In-line optical and x-ray measurements of thickness and composition for manufacturing of heterostructure bipolar transistors

Stefan Zollner, Mariam G. Sadaka, N.V. Edwards, Candi S. Cook, Q. Xie, Ha T. Le, Jill Hildreth, and Andrew S. Morton

Motorola, Inc., DigitalDNA® Laboratories, MD M360, 2200 W. Broadway Rd., Mesa, AZ 85202
(Stefan.Zollner@motorola.com, 480-655-4655)

Abstract

We demonstrate the use of high-resolution x-ray diffraction and spectroscopic ellipsometry as alternatives to transmission electron microscopy to determine thickness and composition of thin epitaxial semiconductor layers used in the manufacturing of III/V and SiGe:C heterojunction bipolar transistors. We also discuss in-line monitoring the emitter and base etches of an InGaP heterojunction bipolar transistor using spectroscopic ellipsometry.

INTRODUCTION

Manufacturing commercial HBTs on large-diameter wafers with high yields is a long, complicated, and expensive process. Screening epitaxial starting materials (for III/V HBTs), controlling the process using test wafers, and inspecting product wafers after critical deposition (SiGe:C HBTs) or etch steps are essential in achieving a manufacturable technology. Non-destructive in-line metrology therefore becomes an integral part of the manufacturing solution. Optical and x-ray techniques are preferred over destructive techniques such as TEM and SIMS, since they are non-destructive, rapid, and because such measurements at multiple spots on the wafer can be inserted in the process flow. Recently, a variety of automated tools (pattern recognition, robot wafer handling) suitable for a manufacturing environment have become available. This presentation will focus on spectroscopic ellipsometry (SE) [1] and high-resolution x-ray diffraction (XRD) [2]. Other optical techniques [3-4] are surface photovoltage spectroscopy, contactless electroreflectance, and Raman spectroscopy. These are suitable to determine built-in electric fields, free carrier concentrations, and strain and therefore are somewhat complementary to SE and XRD.

EXPERIMENTAL TECHNIQUES (SE and XRD)

Spectroscopic ellipsometry [1] (SE) is an all-optical technique, which measures the change of the polarization state of white light reflected by a surface. The measured quantities are the ellipsometric angles ψ and Δ as a function of wavelength (for example 410–750 nm) to describe the polarization change. We can also express the same data as a pseudo-dielectric function ε. For analysis of these raw data, we need to know the optical constants (complex refractive index $n+ik$) for each layer material, including the dependence on composition for alloys. The dependence on doping is usually ignored, except for the base with its high carrier concentration exceeding 10^{19} cm^{-3}. From the raw data, it is possible (at least in principle) to determine the thickness and alloy composition of each layer in the epitaxial stack, and also the thickness of a native oxide or surface roughness layer. A commercial software package (usually sold with the instrument) is needed to solve Fresnel's equations based on the input parameters (thicknesses, optical constants) and compare the calculated ellipsometric angles with the measured ones. In reality, the uncertainties increase with the number of layers. Even for complicated structures, we are usually able to determine thickness and composition of the top layer (and its oxide or roughness thickness) with very high accuracy, since these top layers dominate the ellipsometric response at sufficiently short wavelengths (for photon energies above the band gap). Because of this surface sensitivity, SE is ideally suited as an in-line etch monitoring tool for III/V HBTs. How useful an instrument will be depends on the flexibility of the analysis software, the accuracy of the ellipsometric angles, the width of the spectral range, and the speed, automation features, application support, and reliability of the tool.
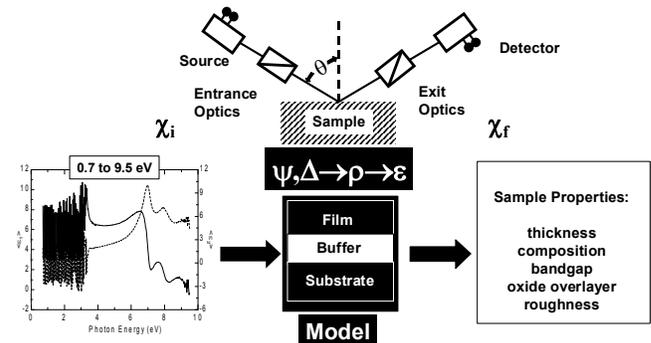

Fig. 1: Experimental setup for a spectroscopic research ellipsometer and schematic algorithm to extract sample information from the experimental data. A manufacturing tool would typically include a wafer robot, beam folding and focussing optics, and a multiple wavelength array detector.

