Metrology of Thin Silicon Epitaxial Films: Determination of Epitaxial Film thickness by Fourier-Transform Infra-Red Spectrometry

by

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Submitted to the Department of Electrical Engineering and Computer Science in partial fulfillment of the requirements for the degree of Master of Science in Electrical Engineering at the Massachusetts Institute of Technology

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Abstract
The objective of this thesis is to investigate the application of Fourier-Transform Infra-Red Spectrometry (FTIR) to the non-destructive determination of the thickness of thin (sub-1 um) silicon epitaxial films on heavily doped silicon substrates. FTIR in the interferogram domain has been used by the semiconductor industry to measure thickness of relatively thick (1 um +) epitaxial films. The technique has the advantage of being non-destructive, fast (an interferogram collection typically takes less than a minute) making it suitable for real-time in-situ control applications, and fairly accurate (an accuracy on the order of 10A is obtained for the case of thicker films). The accuracy rapidly deteriorates for the case of thinner films. While the conventional limit of 0.5 um is quoted by the manufacturers, the industry rarely uses the technique for films thinner than 1 um. In this thesis a thorough investigation of the limitations of the FTIR in the interferogram domain to the determination of the thin epi film thickness is performed. As part of this effort, a comprehensive signal-processing model of the FTIR/epi/substrate system is derived. It is determined that 2 chief factors are responsible for the limitation of the technique:
limited bandwidth over which the optical contrast between the epitaxial film and the heavily doped substrate exists;
non-ideal behavior of the electronic and optical components of FTIR, primarily the source, the detector, and the beam-splitter;
It is determined that the first limitation can be overcome by constructing an accurate model of the silicon optical constants in the infra-red. The second factor was determined to be the fundamental limitation of the technique. An investigation was further performed in the use of FTIR in the frequency domain. Here the IR reflectance spectrum was obtained by referencing its reflected intensity to that produced by a highly reflecting gold mirror. By doing this, the parasitic frequency responses of the electronic and optical components of FTIR are eliminated, removing the second factor as the chief limitation of FTIR. In addition, the reflectance waveforms of the epi on substrate are functions of substrate resistivity and dopant concentration as

2
well as film thickness, providing additional advantage over the conventional FTIR interferogram domain measurements. The reflectance sensitivity to the substrate doping concentration and resistivity was verified experimentally on a set of substrates with varying dopant type and concentration. The reflectance sensitivity to epi film thickness was verified on 2 sets of wafers which respectively use same substrates and varying film thickness. It was determined that FTIR in the reflectance (frequency) mode is sensitive to epi films as thin as 50 nm. In order to determine the epi film thickness as well as substrate resistivity and dopant concentration, the above mentioned signal processing model of FTIR-epi-substrate system was combined with the model of silicon optical constants in the infra-red in a single parametrized DSP model. By optimizing model parameters for the best fit against experimentally obtained reflectance from the epi on substrate, the film thickness, substrate dopant concentration and resistivity are obtained. Finally, the optimization procedure was carried out for the case of a 200 nm epi film: (nominally) on substrate of known dopant type and resistivity.

Thesis supervisor: Professor Rafael Reif
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Thesis Organization

The thesis is organized in 5 chapters. Chapter 1 in an introduction. The use of silicon epitaxy in the IC fabrication technology is described and the need for non-destructive means of thin epi measurement is explained. Ellipsometry and FTIR are presented as the natural techniques for thin epi analysis. Advantages and disadvantages of each conventional method are presented.

Chapter 2 describes the experimental set-up and presents the fundamentals of FTIR from the signal processing point of view. The IR source is treated as an ideal white noise process with randomly distributed phases and polarizations passing through a shaping filter. Michelson interferometer is treated as a correlator device which determines the real part of the covariance function of this random process, which is the resultant interferogram. Using Wiener-Kinchine theorem, the corresponding intensity is obtained by performing inverse Fourier transform of the interferogram. The parasitic responses of the electronic and optical components of the FTIR are considered and the overall signal processing model of FTIR is presented.

Chapter 3 deals with the issues of reflection and transmission of chaotic light in the dispersive media of heavily doped silicon substrate at non-normal angle of incidence as well as in the film-on-dispersive-substrate system. The effects of native oxide are considered. The Fresnel reflection and transmission coefficients are determined using a
hypothetical complex refractive index and the overall reflectance is obtained. The required complex refractive index of heavily doped silicon is considered next. The Drude model is used to obtain the substrate conductivity and the refractive index and the extinction coefficient are obtained phenomenologically from the complex Maxwell equations.

In Chapter 4 the stochastic signal processing model of FTIR is combined with the dispersive model of the epi-substrate sample's reflected intensity to obtain a rigorous mathematical expression for the expected interferogram. DSP techniques are used to convert a continuous frequency continuous time model into discrete frequency discrete time counterpart. DSP simulations are performed and compared to the experimental results. Limitations of interferogram-domain modeling stemming from the uncertainties about the responses of electronic and optical components of FTIR are discussed.

