting in the emission of secondary particles (elemental ions, molecular ions, neutrals). The secondary ions are then mass analyzed by a magnetic sector, quadrupole, or time-of-flight mass spectrometer. The primary ion beam species (e.g., Cs^+) and its impact energy (e.g., 700 eV) and angle of incidence (e.g., 60°) are important factors in optimizing the depth resolution for measuring the Ge outdiffusion into a thin (~10 nm) strained Si cap. Precision of the outdiffusion measurement is affected by the ion collection optics and data processing procedures, and the procedures for accurately measuring the sputter rate. The latter is non-trivial because one cannot measure a shallow crater accurately by conventional techniques. In addition, the surface of the strained Si channel on relaxed SiGe is not fully flat due to residual cross-hatch undulations, even if an intermediate CMP step is used in the SiGe epi growth process.

The technology issues facing the accurate and precise measurement of Ge mole fraction in the SiGe relaxed layer are further discussed in the sections on the SIMS measurement of Ge.

SIMS MEASUREMENT OF GE OUTDIFFUSION

Figure 1 shows the SIMS profile for Ge, O and C, at the interface of a thin strained Si cap on a relaxed SiGe layer. The Si cap is 19.1 nm in this case and the Ge mole fraction in the relaxed SiGe layer is 19.9%. The sharpness of this interface is determined by the slope of the Ge profile which in this case is 0.6 nm per decade of change in the Ge signal. The width of this measured interface is affected both by the primary ion beam mixing from SIMS and by the epi growth process. This particular sample was grown under specific conditions in order to minimize the effect from the epi growth process. The SIMS measurements were acquired using a Physical Electronics Adept 1010 quadrupole SIMS instrument, and using a Cs^+ primary ion beam impacting the surface at 700 eV and 60°.

Figure 1 also shows the SIMS profile for C and O. The C and O in the Si cap is an artifact from the ion beam mixing of surface C and O, with the difference in slope being caused by a Cs^+-induced segregation of the C during the sputtering process. The O and C levels in the deeper relaxed SiGe layer are background levels from O and C absorption in the SIMS chamber, and are not actual concentrations in the SiGe. However, if there had been C and/or O at the Si/SiGe interface above background levels, the SIMS profile would have shown a "spike" of O or C at that interface. Obviously, the ability to detect such spikes depends on how low the backgrounds are, something that can vary significantly with instrumentation and analysis protocols.

The work of Leitz *et al* [2] at AmberWave Systems Corporation illustrates of the value of this SIMS measurement of Ge, C, and O. While studying interfacial oxygen contamination, Leitz *et al* determined that by depositing the strained Si layer at 750^oC or higher, the oxygen spike could be eliminated. However, at these growth temperatures the interface abruptness was severely degraded with SiH_4 precursors, effectively reducing the Si thickness. As shown in Figure 2, by switching from SiH_4 (Gas A) to SiH_2Cl_2 (Gas B) precursors, extremely abrupt interfaces (<0.6 nm/decade) at 750^oC were achieved. This example demonstrates the ability of SIMS characterization to assist in the optimization of the cost of processing. Higher growth temperatures result in faster film growth. Thus, the SiH_2Cl_2 (Gas B) allows sharper interfaces, lower interfacial contamination, and faster film growth – higher performance at lower cost.

SIMS MEASUREMENT OF SI CAP THICKNESS

Figure 1 indicates the Si cap is 19.1 nm thick. This is taken from the SIMS profile assuming the 50% rise in Ge signal is the correct interface depth. The depth scale for

SIMS is normally determined by measuring the depth of the final SIMS crater, assuming a constant erosion rate, and measuring the total time of the SIMS profile. In very shallow SIMS craters the method for measuring the crater depth, i.e., a profilometer, has significant precision problems. An alternative is to determine the sputter rate using a SIMS thickness reference sample. This procedure significantly improves the precision of the sputter rate determination.

There is another SIMS issue to consider in measuring the Si cap thickness, and that is the erosion rate can be a function of the Ge mole fraction. An example of experimental data showing such an effect can be seen in Figure 3. Up to about 20% Ge mole fraction the effect is negligible. From 20% to 100% Ge mole fraction there is a linear increase in sputter rate of about 40%. The dependence of the sputter rate on composition is a function of the SIMS analysis conditions, and must be characterized for each distinct condition used. Once determined, the sputter rate dependence upon the Ge mole fraction can be implemented into a point-by-point correction using appropriate data reduction software.