High-resolution x-ray diffraction [2] (XRD) is similar to SE, except that the radiation consists of monochromatic x-

rays (λ=1.54 Å) and we detect only reflected intensity (no polarization information) as we rotate the sample (θ) and the detector (2θ). The measured quantity is reflected intensity as a function of sample rotation angle (θ). For analysis of the raw data, we need to know the lattice constant and elastic properties (Poisson's ratio) for each material, including variation with alloy composition. Similar to SE, we are able to extract layer thicknesses and compositions by comparing a numerical solution of the Takagi-Taupin equations with the measured spectra. For coherently strained (pseudomorphic) samples, each epitaxial layer yields a Bragg diffraction peak determined by its lattice constant and strain. The peak widths increase with decreasing layer thickness and are accompanied by *Pendellösung* (interference) fringes. Because of the large penetration depth of the x-rays, which is 7.1 µm for the (004) GaAs Bragg reflection, XRD has no surface sensitivity. All layers contribute to the pattern. For quantitative XRD analysis within the context discussed here, all layers need to be pseudomorphically strained (without dislocations). Relaxed and heavily dislocated layers require a different framework not discussed here.

EXAMPLE I: INGAP HBT

As an example, we use a generic InGaP HBT structure [4,5]. The epitaxial layer structure of this HBT (from Ref. [4]) is shown in Fig. 2. A typical TEM image for an HBT structure is given in Fig. 3. It is obvious that SEM and TEM are indispensable tools for developing a semiconductor technology. Literally hundreds of TEM and thousands of SEM images were acquired during development and process startup of our InGaP HBT [6]. TEM is capable of determining thicknesses of epitaxial layers with very high accuracy and can also estimate composition from the contrast of the layers or using other analytical capabilities in the microscope (nano-EDS, EELS). TEM also images defects (dislocations, As-rich precipitates), strain fields, and Ohmic grain formation. SEM is used for imaging the transistor etch profiles and for back-end development, such as interconnects, air bridges, photoresist profiles for metal lift-off, substrate vias, etc.
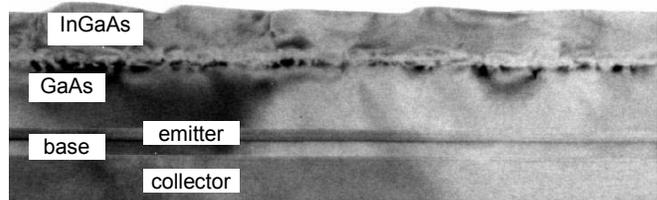
Fig. 3: TEM image of the InGaP HBT structure similar to the schematic in Fig. 2. The top InGaAs layer is rough and defective. The lattice mismatch leads to strain contrast in the GaAs layer underneath.

The complete epitaxial layer structure (as shown in Fig. 3) is not particularly suitable for analysis with SE or XRD because of the heavily dislocated and rough InGaAs top layer, the In grading, and the thick interfacial region between GaAs and InGaAs. Significant surface roughness is an unsolved problem for SE. For XRD, the dislocations cause a mosaic tilt which broadens the Bragg peaks and weakens the interference fringes, making a comparison between measured and calculated XRD spectra unreliable. Since these top layers are primarily intended to form the emitter Ohmic contact, process control of these layers is not as critical.

Instead, we consider measurement of the structure after Etch 1, which removes the InGaAs and GaAs top layers and stops on the InGaP emitter (see Fig. 2). It is important that this etch clears all of the InGaAs and GaAs layer, does not cut significantly into the InGaP emitter, and leaves a smooth InGaP top surface. To ensure that these criteria are met, an SE measurement was inserted in the flow after Etch 1 [6]. Because of the small optical contrast between the different doped and undoped GaAs layers below the InGaP emitter, only an InGaP layer and the GaAs substrate is considered in the model. This model leads to an accurate determination of the InGaP thickness with across-wafer variations of less than 1%. Two wafers out of every 12-wafer lot are measured. Processing is halted when the thickness of the InGaP emitter is outside of the control limits or if the mean squared deviation between the measured and modeled data is more than five times the statistical uncertainty of the ellipsometric angles. (This deviation increases with the number of layers.) It would be possible to also determine the composition of the InGaP layer, but this is not done routinely in manufacturing.

