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Robust Optical Modeling of SiGe Layers

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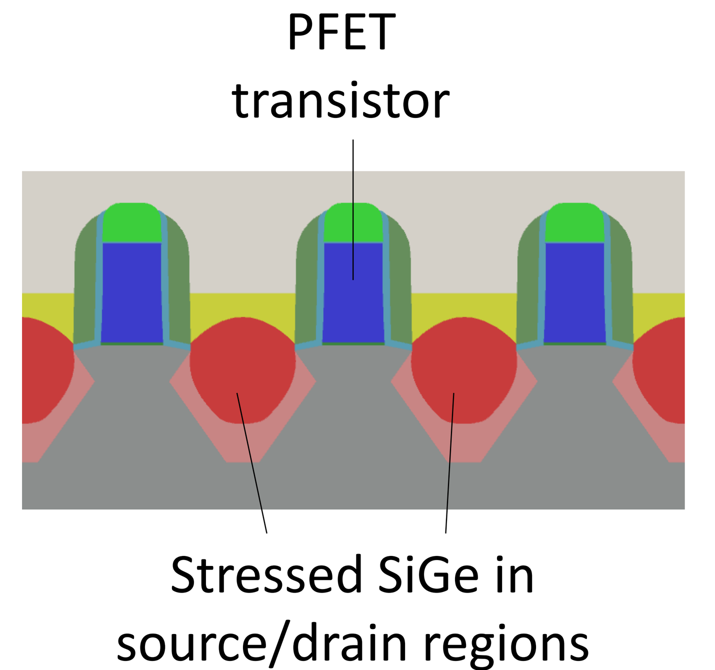
Introduction

Epitaxial Silicon Germanium layers are commonly used in the semiconductor industry to compress the P-FET transistor channel and thus increase its drive current. Accurate metrology of SiGe thickness and Ge content is required, preferably by a fast and nondestructive method, such as spectroscopic ellipsometry. In principle, an optical measurement of Ge concentration is possible, since the composition of a single-crystalline SiGe alloy determines its optical properties. However, the complex nature of this relationship makes the analysis difficult in general. In addition, more than a single SiGe layer is often present due to manufacturing constraints, which complicates the analysis of ellipsometric spectra even further. An analytical description for the dielectric function of SiGe is developed that enables robust and accurate analysis of ellipsometric data for Ge concentrations up to 50%.



SiGe dielectric function parametrization

The fundamental basis for accurate ellipsometric measurements of SiGe layers is a precise mathematical model for the optical properties (dielectric function, DF) of SiGe, for all Ge concentrations up to the maximum amount encountered in production. Commonly, a series of SiGe layers, which cover the needed composition range, are analysed by Spectroscopic Ellipsometry, and a reference method, such as Auger Electron Spectroscopy, is used to measure the true Ge concentration. The SiGe DF extracted for each individual composition is then stored in a lookup-type model along with the reference Ge concentration. A spectroscopic ellipsometry measurement of an unknown SiGe alloy is then matched to the best-fitting database entry. Some kind of spectrum interpolation is employed to find best fits for intermediate compositions.

The problem with this approach is that there are never enough reference spectra to densely cover the needed composition range and that even with smart interpolation approaches (critical point shift, for example), the results are not optimal. Therefore, we take a different approach, which extracts from a series of reference measurements an analytical formula for the SiGe DF that depends solely on the Ge concentration.

The imaginary part of the SiGe DF is shown in figure 1. It is composed of a number of peaks, whose shape in the vicinity of the critical points is described in the literature by various functions [1]. These are based on the physical absorption processes at those specific critical points. In order to describe the DF over the whole spectrum with as few parameters as possible, we use a superposition of N Tauc-Lorentz oscillators [2], which is a very good approximation to the true SiGe DF for N>4. (The complex TL oscillator is inherently Kramers-Kronig consistent, i.e. the real part of the DF is described correctly as well). Each TL oscillator is a function of 4 parameters: amplitude A, energy E, width C, and gap energy Eg. Thus, a set of 4N parameters describes the DF for each SiGe composition. Figure 1 shows how the DF varies with Ge concentration: the first peak shows the strongest shift in energy and amplitude, but in fact all 4N peak parameters vary more or less strongly with the Ge content.