The overall result is the Si cap thickness can be measured accurately, and with precision of $\pm$ 0.2 nm.

ACCURACY OF SIMS MEASUREMENT OF GE

In the SIMS technique, ion counts are converted to concentration using Relative Sensitivity Factors (RSFs). RSFs are determined using reference samples of known composition and impurity content.

For traditional Si semiconductors the RSFs are normally determined from SIMS analysis of reference materials made from implanting elemental ions (e.g., B, P, As, O, C, Fe, Cu, etc.) of known doses into a Si substrate. For a compound semiconductor, such as GaAs, this procedure is also used effectively.

However, for a semiconductor alloy, such as SiGe, this procedure can have problems if the alloy composition (mole fractions of Si and Ge) is either (a) different from the reference material or (b) varies within the sample to be analyzed. The reason for this problem is the ion counts (really the ion yield) generated from a species in a SiGe matrix can be different depending upon the Ge mole fraction. Therefore, an RSF for B or P determined from a $Si_{0.7}Ge_{0.3}$ alloy reference material may not be accurate for B or P in a $Si_{0.5}Ge_{0.5}$ alloy. Likewise, if the Ge mole fraction changes within a sample, the RSF for B or P determined from a $Si_{0.7}Ge_{0.3}$ alloy reference material may be accurate in some parts of the sample but not others.

The solution to this problem is to determine RSF functions (rather than a single value) where the independent variable is the Ge mole fraction, and then to apply these functions on a point-by-point basis throughout the SIMS profile. The RSF functions can be experimentally determined by implanting elemental species of known doses into a range of $Si_{1-x}Ge_x$ materials, measuring the RSFs in each SiGe sample, and then fitting the RSF versus mole fraction (x) data with a correlation curve. The accuracy of this function will be affected by the variability of the individual data points. One way to improve on the accuracy of the RSF functions is to develop models of the functions which are then used in the fitting of the data.

The situation with accurately measuring the Ge mole fraction by SIMS is similar except Ge ion implants into Si are not the best approach to making the reference materials. In this case, bulk (or epi-grown) $Si_{1-x}Ge_x$ materials are best, where x is varied from reference material to reference material. The assignment of the Ge mole fraction in this case cannot be done via an implant dosimeter, but must be made by a separate, and preferably standard-less technique, such as Rutherford Backscattering Spectrometry (RBS) or X-Ray Diffraction (XRD). For our work we are interested in RSF functions for Ge mole fractions from 0 to 1, because of the wide range of Ge mole fractions that we see in our work. RBS meets this requirement, whereas the need for experimental corrections to Vegard's Law at $x > 0.3$ makes XRD uncertainties greater.

Figure 4 shows an example of the variation in the normalized Ge RSF with Ge mole fraction (x determined by RBS) for $Si_{1-x}Ge_x$ where x varies from 0.1 to 0.6. The exact form of the relationship again depends upon the analytical conditions that are used, in this case a Cs^+ primary ion beam impacting the surface at 3 keV and 25°. The data are fit with a function which can then be implemented into data processing software for a point-by-point calibration of Ge in a test sample of $Si_{1-x}Ge_x$.

PRECISION OF SIMS MEASUREMENT OF GE

The long-term precision of the SIMS measurement of Ge in $Si_{1-x}Ge_x$ depends upon the analytical conditions and equipment used for the measurement. Figure 5 shows the long-term precision for a 110 nm box $Si_{1-x}Ge_x$ where x=14.45%, and for a 50 nm graded $Si_{1-x}Ge_x$ where x increases from 0% to 10%. A SIMS profile of each of these is shown in Figures 6 (Box) and 7 (Graded) respectively. The long-term relative standard deviation for both structures is $\pm$ 2.2%. These measurements were made using conditions that allow the measurement of other elements in the same profile. Improvements in the precision can be made if only Ge is measured.

CONCLUSION

SIMS can provide critical characterization of strained Si/SiGe structures and assist in the optimization of the process performance/cost ratio. The use of appropriate instrumentation and advanced protocols and data processing are essential for achieving the benefits of SIMS.