Etch 2 removes the InGaP emitter and stops on the carbon-doped GaAs base. The small optical contrast between the heavily doped GaAs base and the lightly doped GaAs collector is sufficient to determine the thickness of the base and that of the oxide/roughness surface layer. Finally, Etch 3 removes the GaAs base and collector and stops on the GaAs subcollector. This time, we only measure the thickness of the oxide/surface roughness layer.

By inserting these SE measurements in the process flow, a stringent process control of the difficult InGaP HBT etch steps is in place. Since these etch steps are among the first
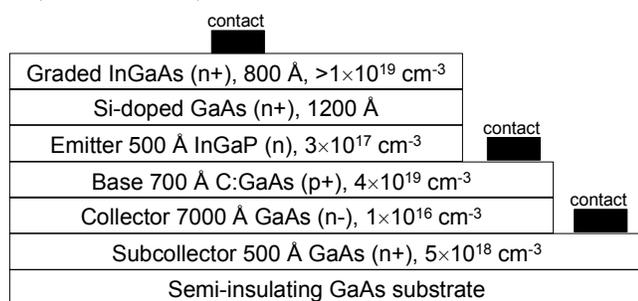

Fig. 2: Generic InGaP HBT structure (see Fig. 1, Ref. [4]), consisting of Te-doped graded InGaAs and Si-doped GaAs as emitter contact, a Si-doped InGaP emitter, a heavily C-doped GaAs base, and GaAs layers as collector and subcollector. Etch 1 removes the InGaAs/GaAs cap layer, etch 2 removes the InGaP emitter, and etch 3 removes the GaAs base and collector.

process steps, errors can be detected early in the flow. Misprocessed wafers can be scrapped early and avoid the cost of additional processing until electrical measurements are possible. Some typical problems that can be discovered during in-line measurements are the following: (1) missing epitaxial layers, additional layers, or improper thicknesses. (2) When experimenting with etch stops, we suspected that As-rich defects (precipitates) in the etch stop might lead to residue (haze) on the surface. (The SE measurement would see this haze as roughness.) The residue may mask subsequent etch steps. (3) Improper etch conditions may lead to redeposition of the etched material. Again, this will be reflected in the SE spectrum as roughness or thickness variation.

To implement in-line monitoring using SE we need accurate optical constants of all layers. While optical constants exist for GaAs [7] and InGaP [8], we made sure that measurements on our own structures agreed with the databases supplied with the instrument. In some cases, refinements were needed. For example, the optical constants of InGaP depend on the degree of ordering, which will depend on the growth conditions. Sample data from research and production ellipsometers are shown in Figs. 4-6.
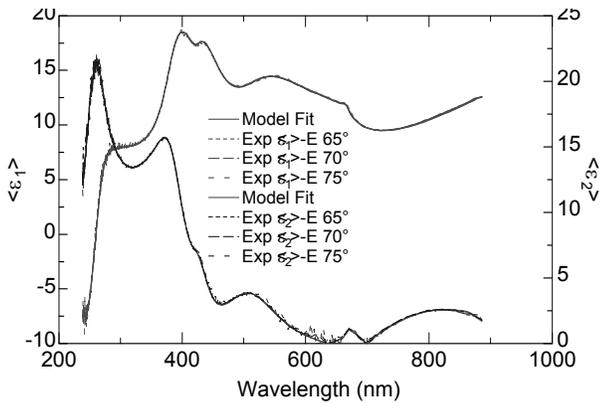

Fig. 4: Pseudodielectric function of 1546 Å of InGaP (disordered) on GaAs.
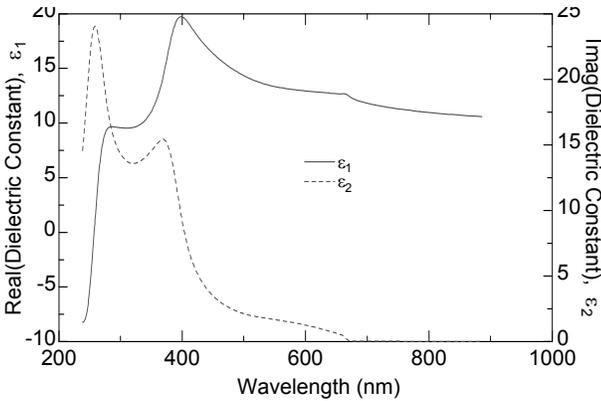