Since the SiGe layer is single crystalline due to the epitaxial matching to the underlying Si substrate, its crystal structure and thus optical properties are uniquely defined by the Ge concentration (assuming statistical distribution of Si and Ge atoms on the lattice). This means that 4N-1 peak parameters are perfectly correlated to each other. Only one parameter is truly free, and each peak parameter can thus be written in principle as a unique function of the Ge concentration. The challenge is to find those functions. In an iterative approach, similar to the one described in detail in [3] for the DF of mechanically stressed Si, a polynomial relationship to the Ge concentration is first assumed for the most sensitive peak parameters, which constrains the functional dependence for the others. This is repeated until a functional relationship is established for all peak parameters. As a result, the SiGe DF is fully parameterized to the Ge concentration as a single parameter, but to a rough approximation only. In the final step, the polynomial constants (up to 3 per peak parameter) are determined in a multi-sample fit involving the ellipsometric spectra of all reference samples [4]. We used 10 reference Ge concentrations, spaced roughly equally from 0 to 47% (i.e., including pure Si). This results in a large, highly non-linear optimization problem to simultaneously find a fit optimum for a set of up to 3·4N (typically 30 to 100) free parameters.

In this way we were able to describe the DF of fully strained SiGe alloys by a self-contained analytical function with Ge concentration as the single dependent parameter, valid in the range of 0 to 50% Ge. With this functional approach, the fitted Ge concentration smoothly follows the true Ge content and avoids problems related to the reference concentration points in the conventional lookup & interpolate approach (e.g., fit trending toward the reference points, since interpolated spectra have inherently higher fit error). Figure 2 illustrates this point for a very simple interpolation model.

Comparing Ge concentration fit results to reference measurements for a large number of samples of various thicknesses and concentrations shows that the accuracy is about 1% (percentage point), precision and repeatability are <0.1% (single SiGe layer with native oxide). This accuracy is achieved if all model assumptions are fulfilled, i.e, epitaxial SiGe film on Si(100), fully strained and homogeneous. Non-ideal conditions can be detected by an increase in the mean-squared error of the fit.

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2. G. E. Jellison and F. A. Modine, *Appl. Phys. Lett.* **69**, 371-373 (1996)
3. Z. Chong, M. Weisheit, M. Hecker, and E. Zschech, *Semicond. Sci. Technol.* **24**, 045013 (2009)
4. B. Johs, C. Herzinger, B. Guenther, WVASE32 Version 3.686 (2008)