Chapter 5 discusses the reflectance measurements by FTIR. The advantages of frequency-domain measurements and modeling over the conventional interferogram-domain methods are discussed. The experimental results from the measurements on the bare substrates and the epi-on-substrate samples are presented. The previously derived model of FTIR-epi/substrate system is used in the frequency domain to determine the substrate doping concentration and resistivity for the case of bare substrates, and epi film thickness in addition to the substrate doping concentration and resistivity for the case of
epi film on substrate. The comparisons between the experimental results and the model predictions are presented for both the bare substrates and epi-on-substrate samples.

The Summary section concludes the thesis by summarizing the results and discussing some ideas for the follow-on work.
Chapter 1: Introduction

1.1 Thin Epitaxial Films and the Need for Their Control

Silicon epitaxy is a process where a thin layer of crystalline silicon is grown on a crystalline silicon substrate. It is one of the most common steps in the modern IC fabrication process, used to manufacture analog and digital, discrete and integrated devices in CMOS, BiCMOS and bipolar technologies\(^1\). The reasons for using epi in the IC fabrication are many and varied, but the overwhelming majority of cases include growing a lightly doped epi on a heavily doped substrate. Modern CMOS and BiCMOS processes use heavily doped substrate to improve resistance to latch-up, while the lightly doped oxygen- and carbon-free epi preserves high mobility necessary for good device performance\(^2\). In the discrete and analog bipolar processes, the lightly doped epi is used to improve the breakdown voltage of the device while heavily doped buried layer improves collector resistance\(^3\). The low end of the epi film thickness in the modern IC process currently stands at 0.5 um - 1um. Continuing lateral and vertical scaling of the IC features will undoubtedly cause this number to decrease. In addition, some advanced device structures such as elevated source/drain in sub-0.1 um MOSFETs and heterojunctions in advanced Si-Ge HBTs already utilize epi layers as thin as 100 nm. As the traditional IC devices continue to shrink and advanced structures emerge from the research environment, accurate control, preferably in-situ, of epitaxial film thickness becomes increasingly important. In order to achieve this, an accurate fast non-destructive method of determining epi film thickness is necessary.
1.2 Optical Characterization Techniques: Ellipsometry vs FTIR

Optical techniques have traditionally been utilized to perform thin film and surface analysis of materials and are natural applications for thin epi measurements. In order to utilize optical techniques for thin epi analysis, an optical contrast must exist between epi and the substrate. Such contrast indeed exists due to the difference in the doping levels and is discussed in some detail in Chapter 3. 2 techniques are most promising: ellipsometry and Fourier Transform Infra-Red Spectrometry (FTIR). Both have their pros and cons.

1.2.1 Ellipsometry

Ellipsometry has been particularly popular in thin film analysis\textsuperscript{4,5}. Ellipsometry as applied to thin film analysis measures two quantities: $\tan \Psi$ is the ratio of the amplitudes of the reflected p (parallel) and s (perpendicular) polarized electric fields; and $\Delta$: the phase difference of the above p- and s- polarized fields. The combined complex quantity is expressed as

$$\tan \Psi e^{i\Delta}$$

As ellipsometry utilizes visible light as the source, it is very well suited to measurement of films of thickness comparable to the wavelength of the light - sub-1 um and below. As ellipsometry provides information on both amplitude and phase of the reflected intensity, it is a valuable tool for material analysis. The problem with this technique as applied to thin epi analysis is that the optical contrast between silicon epi and substrate exists only in the infra-red range of frequencies: the wavelengths of 2.5 um and and longer. The
typical ellipsometers utilize the wavelengths shorter than 1 um which are incapable of
detecting the optical interface. The required infra-red ellipsometers are proving to be
difficult to construct due to the problems with polarizers and detectors. The field of infra-
red ellipsometry is still in its infancy, and significant efforts must be made for the
technique to achieve its potential. Nevertheless, infra-red ellipsometry holds significant
promise for thin epi measurements.

1.2.2 FTIR

As an instrument, FTIR consists of a Michelson interferometer coupled to a computer
system\(^6\). A schematical representation of a Michelson interferometer is shown in Figure
1.

![THE MICHELSON INTERFEROMETER](image)

**Figure 1: Schematic of Michelson interferometer**
A Michelson interferometer divides a beam of radiation from an ir coherent infra-red source into two paths and recombines them at the detector after a path difference has been introduced, creating a condition under which an interference between the two beams can occur. The intensity variation as a function of the path difference is captured by the detector and results in the interferogram.

The typical interferogram of the epi film on substrate is shown in Figure 2. The interferogram consists of a strong center burst and two similar smaller bursts positioned symmetrically to the sides of the center burst. The epi film thickness is determined according to the following formula:

\[ d = \frac{\Delta}{2n\cos \theta} \]

where \( d \) is the epi film thickness, \( 2\Delta \) is the distance between the side-bursts in the interferograms (same as the path difference between the two beams), \( n \) is the refractive index of silicon epi, and \( \theta \) is the angle of refraction in epi.
Epi film thickness measurements by FTIR has several key advantages over ellipsometry:

- interferogram collection is fast: an interferogram is typically collected in less than a minute, making it suitable for real-time in-situ control/monitoring application;
- FTIR uses infra-red source in the range of 2.5 um to 40 um, which captures most of the range in which the optical contrast between epi and substrate occurs;
- The instrument (Michelson interferometer) is simpler than ellipsometer with fewer optical components: therefore it's less prone to suffer from instrument errors/components imperfections, and cheaper to acquire and operate;
- Sidebursts can be easily identified, resulting in the simpler thickness readout.