REFERENCES

1. *International Technology Roadmap for Semiconductors 2003 Edition*, Semiconductor Industry Association (2003).
2. Christopher Leitz, Vicky Yang, Mark Carroll, Thomas Langdo, Richard Westhoff, Christopher Vineis, and Mayank Bulsara, "A High-Throughput, Ultra-Low Roughness, SiGe-Free Strained Si Regrowth Process," Extended Abstract, 2nd International SiGe Technology and Device Meeting, May 16 - 19, 2004, Frankfurt (Oder), Germany.

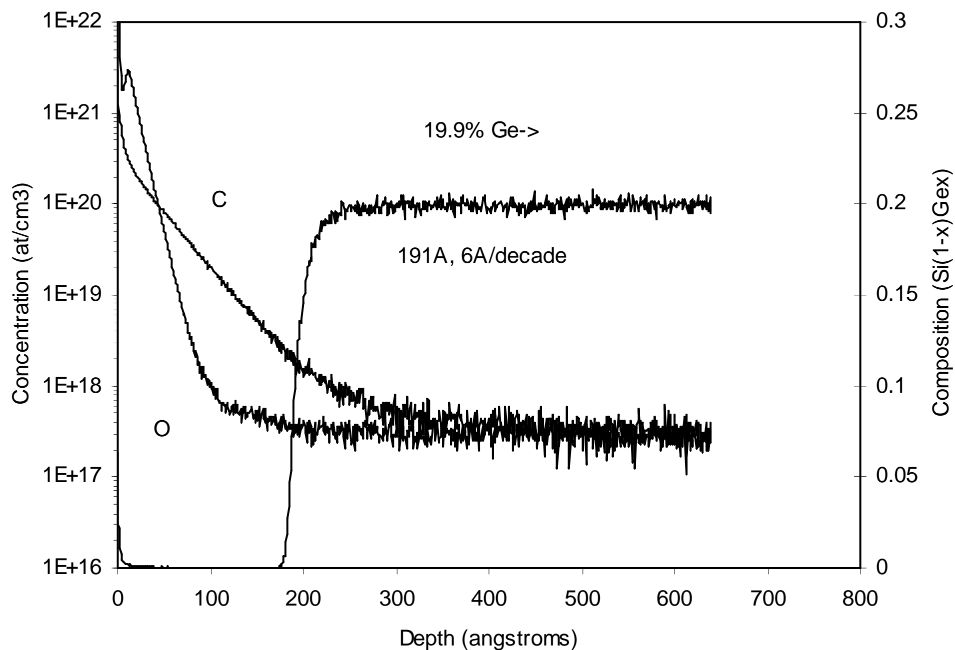

Figure 1. Ultra Low Energy SIMS profile of a strained Si on SiGe buffer layer. A single profile can demonstrate the thickness of the strained Si cap, Ge composition, interface abruptness, and atmospheric contamination with high sensitivity.

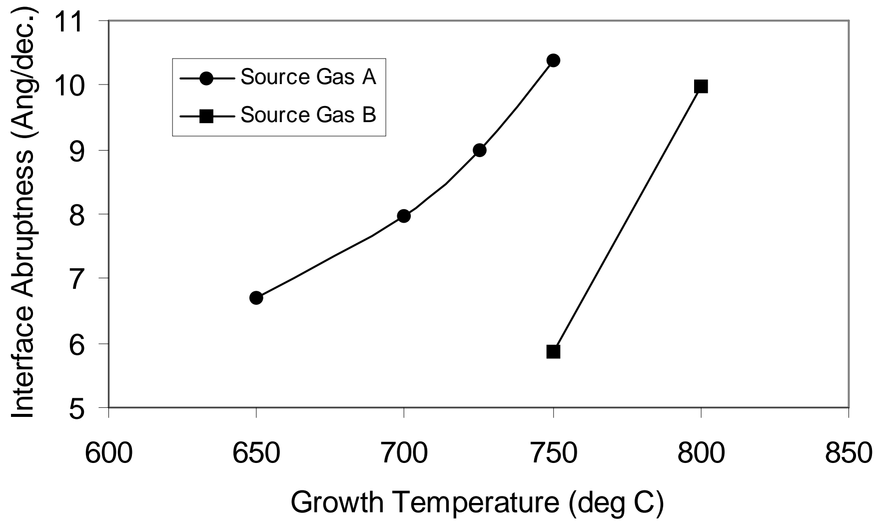

Figure 2. Interface Abruptness versus growth temperature and source gas (A=SiH_4, B=SiH_2Cl_2) [2]