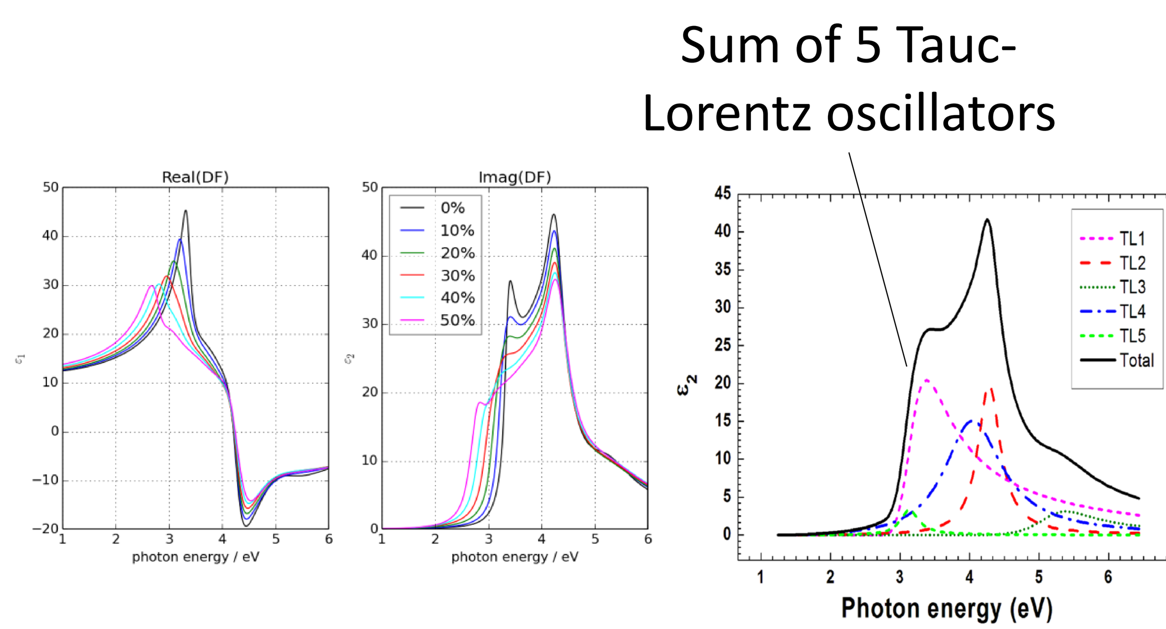


FIGURE 1. Real and imaginary part of the dielectric function of fully strained epitaxial SiGe layers on Si (a) and functional description by superposition of Tauc-Lorentz oscillators (b)

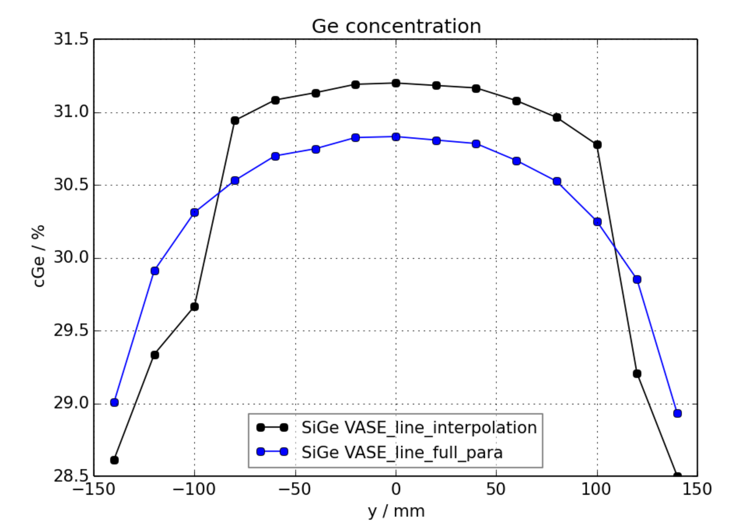
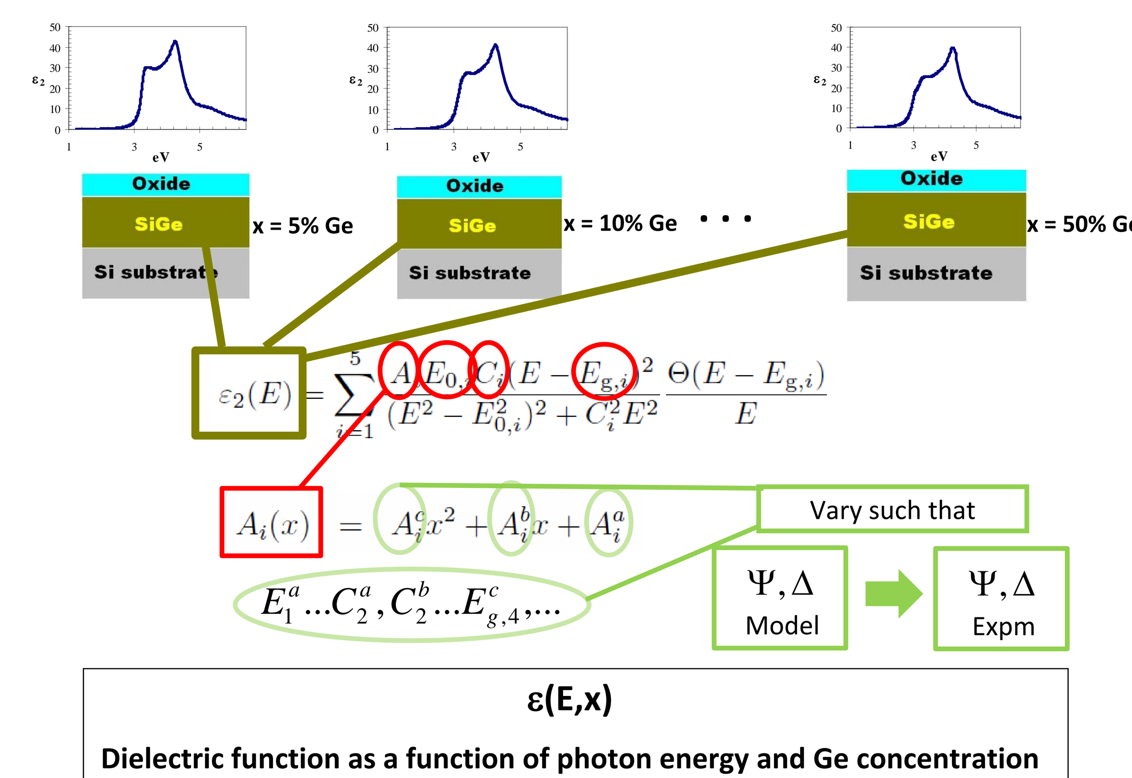