FTIR has been the traditional tool in the semiconductor industry for thick epi analysis.
Nevertheless, epi thickness measurements by FTIR are less successful in the case of thinner films. From Eq 1.1 it can be seen that as the film thickness $d$ get smaller, the sidebursts move closer together and eventually get swamped by the centerburst. Figure 3 shows the interferogram of the 0.5 um epi film. It can bee seen that the sidebursts can not be identified in this interferogram.

![Interferogram of 0.5 um epi film on P substrate](image)

**Figure 3: Interferogram of 0.5 um epi film on P' substrate**

Clearly, the epi thickness reading by the identification of the side-bursts in no longer available for the case of thinner films. However, the shape of the interferogram is still a function of the film thickness, and therefore can be used to obtain it. The rest of this thesis deals with the techniques for achieving this.
Chapter 2: FTIR Fundamentals and Statistical Signal Processing

The measurements presented in this thesis were performed using FTS-40 series FTIR manufactured by BioRad corporation. The schematic of the instrument is shown in Fig 4. As can be seen, the instrument is considerably more complicated than the simplified schematic presented in Fig. 1 earlier.

![Figure 4: Schematic of BioRad FTS 40 FTIR](image)

Yet it functions in the same way: divide the incident beam in two; introduce the path difference; recombine the beams at the detector. Let $E_0$ be the (complex) electric field entering the FTIR. Let path 1 be the path traveled by the field reflected from the fixed mirror, and path 2 for the field reflected from the moving mirror. If the length of the Path 1 is $X$, then the length of the Path 2 is $X-\Delta$, where $\Delta/2$ is the position of the moving mirror from its equilibrium point. Then the intensity at the detector is given by:

$$I(\Delta) = \left\langle \frac{1}{4} \times |E(x) + E(x - \Delta)|^2 \right\rangle$$

$$= \frac{1}{4} \left\langle |E(x)|^2 + |E(x - \Delta)|^2 + 2 \text{Re}[E(x)^* E(x - \Delta)^*] \right\rangle$$
Here, \( < > \) indicate time average quantity, * indicate complex conjugation, and \( || \) absolute quantity magnitude.

### 2.1 Statistical properties of white light

White light or chaotic light can be described as resulting from radiation of a number of oscillators at a variety of frequencies whose phases are statistically distributed random variables\(^7\). A good example of chaotic light is the gas discharge lamp, where the different atoms are excited by the electronic discharge and emit their radiation independently of one another. The shape of the resulting intensity is a function of the statistical distribution of the atomic velocities and the occurrence of collisions. Other examples of chaotic light include thermal cavity and the filament lamp. The IR source for the BioRad FTIR, the high temperature cooled ceramic source, is an example of the latter. It is clear that the electric field of the chaotic light will be randomly distributed in time, and as such, will be a random process.

Figure 6 shows electric field radiated by a single atom, which experiences random collisions.

![Electric field](image)

**Figure 5**: The electric field amplitude of a single atom suffering random collisions.
2.2 Wide Sense Stationarity and Ergodicity

A random process is a time-varying quantity (e.g. electric field in case of chaotic light) whose value at a given point in time is a random variable. A random process in general is characterized by the joint probability density of all of its values in time:

\[ p_{x(t_1), x(t_2), \ldots, x(t_n)}(X_1, X_2, \ldots, X_n) \]

For many processes, the quantities of interest are their mean and covariance function. A mean of a process is given as:

\[ m_x(t) = \int X(t) p_x(X)dX \]

And the covariance is:

\[ K_{xx}(t, s) = \int \int X(t) X^*(s) \cdot p_{x(t), x(s)}(X(t), X(s))dX(t)dX(s) \]

\[ = X(t)X^*(s) \]

Where \{ \} indicates statistical average.

Chaotic light belongs to a class of processes called Wide Sense Stationary (or WSS) and Ergotic. For WSS process, it's covariance function \( K_{xx} \) is only a function of the separation between \( t \) and \( s \) (call it \( \tau \)). For ergotic process, the statistical average is equivalent to time average. This allows us to replace our earlier expression for the intensity at the detector by a much simpler expression:

\[ I = 1/2|E(x)|^2 + 1/2 \Re K_{EE}(\Delta) \]

As \( |E(x)|^2 \) is a constant independent of \( \Delta \), it can be easily removed from the interferogram, and the resulting item is nothing more than a half of the real part of the covariance function of the chaotic light emitted by our source.
2.3 Power Spectral Density and the Wiener-Khinchine Theorem

