Graded $\text{Si}_{1-x}\text{Ge}_x$ Metrology Using a Multi-Technology Optical System

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Abstract. Graded $\text{Si}_{1-x}\text{Ge}_x$ structures have been measured with good accuracy, stability and tool-tool matching by utilizing different measurement methods in one system (Opti-Probe®). The measurement methods utilized are (i) laser reflectivity versus angle for S and P polarization (BPR®), (ii) visible-DUV reflectometry (BB), and (iii) spectroscopic ellipsometry (SE). An alloy dispersion model, along with a multi-layer linear graded-material model, were used to process the data and extract the thickness of the cap-Si, graded and spacer $\text{Si}_{1-x}\text{Ge}_x$ layers, as well as the Ge%, simultaneously. The results were found to be in agreement with subsequent SIMS analysis to within 50Å for all layers and 0.5% atomic Ge%. Stability and matching results for thickness were <13Å (3σ) for all layers, and for the Ge% the stability was <0.25-0.6% (3σ).

Keywords: $\text{Si}_{1-x}\text{Ge}_x$, optical metrology, multi-layer film stacks, reflectance, spectroscopic ellipsometry

INTRODUCTION

In order to meet the demand for increased speed, reduced size and resistivity for semiconductor devices, new alloy materials have been vigorously pursued as candidates for replacing the standard c-Si structures that have been successful for the past several decades. Strained $\text{Si}_{1-x}\text{Ge}_x$ (where x defines the Ge atomic fraction) has been successfully implemented as material for bi-polar transistors and HBT's (Heterojunction bi-polar transistors) [1,2], and shows promise for faster logic gate devices at 90nm and below.

The larger lattice spacing of Ge relative to Si creates a lattice strain in the $\text{Si}_{1-x}\text{Ge}_x$ film that narrows the bandgap, and results in an increased mobility of electrons. This ultimately reduces the resistivity and allows for higher frequency, and lower power consumption for applications in optical and fast wireless devices. Measurement of $\text{Si}_{1-x}\text{Ge}_x$ films in single and multi-layer structures is a challenging requirement for optical metrology, since the optical dispersion for SiGe is not significantly different from c-Si [3]. Figure 1 shows the index, extinction curves for c-Si relative to Ge%=5%, 10% and 15%.

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With the additional presence of a c-Si cap layer typically seen in the HBT structures, the difficulty of optical measurements is further compounded, as the limited penetration depth of the incident light at the interband transition regions of the silicon over-layer can obscure the critical point shifts caused by Ge incorporation into the buried epitaxial layer. Despite these limitations, the optical characterization of buried Si$_{1-x}$Ge$_x$ [4] and full HBT stacks is possible [5].

Recent Si$_{1-x}$Ge$_x$ developments have included a graded Si$_{1-x}$Ge$_x$ structure, where a linear variation of atomic Ge% is deposited vs. depth in order to further enhance the device performance. This film stack structure leads to additional metrology challenges above and beyond the difficulties of optically characterizing and measuring the thickness and Ge content of multi-layer homogeneous film-stack structures. Nonetheless, the results presented here demonstrate that an optical metrology technology can measure a buried, graded Si$_{1-x}$Ge$_x$ film stack as well with good stability and matching.

**GRADED Si$_{1-x}$Ge$_x$ FILM STACK MODELING**

The typical graded Si$_{1-x}$Ge$_x$ film stack structure involves a cap-Si layer on top of a graded Si$_{1-x}$Ge$_x$ layer, and a final homogeneous spacer (and uniform) Si$_{1-x}$Ge$_x$ layer on silicon substrate. The total stack thickness typically ranges from 500-1200Å. The production metrology requirement is to measure the cap-Si thickness (t$_{cSi}$), the graded Si$_{1-x}$Ge$_x$ layer (t$_{gSiGe}$), the spacer Si$_{1-x}$Ge$_x$ layer (t$_{sGe}$) and the Ge% as a function of depth.

**Si$_{1-x}$Ge$_x$ Alloy Dispersion Modeling**

Previous analysis has been performed to characterize the optical properties of both strained and relaxed Si$_{1-x}$Ge$_x$ [6,7]; the differences between the two are relevant for our graded Si$_{1-x}$Ge$_x$ analysis. In order to obtain the most accurate reference dispersions possible, a set of single-layer, strained Si$_{1-x}$Ge$_x$ standards ranging from 0-27% Ge were grown and analyzed. Care was taken to ensure that the mechanical equilibrium critical thickness for misfit dislocation formation for each was not exceeded. The optical dispersion for these standards were characterized using the combination of BPR®, BB and SE technologies. It was the combination and resultant consistency of these technologies that provides added information in generating the most accurate and reliable set of dispersion standards for strained Si$_{1-x}$Ge$_x$. The samples were independently calibrated by RBS, TEM and SIMS analysis in order to establish the Ge% for each.