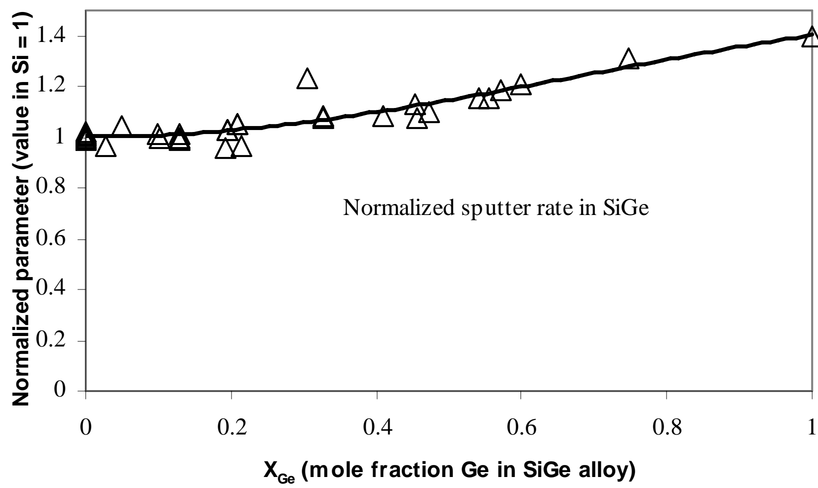

Figure 3. Normalized sputter rate versus the mole fraction of Ge in the SiGe alloy. (2 keV Cs^+ bombardment at 60° angle of incidence.)

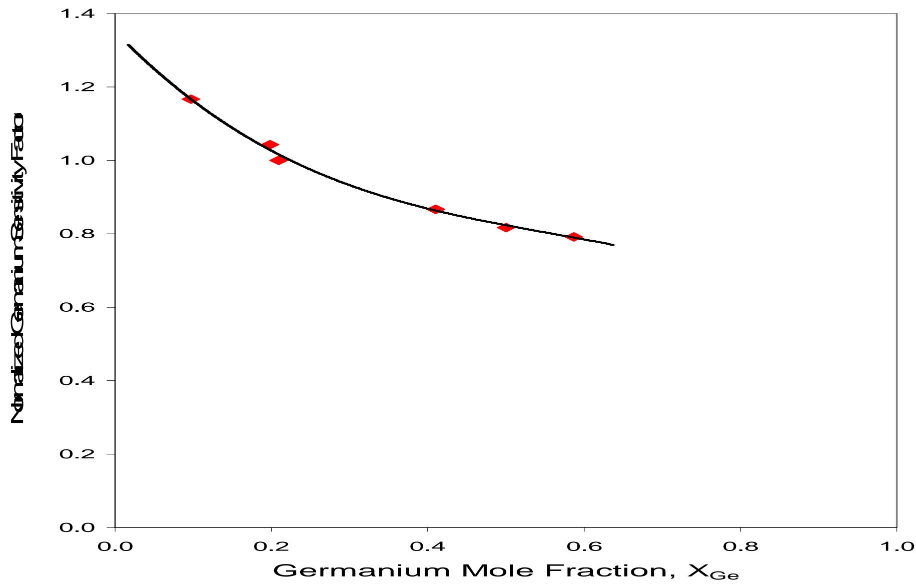

Figure 4. Normalized Relative Sensitivity Factor (RSF) for Ge versus the Ge mole fraction in $Si_{1-x}Ge_x$. The Ge mole fraction was determined by RBS.