Power Spectral Density of a process, or \(S_{xx}(j\omega)\) is the amount of energy contained in the process at frequency \(\omega\). It is also mathematically defined as the variance of the random process when filtered by the bandpass filter whose frequency response \(H(j\omega)\) is:

\[
H_{\omega}(j\omega) = \frac{\sqrt{2\pi / \epsilon}}{\epsilon} \quad \text{for } |\omega - \omega_0| < \epsilon / 2
\]

\[0 \quad \text{otherwise}
\]

Wiener-Kinchine theorem states that Power Spectral Density \(S_{xx}(j\omega)\) of a WSS process \(X(t)\) is the Fourier Transform of its covariance function \(K_{xx}(\tau)\)

\[
S_{xx}(j\omega) = \int_{-\infty}^{\infty} K_{xx}(\tau)e^{-j\omega \tau} d\tau
\]

Therefore the spectral intensity of our IR source is easily obtained from the interferogram by performing a Fourier Transform. It also becomes clear why this technique is called Fourier Transform Infra-Red Spectroscopy: the power spectrum and the interferogram are the Fourier Transform pairs.

2.4 White Light and the Paley-Wiener Theorem

A class of processes is called White Noise process if \(K_{xx}(\tau) = \delta(\tau)\), where \(\delta(\tau)\) is the Dirac delta function. Applying the Wiener-Kinchine theorem, it’s easy to see that the Power Spectral Density \(S_{xx}(j\omega)\) of a White Noise process is uniform unit amplitude everywhere. Pawley-Wiener Theorem allows to represent a WSS process \(X(t)\) with a non-uniform \(S_{xx}\) as a response of a certain filter \(H(j\omega)\) to a White Noise process subject to a constraint

\[
\int \left| \frac{\ln S_{xx}(j\omega)}{1 + (\omega / 2\pi)} \right| d\omega < \infty
\]
The filter response $H(j\omega)$ is given by:

$$S_{xx}(j\omega) = |H(j\omega)|^2$$

Now we can see that for the case of the ideal Michelson interferometer we can represent the intensity falling on the FTIR detector as the following system function in the frequency domain:

$$I_w \quad \frac{|H_s(j\omega)|^2}{\quad} \quad I_d$$

Where $I_w$ is the intensity of the white noise process, and $I_d$ is the intensity reaching the detector.

2.5 FTIR non-idealities and the signal processing model of the real FTIR

So far we only considered the ideal FTIR driven by the non-ideal IR source. We showed that the resultant intensity is equivalent to that produced by an ideal white noise process passing through a shaping filter $H_s(j\omega)$. However, the real FTIR contains certain components whose non-ideal behavior must be accounted for. These components are the beam splitter and the detector. Let $H_b(j\omega)$ be the response of the beam splitter to the incident electric field, and $H_d(j\omega)$ be the response of the detector to the incident intensity.

Then the overall system function of the FTIR is seen as following:

$$I_w(j\omega) \quad \frac{|H_s(j\omega)|^2}{\quad} \quad \frac{|H_b(j\omega)|^2}{\quad} \quad H_d(j\omega) \quad I_d(j\omega)$$

Figure 6: Signal Processing Model of non-Ideal FTIR
Notice the absence of the magnitude squared in the third system function. This is because the detector responds to the intensity, and not the electric field. This has certain implications which will be discussed in the follow-on chapters (see Chapter 4).
Chapter 3: Dispersive Optics of Silicon

In our construction of the signal processing model of FTIR, the Michelson interferometer was driven by the IR source. In the case of epi measurements, the IR source is reflected from the sample prior to entering the FTIR. The schematic of the measurement set-up is shown in Fig. 7.

![Figure 7: Schematic of epi thickness measurement set-up](image)

Chapter 2 showed that the Fourier transform of an interferogram is the intensity entering the FTIR. In order to be able to model the FTIR interferogram as the function of epi film thickness, an accurate model of the intensity reflected off the sample needs to be constructed. This is the subject of the present chapter.
3.1 Complex Maxwell equations and complex index of refraction

The complex Maxwell equations for the case of linear media are presented below:\(^9\):

\[
\begin{align*}
\nabla \times \mathbf{E} &= -j\omega\mu\mathbf{H} \\
\nabla \times \mathbf{H} &= j\omega\varepsilon\mathbf{E} + \mathbf{J} \\
\nabla \times \varepsilon\mathbf{E} &= \rho \\
\nabla \times \mu\mathbf{H} &= 0
\end{align*}
\]

These can be combined in the wave equation:

\[
\nabla^2 \mathbf{E} = \omega^2 \varepsilon\mu\mathbf{E}
\]

The solution of the equation is a monochromatic wave:

\[
\Psi(\mathbf{r}, t) = A e^{i(\omega t - k\mathbf{r})}
\]

where \(k\) is the wave vector, \(\mathbf{r}\) is the coordinate vector, \(\omega\) is the angular frequency, \(\varepsilon\) is the polarization, and \(\mu\) is permittivity. One defines \(c\) the speed of light in medium as \(\omega / k\).