FIGURE 2. Fitted Ge concentration of a 4nm thick epitaxial SiGe film along the wafer diameter for a simple interpolation model (black curve) and the fully parameterized SiGe model described here (blue curve). The discontinuous Ge concentration jump at 100mm radius in the interpolation model is an artifact of the large discrete spacing of reference spectra.

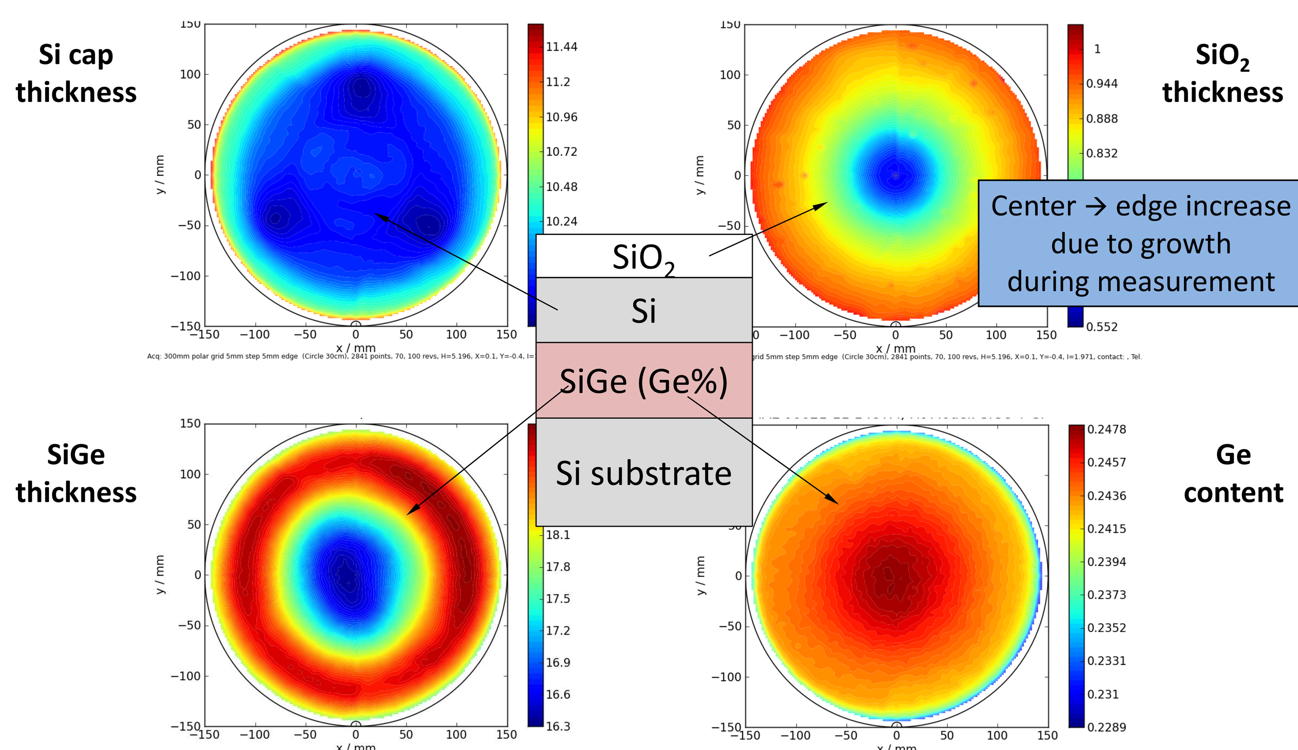
Fit strategy

In order to find the true thickness and Ge concentration for an unknown SiGe film, a robust fit strategy is needed to avoid getting trapped in local optimization minima of the fit error landscape. The fit error landscape can be visualized in this case as a 2-dimensional function of SiGe thickness and Ge concentration (the native oxide on top, which is also a fit parameter, can be safely ignored due to its low thickness). A number of local minima will be evident, which must be avoided by choosing starting values close enough to the true global minimum. By analyzing a number of such fit error landscapes