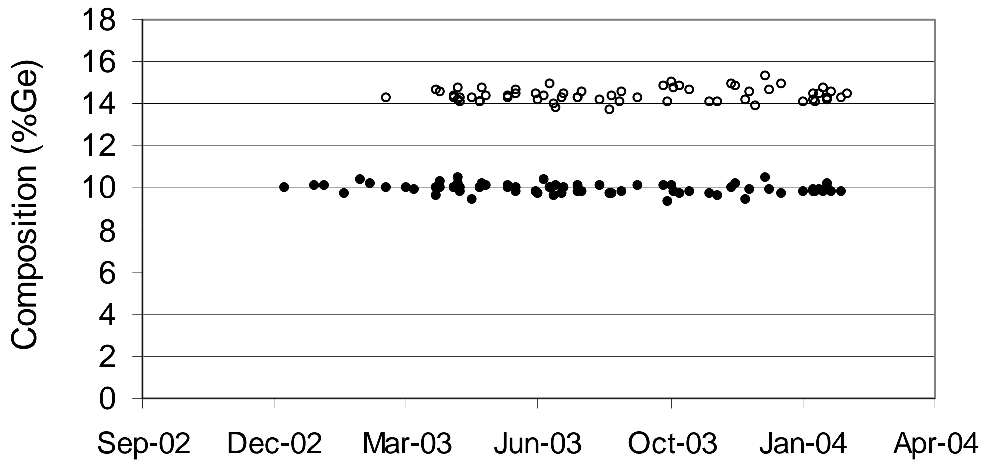

Figure 5. Long-term reproducibility of Ge composition. (Open circles, 14.45% SiGe box control sample; filled circles, 0-10% SiGe grade control sample – maximum value plotted)

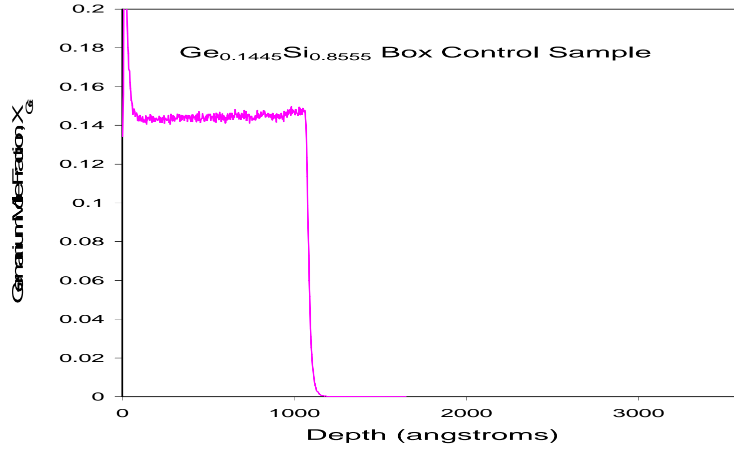

Figure 6. One SIMS profile of a 110 nm box $Si_{1-x}Ge_x$ where x=14.45%.

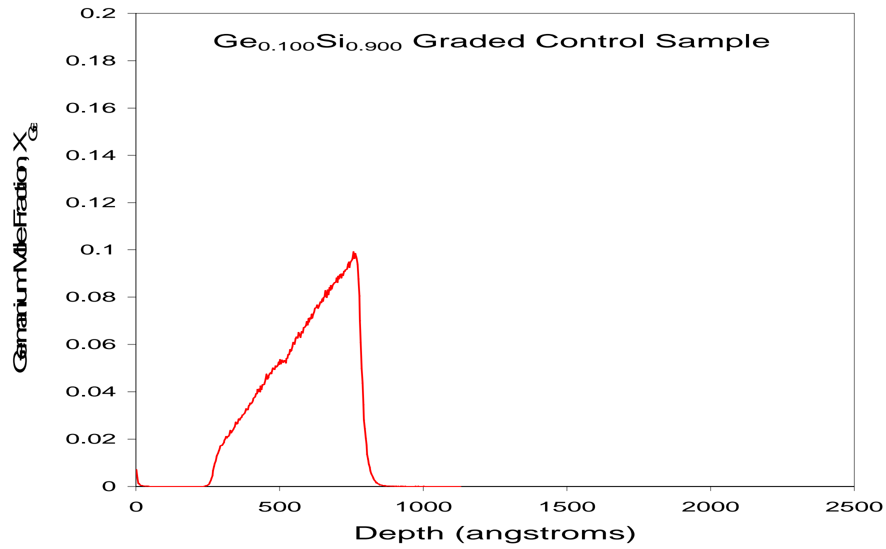

Figure 7. One SIMS profile of a 50 nm graded $Si_{1-x}Ge_x$ where x was increased from 0% to 10%.

Key Words

SiGe, strained silicon, SIMS, Ge diffusion