From the wave equation

\[
c = \frac{\omega}{k} = \sqrt{\frac{1}{\mu\varepsilon}}
\]

One defines \(n\) the complex index of refraction as the ratio of the speed of light in the media to that in vacuum. Thus in vacuum, \(n\) is real and unity. The complex refractive index \(n\) can be written as

\[
n = n - ik
\]

where \(n\) is the refractive index and \(k\) is the extinction coefficient. The are usually frequency dependent quantities.
3.2 Reflection from epi-substrate, Fresnel coefficients, and the total reflected intensity.

The subject of transmission and reflection of E&M waves in layered media has been treated in several books\(^{10,5}\). The schematic presentation of the situation pertaining to epi on substrate is presented in Fig. 8.

![Diagram of reflection and transmission in the epi-substrate system](image)

**Figure 8: Reflection and transmission in the epi-substrate system**

Let \(n_0\), \(n_1\), and \(n_2\) be the corresponding indexes of refraction in the air, epi, and substrate, and \(\varphi_0\), \(\varphi_1\), \(\varphi_2\) be their (complex) angles of incidence/refraction. The Fresnel reflection coefficient \(r_{jk}\) is defined as the ratio (complex) of the reflected electric field from the media \(k\) to the incident in the media \(j\). Like wise, the Fresnel transmission coefficient \(t_{jk}\) is defined as the ration of the transmitted electric field in the media \(k\) to the incident in the media \(j\). The overall Fresnel reflection coefficient \(R\) is the ratio in the reflected electric field from the overall epi-substrate system to the incident. In addition, the field polarizations must be considered as well. S-polarization stands for perpendicular, and p-
polarization for parallel. Solving the Maxwell equations with the corresponding boundary conditions for the air-epi-substrate system, we get the following expressions for the overall Fresnel reflection coefficient $R$:

\[
R_p = \frac{r_{01p} + r_{12p}e^{-j2\beta}}{1 + r_{01p}r_{12p}e^{-j2\beta}}
\]

\[
R_s = \frac{r_{01s} + r_{12s}e^{-j2\beta}}{1 + r_{01s}r_{12s}e^{-j2\beta}}
\]

where

\[
r_{01p} = \frac{n_1 \cos \varphi_0 - n_0 \cos \varphi_1}{n_1 \cos \varphi_0 + n_0 \cos \varphi_1}
\]

\[
r_{12p} = \frac{n_2 \cos \varphi_1 - n_1 \cos \varphi_2}{n_2 \cos \varphi_1 + n_1 \cos \varphi_2}
\]

\[
r_{01s} = \frac{n_0 \cos \varphi_0 - n_1 \cos \varphi_1}{n_0 \cos \varphi_0 + n_1 \cos \varphi_1}
\]

\[
r_{12s} = \frac{n_1 \cos \varphi_1 - n_2 \cos \varphi_2}{n_1 \cos \varphi_1 + n_2 \cos \varphi_2}
\]

and

\[
\beta = 2\pi \left( \frac{d_1}{\lambda} \right) \left( n_1^2 - n_0^2 \sin^2 \varphi_0 \right)^{1/2}
\]

Here, $\beta$ is the phase difference between the incident and reflected waves due to the wave travelling in the film.

The overall reflectance $R$ is the ratio in the reflected and incident intensities and is

\[
R = |R|^2
\]

for the corresponding polarization.
3.3 Silicon optical constants in the infra-red

Having derived the required reflection coefficients and reflectance, we must now turn attention to the determination of the complex index of refraction $n$. In order to do this, we have to go back to the complex Maxwell equations. In particular, replace the term $J$ in the second equation by

$$J = \sigma E$$

we obtain for the second equation:

$$\nabla \times H = j \omega E + \sigma E$$

$$= j \omega E (1 - j \sigma_0 \omega) E$$

and we can define complex dielectric constant $\varepsilon$ as

$$\varepsilon = \varepsilon (1 - j \sigma_0 / \omega \varepsilon)$$

and the previous solutions to the Maxwell equations including our expressions for the reflection coefficients and reflectance hold true with the new $\varepsilon$.

We are not quite finished yet, as we need to determine the conductivity $\sigma$.

For that, we can use the Drude model of conductivity\(^1\), where

$$\sigma(\omega) = \frac{\sigma_0}{1 - j \omega \tau}$$

and

$$\sigma_0 = \frac{ne^2}{m}$$
Here, $\tau$ is the scattering time, $n$ is the carrier concentration in the substrate, $m$ is the effective mass of electron or hole in the substrate, and $e$ is the electron/hole charge. The scattering time $\tau$ can also be obtained from resistivity $\rho$ as $\tau = \frac{m}{\rho ne^2}$.

Using these expressions, we can determine the overall complex dielectric constant as

$$\varepsilon = \varepsilon' - j\varepsilon'' = [\varepsilon(\omega) - \frac{\tau}{1 + \omega^2 \tau^2}; \sigma_0] + j\sigma_0 \left[\frac{1}{\omega (1 + \omega^2 \tau^2)}\right]$$

where $\varepsilon'$ and $\varepsilon''$ are the real and imaginary parts of the complex dielectric constant.