An "alloy model" (library based) was used to characterize the optical dispersion of the homogeneous strained Si$_{1-x}$Ge$_x$ layer. In order to estimate the dispersion for intermediate values of x, the alloy model interpolates the look-up tables at each wavelength, and reports the interpolated value. In the final fitting procedure, the value of x is floated, along with the thickness of all other layers, and an optimal value is determined by using a non-linear (Levenberg Marquardt) least-squares minimization procedure.

**Graded Layer Film Modeling**

The modeling of the Si$_{1-x}$Ge$_x$ graded layer was performed using a set of N discrete (and equal t$_{i}=t_{i-1}=...=t_{0}$) sub-layers such that $\sum_{i=1..N} t_i = t_{gSiGe}$. In addition, the dispersion of the graded layer was constrained to be consistent with the layer above (cap-Si) and below (homogeneous Si$_{1-x}$Ge$_x$), with a linear variation between. With a discrete-layer model, there is inevitably going to be a systematic error relative to a true, uniformly varying graded layer. In addition, from a computational point of view, as N gets larger, the calculation will also take longer, and a practical value of N must be chosen. Based on these considerations, N=8 was chosen for all subsequent film modeling and fitting.
LIMITATIONS OF SE

Spectroscopic ellipsometry (SE) has been the technology of choice for existing metrology approaches to thin-film measurement, including Si$_{1-x}$Ge$_x$. This is not surprising, because the information contained in the $\tan \Psi = |R_p/R_s|$, $\cos \Delta$ (where $\Delta$ is the sample phase shift) sample data [8] at each wavelength enables SE in principle to independently determine the sample dispersion over a spectral range.

However, in the case of a “buried Si$_{1-x}$Ge$_x$” layer, where the Si$_{1-x}$Ge$_x$ layer lies beneath an epi-Si layer, the benefit of SE in determining the Si$_{1-x}$Ge$_x$ film properties is reduced. In general, the sensitivity of ellipsometry is greatest near Brewster’s angle, $\theta_B$ (for a given interface). For the c-Si/SiGe interface (assuming $n_{cSi}=3.822$, $n_{SiGe}=3.9$), $\theta_B \approx -45$ degrees. On the other hand, for an SE incident angle $\theta_i \approx 65$ degrees, the angle of the signal entering the c-Si/SiGe interface is only $-13$ degrees, far away from $-45$ degrees, and it is in fact not far from normal incidence where $R_p$ and $R_s$ are no longer defined. This ultimately reduces the overall sensitivity of the SE to the measurement of the “buried” Si$_{1-x}$Ge$_x$ layers.

STRENGTH OF BB

In order to evaluate the capability of SE relative to other technologies and to determine the best overall combination of technologies, a numerical sensitivity study [9] was performed for all technologies for a 300Å cap-Si/350Å graded SiGe/300Å S$_{0.6}$Ge$_{0.4}$ filmstack, and evaluating different technology combinations in order to choose the best combination. In addition to SE, broadband spectral reflectance (BB) from 190 nm to 840 nm as well as BPR® (Beam Profile Reflectometry [10]) and AE® (Absolute Ellipsometer) technologies were considered.

This analysis determines the true “information content” of different technologies singly and in combination by effectively calculating the local curvature of the residual in the multi-dimensional parameter space in a correlated direction. Overall, the BB-only technology, an intensity measurement, was found to have the greatest information content for all measurement parameters (except for the top native oxide). All other technologies and their combinations (including other technologies in combination with BB) have reduced information content relative to BB only. This includes BPR®, and both AE® and SE, as they all suffer from a reduction in sensitivity due to the high-index cap layer. Overall, the information content of SE relative to BB for the $t_{cSi}$, $t_{SiGe}$, $t_{cSi}$ and Ge% parameters of interest was $\approx 50\%$, a reduction by a factor of two.

![Graded SiGe BB Spectral Fit](image)

**FIGURE 2.** Reflectivity vs. wavelength for broadband (BB) spectral fit (data vs. model) for sample 2.

Figure 2 shows an example of reflectivity vs. wavelength for a graded Si$_{1-x}$Ge$_x$ film stack. For the films considered here, i) the Ge% is determined by the amplitude of the spectral fringes, ii) the total film stack optical thickness is determined by the number of fringes (for $\lambda>400$nm), and iii) the relative thickness of the cap-Si and Si$_{1-x}$Ge$_x$ layers drives the modulation of the spectral data.