Fig. 5: Real (solid) and imaginary (dashed) part of the dielectric function of disordered InGaP determined from the raw data in Fig. 4. The direct band gap is clearly visible at 671 nm (1.85 eV), indicating a high degree of disorder. The E_1 edge appears near 390 nm (3.2 eV).
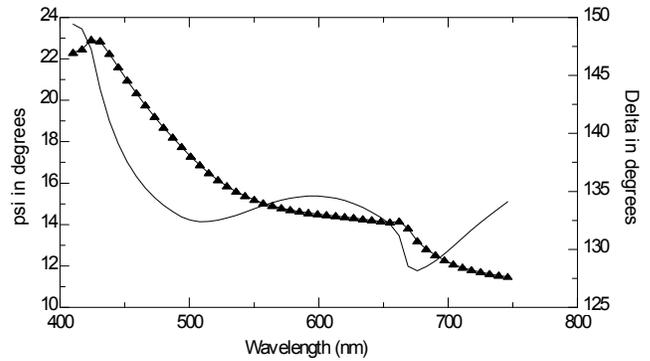

Fig. 6: Calculated ellipsometric angles ψ (symbols) and Δ (line) as a function of wavelength (410 to 750 nm) for 500 Å InGaP on GaAs (HBT after etch 1). A 45° Δ-offset and a seven-degree angular spread around the average angle of incidence (65°), similar to a production tool, were added.

EXAMPLE II: SIGE:C HBT

The second example, a SiGe:C HBT for a BiCMOS technology, is different. Unlike the InGaP HBT, where all processing is done by etching into an epitaxial starting material (see Fig. 2) the SiGe:C HBT layers are grown epitaxially after most of the CMOS processing is already completed. The SiGe base layer, visible in the TEM image shown in Fig. 7 as a dark line below the emitter contact, is quite thin and has a compositional grading, which complicates the data analysis. The compositional grading, the doping of the base, and the impurity content in the epitaxial layers (primarily oxygen) are determined in an off-line analysis lab using SIMS and Auger depth profiling. However, in-line SE and XRD are used to monitor a number of variables after growth of special test structures consisting of a SiGe layer with a Si cap: (1) SiGe growth rate (which may depend on C and B doping), (2) Si growth rate, (3) Ge content in the alloy.

Accurate optical constants for SiGe alloys were only available for bulk (unstrained) alloys, whereas the HBT layers are pseudomorphically strained, which changes the optical constants. Therefore, strained SiGe optical constants needed to be determined [9]. Our results for the imaginary part of the dielectric function are shown in Fig. 8. Using these input data, thickness and composition of SiGe layers with uniform composition can be determined by SE. It is also possible to determine thicknesses and composition of a double-layer structure consisting of a SiGe layer and Si cap.

The optical constants of SiGe alloys change only slightly by adding a small amount of carbon. Therefore, SE is not sensitive to the C content, which needs to be determined by XRD. (One percent of carbon compensates the strain of roughly 10% of Ge; therefore XRD is very sensitive to C content.) Typical XRD data for a $Si_{1-y}C_y$ alloy are shown in Fig. 9. The sharp peak at $\Delta\theta=0$ is due to the Si substrate. A $Si_{1-y}C_y$ alloy has a smaller lattice constant than Si; therefore

its XRD peak is shifted to the right. Likewise, a SiGe alloy has an XRD peak shifted to the left relative to the Si substrate. By measuring the shift between the alloy and substrate peak (and assuming one knows the Ge content from a previous SiGe alloy growth without C source), the C content in a SiGe:C alloy layer can be determined. As described by Zaumseil [10], it is also possible to characterize graded SiGe:C base layers with a Si emitter cap.