Using the above expression and remembering that

$$n = n - jk = \sqrt{\varepsilon}$$

we get

$$n^2 = \frac{1}{2}(\sqrt{\varepsilon'^2 + \varepsilon''^2} + \varepsilon') \quad \text{and} \quad k^2 = \frac{1}{2}(\sqrt{\varepsilon'^2 + \varepsilon''^2} - \varepsilon')$$

We now have the necessary expressions to be able to calculate the required silicon optical constants. Fig. 9 and 10 show simulations of the refractive index and extinction coefficient for several silicon substrates.
Figure 9: Plot of refractive index as a function of frequency for 3 different substrates

Figure 10: Plot of extinction coefficient as a function of frequency for 3 different substrates

The *wavenumber* is defined as the inverse of the wavelength in cm: 10000 wavenumbers is equivalent to 1 um.
Here, we can see that as the doping level and conductivity in the substrate decline, the substrate begins to look optically as a dielectric epi. We can also see that the concentration level of 1e18 cm$^{-3}$ is about the lowest concentration at which the optical contrast exists between the epi and the substrate. Yet another observation is that the optical contrast exists only for a limited range of frequencies: at frequencies approaching 5000 wavenumbers, substrate begins to look like a dielectric.

3.4 Effects of the native oxide.

A very thin layer of native oxide (up to a few nm) is usually present on the epi. The question of whether this layer effects the measurements must be considered. From the previously derived expression for the film phase difference $\beta$, consider SiO$_2$ film thickness of 1 nm, and wavenumber $k$ of 4500 (extreme case). A quick calculation produces $\beta = 3.02E-2$, which results in $e^{-j2\beta} = 1$. Substituting this into the expressions for the total reflection coefficients, it's a simple exercise to show that native oxide has no effect on either the measurements or on simulations as long as the requirement $e^{-j2\beta} = 1$ is satisfied.

Physically, this means that as long as there is no interference between the wave reflected from the air-oxide interface and the oxide-epi interface (the two waves are in phase), light emerges from the oxide un-attenuated and undisturbed.
Chapter 4: Signal Processing Model of FTIR/Epi/Substrate System and Interferogram-domain Modeling

4.1 Complete Model

We now have the necessary expressions to obtain the complete signal processing model of the FTIR/Epi/Substrate system in the frequency and interferogram domains. In the frequency domain, the model is shown in the block diagram below:

$$I_w(j\omega) \overset{|H_s(j\omega)|^2}{\to} |H_b(j\omega)|^2 \overset{R(j\omega)}{\to} H_d(j\omega) \to I_d(j\omega)$$

where $H_s$ is the system function of the IR source, $H_b$ is the system function of the beam splitter, $R$ is the total reflectance of the epi-substrate system (see Chapter 3), and $H_d$ is the system function of the detector. $I_w$ is the intensity of the white noise, and $I_d$ is the intensity read by the detector.

4.2 Interferogram domain modeling

We obtain the interferogram by performing inverse Fourier transform of the detected spectral intensity $I_d$ (see Chapter 2). Since we are dealing with a continuous time continuous frequency problem, it is efficient to convert it into its discrete time discrete frequency counterpart and take advantage of the DSP techniques such as Fast Fourier Transform to speed up the calculations. The procedure for accomplishing this is presented in Fig. 1, and simulations for the case of 2 um and 4 um films in Figs 12 and 13.
Figure 11: Interferogram modeling by DSP
4.3 Discussion of the simulated interferograms

Examining the Figs 12 and 13, we can see that the sidebursts which are visible in the 4 um film, disappear in the 2 um film interferogram. Physically, we can understand the shape and position of the centerburst and the sidebursts as follows: the total reflected electric field $E$ is made up of a primary field $E_0$, reflected from the epi, and an infinite series of secondary fields which bounce in the epi before emerging from it. Thus field $E_1$ undergoes one bounce, field $E_2$ two bounces, etc. On each bounce the field is attenuated considerably. The detected intensity is made up of the interference of these fields. The center burst is due to the interference of $E_0$ with itself, and therefore the strongest, the primary sidebursts are due to the interference between $E_0$ and $E_1$, and are considerably weaker. All other interference cases, such as due to $E_1$ and $E_2$ are weaker still and can be neglected. The position of the bursts is the optical path difference between the two interfering waves: for the centerburst it's zero, therefore it's positioned at the center. For the sidebursts it's the distance travelled by the light in the epi. As the epi thickness is reduced, the sidebursts move closer to the centerburst. The width and the shape of the bursts is due to the finite bandwidth and particular shapes of the system functions which make up the signal processing model of the FTIR/Epi/Substrate system. The width of the bursts is inversely proportional to the overall bandwidth by the uncertainty principle. This should also be clear from the discussion in Chapter 2.
4.4 Limitations of the interferogram modeling

