Characterization of Ge Outdiffusion and Si Cap Thickness in Strained Si/SiGe Structures using SIMS

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The outdiffusion of Ge from the SiGe underlayer into the thin Si cap layer in Strained Si/SiGe material systems can greatly affect the mobility of carriers in the Si channel. This outdiffusion can be affected by epi growth temperature, rate and source gas. The Si cap layer is very thin, on the order of 10 nm, such that the required depth resolution information of the Ge out-diffusion is very challenging. Ge out-diffusion is a critical aspect in the proper integration of Strained Si into real devices.

The production and use of Strained Si has led to increased need for proper quantification of these structures including: Si thickness, Ge composition, Ge out-diffusion and quantification of dopants and contaminants. Ultra low energy (ULS) Secondary Ion Mass Spectrometry (SIMS) has been used to characterize these critical parameters. Figure 1 demonstrates the simultaneous quantification of C, O and Ge in one analysis. The Ge composition is obtained with $\pm 3-5\%$ accuracy up to 70% Ge, with very low detection limits for C and O.

A study was performed to measure the interface abruptness at the Si/SiGe interface produced using different growth conditions. Figure 2 presents the results of varying growth temperature and source gas on the interfacial abruptness as monitored using ULE SIMS. The optimal conditions give the most abrupt interface at the highest growth temperature. Such process condition optimization can improve device performance and maximize throughput for the client and thus reduce costs.

A subsequent study is also intended to show the long-term precision of using ULE SIMS to measure the Si cap thickness. It is known that the SiGe sputter rates increase relative to Si with increasing Ge content. Corrections are utilized to adjust the sputter rate on a point-by-point basis as a function of Ge. This allows for a very precise measurement of Si cap thickness with a long-term precision of ± 2 Å.

Excellent long-term reproducibility of SIMS measurements of X_{Ge} under routine analysis conditions is illustrated in Figure 3. Relative standard deviations of $\pm 2.2\%$ have been obtained for two different control samples, a 50nm graded layer with a maximum Ge content of 10%, and a 110nm box structure with an average Ge content of 14.45% (confirmed by RBS). Additional measurement protocols are being developed that will provide substantially higher precision composition measurements for critical applications.

The absolute accuracy of SIMS measurements of X_{Ge} is determined by the accuracy of the reference materials used to calibrate the raw SIMS signals. Current EAG SIMS composition reference materials cover a wide range of X_{Ge} (0.027 to 0.80), and have been extensively characterized using Rutherford backscattering analysis (RBS). RBS is a standardless analysis technique that provides highly accurate ($X_{Ge} \pm 0.005$) Ge composition determinations of suitable samples. SIMS data from a suite of RBS-characterized reference materials provides SIMS relative sensitivity factors (RSF) for X_{Ge}

measurements. For a number of SIMS instrument conditions, such RSF's can be accurately modeled using the known bulk density of SiGe alloys as a function of X_{Ge} along with constant or only slowly varying relative secondary ion yields for Si and Ge ions. This modeling allows accurate point-by-point quantification of SIMS X_{Ge} depth profiles using specialized data reduction software.



Fig. 1. ULE SIMS Profile, 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.



Fig. 2. Interface Abruptness versus growth temperature and source gas (A=SiH₄, B=SiH₂Cl₂)



Fig. 3. 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)

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