for samples of different thicknesses and concentrations, a robust fit strategy can be established: start with a gridded global fit of Ge concentration in 15% steps, SiGe thickness in 20nm steps, to find the best starting value, and finish with Levenberg-Marquardt iterations to the minimum. This procedure will always find the global optimum. SiGe films up to 200nm thickness and up to 50% Ge concentration are thus fitted reliably in a few seconds with a single recipe. A number of examples for single- and multi-layer stacks will be shown in the presentation.

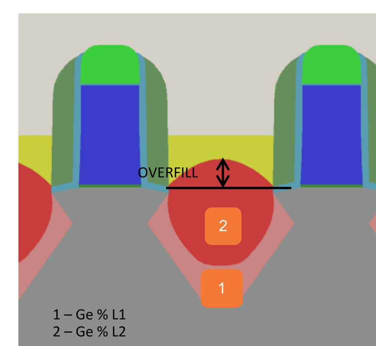
multi-sample fit



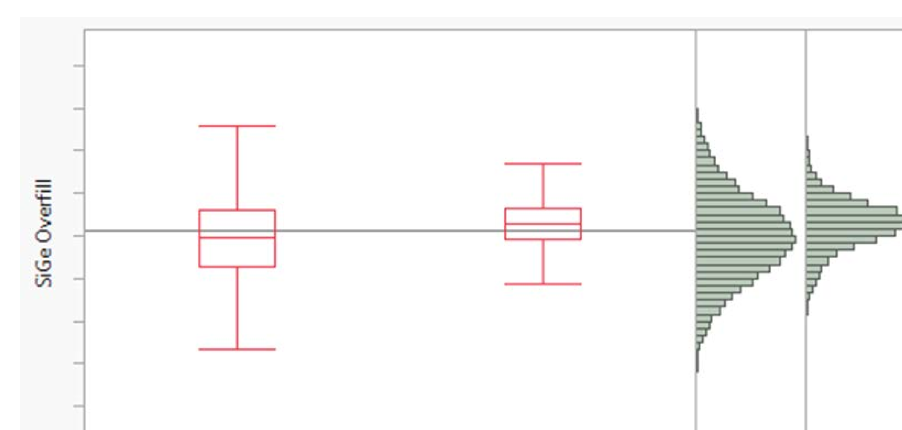
Si on SiGe *blanket wafer*



Si on double-layer SiGe *OCD grating*

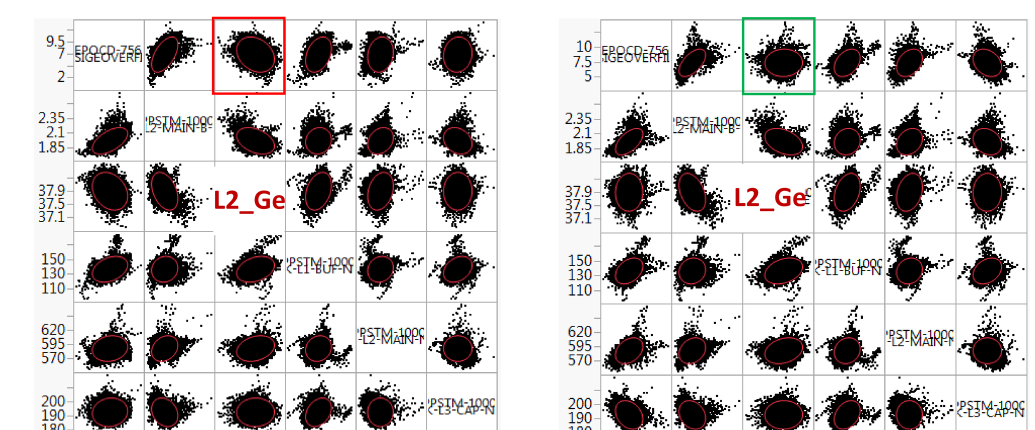


SiGe overfill measurement in device-like test structure by scatterometry



old new

New model helps to break correlation between main layer Ge % and Overfill measurement



-0.26 **0.02**

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