If we compare the simulated interferograms of Figs. 12 and 13 with the experimental ones shown in Figs. 2 and 3, we can see that they are quite different. In particular, the modeled interferograms are symmetric, while the experimental ones exhibit some asymmetry. The asymmetry is due to the fact that the system function of the detector $H_d$ has imaginary component, which we don't know. In addition to the asymmetry, we also have difficulty estimating the responses of the beam splitter and the IR source. While it's possible to characterize a particular FTIR, the instrument-to-instrument variations preclude this from being a viable option.
Chapter 5: Reflectance Measurements

5.1 Advantages of reflectance measurements

In the previous chapter we concluded that interferogram domain modeling has limited accuracy due to the uncertainties in the frequency responses in the electronic and optical components of FTIR. These can be eliminated by performing reflectance measurements. In the reflectance measurements one ratios the intensity reflected from the epi-substrate system by that reflected by a highly reflecting gold mirror. Since the parasitic frequency responses of the optics and electronics appear both in the numerator and denominator, they cancel. Both reflected intensity and the reference intensity are obtained from the corresponding interferograms using the DSP techniques described in Chapter 4.

Fig. 14 shows a typical reference intensity.

![Figure 14: Reference intensity](image)

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5.2 Reflectance measurements of heavily doped substrates: measurements of resistivity and dopant concentrations

5.2.1 Experimental reflectance waveforms of various substrates

As previously shown in Chapter 3, the optical constants in heavily doped silicon substrate depend on the doping level and resistivity. Therefore the shape of the reflectance curve is a function of the latter parameters. This enables to extract these substrate parameters non-destructively from their corresponding reflectance waveforms. Fig. 15 shows experimentally determined reflectance curves from several substrates of varying dopant concentration, resistivity and dopant types. The samples are described in Table 1.

Figure 15: Reflectance spectra of various silicon substrates

<table>
<thead>
<tr>
<th>Sample</th>
<th>Graphical representation</th>
<th>Dopant type</th>
<th>Substrate orientation</th>
<th>Nominal resistivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>S12</td>
<td>------------------------</td>
<td>Boron</td>
<td>100</td>
<td>0.001-0.002</td>
</tr>
<tr>
<td>S44</td>
<td>---</td>
<td>Arsenic</td>
<td>100</td>
<td>0.005-0.01</td>
</tr>
<tr>
<td>Blk1</td>
<td>---</td>
<td>Antimony</td>
<td>100</td>
<td>0.008-0.02</td>
</tr>
</tbody>
</table>

Table 1: Substrate samples for reflectance measurements

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5.2.2 Polarization averaging and determination of substrate dopant concentration and resistivity by optimization of parameters.

We can use previously developed formulas for the reflectance from the epi/substrate system for the case of substrate by setting film thickness \( d \) to zero. By optimizing the parameters \( \rho \) and \( N \) - substrate resistivity and dopant concentration - for the best fit against the experimental reflectance, we can extract the above parameters. Before we attempt to do this, we must consider the question of polarization. From the expressions for the reflectance in Chapter 3, we see that the answers are different for s- and p-polarized light. Fig. 16 shows simulated reflectance for a case of a hypothetical substrate of \( N = 1.25 \times 10^9 \text{cm}^{-3} \) and \( \rho = 0.015 \text{ohm-cm} \).

![Graph of reflectance vs. wavenumbers](image)

**Figure 16:** Substrate reflectance of s- and p-polarized light.
In Chapter 2 we showed that chaotic light can be modeled as that produced by radiators with statistically distributed phases and polarizations. Therefore the total intensity of the randomly polarized light is the sum of the two polarizations. Therefore the right procedure for our simulations is to take the average of the two polarizations and optimize it against the experimental reflectance spectrum. Such optimization was performed for two substrate samples from the Table 1: S12 and Blk1. The resulting waveforms after the optimization are presented in Fig. 17 and 18 on the next page. The extracted parameters are presented in Table 2 below.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Dopant type</th>
<th>Nominal resistivity</th>
<th>Extracted resistivity</th>
<th>Extracted concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>S12</td>
<td>Boron</td>
<td>0.001-0.002</td>
<td>0.0015</td>
<td>1.25E20</td>
</tr>
<tr>
<td>Blk1</td>
<td>Antimony</td>
<td>0.008-0.02</td>
<td>0.02</td>
<td>3E18</td>
</tr>
</tbody>
</table>

Table 2: Extraction of dopant concentration and resistivity
Figure 17: Model vs. experiment for sample S12

Figure 18: Model vs. experiment for sample Blk1
5.3 Reflectance measurements on thin epi films on substrate: determination of epi film thickness and substrate dopant concentration and resistivity

We now turn to the original objective of this thesis: determination of epitaxial film thickness on substrate. We employ methods similar to those of the previous section, except for we must optimize three parameters simultaneously: epi film thickness, substrate dopant concentration, and substrate resistivity.