MEASUREMENT RESULTS

Wafer Uniformity

Nine sites across a (patterned) buried, graded Si$_{1-x}$Ge$_x$ sample using a BB-only, alloy/graded medium recipe were measured; the results are summarized in Table 1. The spatial variation across sample 1 is easily detectable, as all layers have a center (thicker) to edge (thinner) variation that trend together.
Dynamic Repeatability and Matching

Dynamic repeatability measurements (30 load/unloads over 24 hours) were performed on two graded Si_{1-x}Ge_x samples with a cap-Si/graded SiGe/SiGe/c-Si film stack on two systems using the BB spectral data in the fit, and the stability and matching results from two systems were compared. The results for samples 2 and 3 are summarized in Table 2; a sample spectral fit result is also presented in Figure 2. The results represent the mean wafer parameter value, as well as the mean 3σ variability of four sites on the sample. Overall, the mean 3σ stability is <13 Å for all layers, and the mean 3σ Ge% is < 0.6%. Mean wafer matching is <5 Å for all layers on both samples, and <0.5% atomic Ge%.

<table>
<thead>
<tr>
<th>Site#</th>
<th>t_{cap}(Å)</th>
<th>t_{graded}(Å)</th>
<th>t_{SiGe}(Å)</th>
<th>Ge%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>310.1</td>
<td>345.7</td>
<td>215.0</td>
<td>10.06</td>
</tr>
<tr>
<td>2</td>
<td>338.0</td>
<td>349.9</td>
<td>231.1</td>
<td>10.19</td>
</tr>
<tr>
<td>3</td>
<td>345.6</td>
<td>370.2</td>
<td>231.5</td>
<td>10.52</td>
</tr>
<tr>
<td>4</td>
<td>369.9</td>
<td>373.6</td>
<td>235.8</td>
<td>10.56</td>
</tr>
<tr>
<td>5</td>
<td>370.2</td>
<td>385.4</td>
<td>237.8</td>
<td>10.68</td>
</tr>
<tr>
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<td>356.0</td>
<td>379.5</td>
<td>239.7</td>
<td>10.63</td>
</tr>
<tr>
<td>7</td>
<td>330.0</td>
<td>377.7</td>
<td>236.6</td>
<td>10.55</td>
</tr>
<tr>
<td>8</td>
<td>312.1</td>
<td>363.6</td>
<td>239.1</td>
<td>10.49</td>
</tr>
<tr>
<td>9</td>
<td>266.7</td>
<td>364.9</td>
<td>237.0</td>
<td>10.68</td>
</tr>
</tbody>
</table>

TABLE 1. Thickness and Ge% vs. site for graded Si_{1-x}Ge_x sample 1.

<table>
<thead>
<tr>
<th>Sample/Tool</th>
<th>t_{cap-Si} (Å) ±3σ</th>
<th>t_{SiGe} (Å) ±3σ</th>
<th>t_{SiGe} (Å) ±3σ</th>
<th>Ge%±3σ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample 2/Tool 1</td>
<td>436.3±3.9</td>
<td>233.9±7.2</td>
<td>-4.5</td>
<td>13.72±0.21</td>
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<tr>
<td>Sample 2/Tool 2</td>
<td>431.7±7.5</td>
<td>238.4±8.1</td>
<td>4.1</td>
<td>13.46±0.11</td>
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<tr>
<td>Tool 1-Tool 2</td>
<td>689.8±7.8</td>
<td>218.1±12.6</td>
<td>2.0</td>
<td>10.62±0.63</td>
</tr>
<tr>
<td>Sample 3/Tool 1</td>
<td>692.8±7.8</td>
<td>216.1±13.2</td>
<td>1.6</td>
<td>11.0±0.54</td>
</tr>
<tr>
<td>Tool 1-Tool 2</td>
<td>3.0</td>
<td>2.0</td>
<td>-4.8</td>
<td>0.48</td>
</tr>
</tbody>
</table>

TABLE 2. Stability (3σ) and matching results for thickness and Ge% for samples 2 and 3.

SIMS Results

In order to determine the inherent accuracy of the method, sample 1 was measured using BB spectral data, and was subsequently analyzed using SIMS. The comparison of the SIMS vs. OP results are summarized in Figure 3. As can be seen from the figure, the results agree to within ~50 Å to the SIMS results for all layers.

FIGURE 3. Ge percentage versus depth for SIMS vs. Optical (Opti-Probe) measurements for graded Si_{1-x}Ge_x sample 1.
CONCLUSIONS

The results presented here demonstrate that stable and accurate measurements of graded Si$_{x}$Ge$_{y}$ films are possible by utilizing optical metrology technologies along with appropriate graded layer and Si$_{x}$Ge$_{y}$ alloy dispersion modeling. A combination of technologies (BPR®, BB, SE) proved to be valuable in the characterization of an accurate set of reference Si$_{x}$Ge$_{y}$ standards. In the measurement of "buried" Si$_{x}$Ge$_{y}$ filmstacks, the BB technology has the maximal sensitivity and provides the optimal benefit for this particular application. Overall, the results presented here demonstrate that accurate, long-term multi-parameter 3σ stability/matching results of $<$13Å/5Å are possible for $t_{Si}$, $t_{SiGe}$, $t_{Ge}$, and $<$0.6%/0.5% (absolute) for the atomic Ge%.

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REFERENCES