CONCLUSIONS

Spectroscopic ellipsometry and high-resolution diffraction are excellent in-line quality control and inspection tools to manufacture III/V and SiGe HBTs. Commercial tools are available, which are suitable for integration in a manufacturing environment.

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ACRONYMS

HBT: Heterojunction bipolar transistor
XRD: X-ray diffraction
TEM: Transmission electron microscopy
SEM: Scanning electron microscopy
SE: Spectroscopic ellipsometry
SIMS: Secondary ion mass spectrometry
EDS: Energy dispersive spectroscopy
EELS: Electron energy loss spectroscopy
CMOS: complementary metal-oxide semiconductor

Fig. 8: Imaginary part ε_2 of the dielectric function of pseudomorphically strained SiGe alloys grown on Si (001) using chemical vapor deposition. The onset of absorption shifts to lower photon energies with increasing Ge content. Also both peaks in ε_2 decrease in amplitude. The dependence of the optical constants on Ge content provides sufficient optical contrast to determine thickness and composition of $Si_{1-x}Ge_x$ alloys.
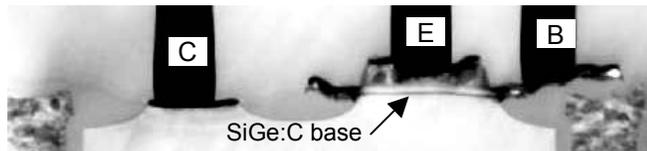
Fig. 7: TEM image of a SiGe:C HBT integrated into a Si CMOS flow. Collector, emitter, and base contacts are shown from left to right. This HBT has a SiGe:C base highly doped with boron, visible as a dark line just below the poly-Si emitter contact.
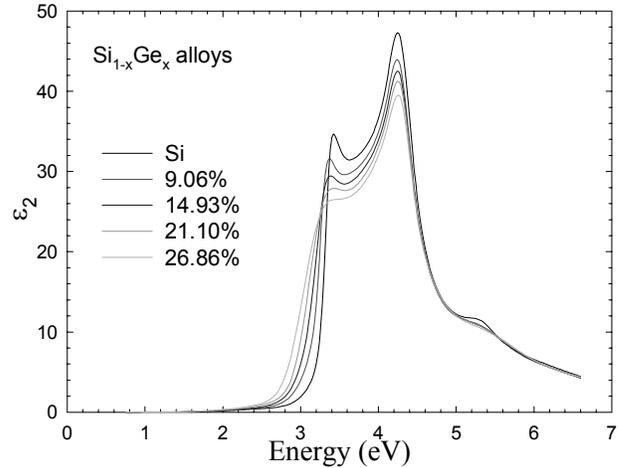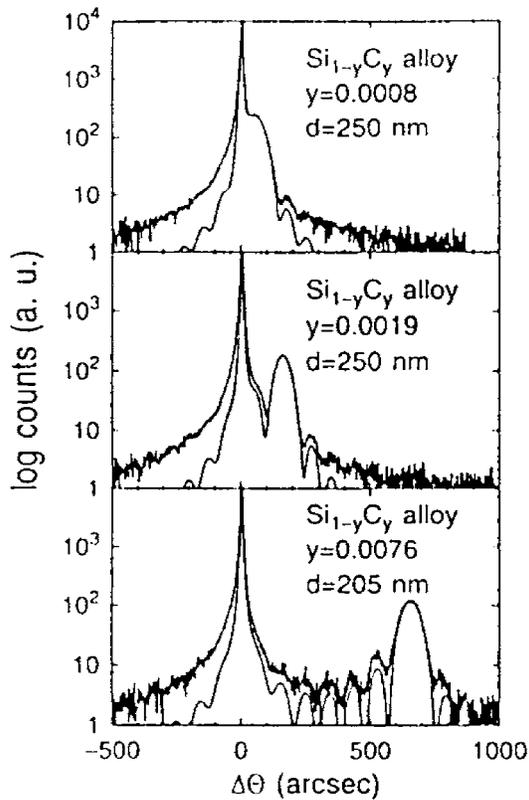
Fig. 9: X-ray rocking curves for $Si_{1-y}C_y$ alloys grown pseudomorphically on Si. Increasing the amount of carbon in Si shifts the alloy peak to the right. The thickness of the alloy layer can be determined from the width of the alloy peak and the interference fringes.