5.3.1 Experimental study of reflection spectra of thin epi films on substrate

In order to verify the previous statement that reflectance measurements by FTIR are sensitive to thin silicon epitaxial films, experiments have been performed on two batches of thin epi samples: batch1 consisted of 5 samples of varying film thickness grown on P⁺-doped (Boron) substrate at 900C. Batch2 consisted of 5 thin epi films on P⁺(Boron) substrate of varying film thickness and a blank substrate. Epi was intrinsic for both cases. Their characteristics are shown in the Tables 3 and 4 below, and the corresponding reflectance spectra are shown in Fig. 19 and 20 on the next page.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Substrate type</th>
<th>Nominal resistivity</th>
<th>Nominal film thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>70sec2</td>
<td>P+ Boron</td>
<td>0.005-0.01 (ohm-cm)</td>
<td>0.1 (um)</td>
</tr>
<tr>
<td>82sea4</td>
<td>-</td>
<td>-</td>
<td>0.2</td>
</tr>
<tr>
<td>85sea7</td>
<td>-</td>
<td>-</td>
<td>0.3</td>
</tr>
<tr>
<td>80seg4</td>
<td>-</td>
<td>-</td>
<td>0.4</td>
</tr>
<tr>
<td>27sec1</td>
<td>-</td>
<td>-</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Table 3: Batch 1 characteristics

<table>
<thead>
<tr>
<th>Sample</th>
<th>Substrate type</th>
<th>Nominal resistivity</th>
<th>Nominal film thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>s12</td>
<td>P+ Boron</td>
<td>0.001-0.002 (ohm-cm)</td>
<td>substrate</td>
</tr>
<tr>
<td>s61</td>
<td>-</td>
<td>-</td>
<td>50 (nm)</td>
</tr>
<tr>
<td>s62</td>
<td>-</td>
<td>-</td>
<td>100</td>
</tr>
<tr>
<td>s63</td>
<td>-</td>
<td>-</td>
<td>150</td>
</tr>
<tr>
<td>s64</td>
<td>-</td>
<td>-</td>
<td>200</td>
</tr>
<tr>
<td>s66</td>
<td>-</td>
<td>-</td>
<td>300</td>
</tr>
</tbody>
</table>

Table 4: Batch 2 characteristics
Figure 19: Batch 1 reflection spectra

Figure 20: Batch 2 reflection spectra
From Figs 16 and 17 we can see that given the assumption of the same substrate characteristics for each batch, the reflectance measurements by FTIR are clearly capable of resolving the thin epi films down to 50 nm range.

5.3.2 Determination of epi film thickness, substrate doping level and resistivity by parameter optimization

Having established the sensitivity of the FTIR in the reflectance mode to the epitaxial film thickness, we use methods similar to those of section 5.2.2 to extract the film thickness, and substrate doping concentration and resistivity from their reflectance spectra. The optimization procedure is an order of magnitude more complex due to the inclusion of the extra parameter and was carried out for the case of sample S64 with considerable manual intervention. The waveform after optimization is shown in Fig. 21 below.

![Graph showing experimental and model comparisons for epi thickness extraction](image)

**Figure 21: Model vs. experiment: epi thickness extraction sample S64**
Summary

FTIR in the reflectance mode in combination with accurate models of chaotic light and dispersive optical properties of silicon, and DSP software, appear to be promising tools for non-destructive characterization of thin silicon epitaxial films on highly doped substrate. The work described here focused on intrinsic epi on extrinsic substrate. Similar techniques can potentially be applied to the case of heavily doped epi on extrinsic substrate. It is a reasonable guess to assume that heavily doped epi will be of interest to the semiconductor industry as the push to smaller feature size continues. Heavily doped epi on substrate will result in smaller depletion layer thickness, which tightens the vertical dimensions/tolerances. Extrinsic epi characterization by FTIR would be more challenging than the intrinsic case, since the electric field will be attenuated considerably in the heavily doped epi: a quick calculation for a hypothetical case of P+ epi with \( N = 1.25 \times 10^{19} \text{ cm}^{-3}, \rho = 0.01 \), and film thickness of 1 um shows that the field will be attenuated by approximately factor of 2 with the corresponding reduction in signal strength. In addition, a 3-parameter optimization of the intrinsic epi is replaced with 5-parameter optimization for the extrinsic case. Sophisticated DSP and optimization algorithms will have to be explored to make this method work.

This work also employed the phenomenological theory based on the Drude model for the substrate conductivity to derive the optical constants of the extrinsic silicon substrate. Examining Fig. 17 we can see that the model is more accurate at the shorter wavelength range. At the far-IR the agreement between the model and the experiment, while still
reasonably good, is not as precise. This leads one to consider the applications of other
more physically based models, such as based on Boltzmann transport, to attempt to obtain
a closer agreement between the model and the experiment.

Presently, the majority of FTIRs, including the one utilized in this work, operate between
the wavelengths of 2.5um and 40um for a variety of reasons, which corresponds to
between 250 and 4000 wavenumbers. Since the strongest optical contrast between the epi
and the substrate exists in the far-IR range (see Figs. 9 and 10), it would be advantageous
to extend the FTIR range beyond the current 40 um limit. This will be particularly useful
in the case of heavily doped epi.
References


