Refractive index and extinction coefficient of doped polycrystalline silicon films in infrared spectrum

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Abstract. The refractive index and extinction coefficient in infrared spectrum of the polycrystalline silicon films with different doped dosages, base on the inverse calculation, are obtained by means of utilizing the measured reflectance and transmittance of a layer of material and multilayer films, and the equations derived from photonics and electromagnetic theory. The calculation results demonstrate that the refractive index of the doped polycrystalline silicon films decreases with the doped dosages increasing and the extinction coefficient increases with the doped dosages increasing for a given wavelength. This method used for determining the refractive index and extinction coefficient of the polycrystalline silicon films is effective and has the advantage of that the measured samples are fabricated simply.

1. Introduction
Polycrystalline silicon (Poly-Si) thin film is commonly used for movable structures in the micro sensor base on microelectronics technology, as its fabrication method is compatible with integrated circuit processes, it exhibits excellent mechanical performance and the heavily doped Poly-Si is a conductor. The physical properties of thin films are different from that of bulk materials. Therefore, the research on the properties of the doped Poly-Si film is helpful for micro sensor design. Various methods for the determination of thin film parameters was reported due to thin films can be widely applied in modern optical instrument [1]. In the paper, based on the equations derived from photonics and electromagnetic theory, utilizing the value of the measured reflectance and transmittance of a layer of plate and the multi-layer films, the refractive index and extinction coefficient in infrared spectrum of a layer of Poly-Si film with a certain doped dosage are obtained by means of using the inverse calculation.

2. Measurement equipment
A Fourier transform infrared spectrometer, as shown in Fig. 1, is used for measuring the spectral reflectance and transmittance of samples, which has advantages of higher precision, resolution and efficiency. As the surface of the measured samples is not smooth enough, there are specula reflection and diffuse reflection. Therefore, a non-standard auxiliary integrating sphere, as shown in Fig. 2, is employed in the test to collect reflected and transmitted energy [2].

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In order to provide a high single to noise ratio, the detector in Fourier transform infrared spectrometer is cooled by liquid nitrogen.

3. Sample design and parameter determination

3.1. Sample design

A practical measurement setup requires millimetres size membranes for a reasonable signal level, to ensure the reflected and transmitted energy to be measured accurately [3]. However, the fabrication of the sample in which the free-standing suspended poly-Si film with a thickness of 1-2μm or less satisfies this size is more complex.

In order to solve the problem brought by the dimensions feature above, a series of samples are designed, fabricated and measured, including a silicon (Si) substrate, silicon oxide (SiO$_2$) film/Si substrate, and Poly-Si film with different doped dosages, SiO$_2$ film and Si substrate forming a sandwich structure. In the structure, a layer of SiO$_2$ film grown on the silicon substrate is used for avoiding doped phosphorus into the silicon substrate, to ensure the accuracy of concentration and uniformity of the impurity doped in the Poly-Si film.

3.2. Parameter determination

3.2.1. A layer of material

The spectral reflectance is the ratio of spectral intensity reflected $I_R$ by a sample to the incident spectral intensity $I_0$ upon the sample surface. The spectral transmittance is the ratio of the transmitted spectral intensity $I_T$ to the incident spectral intensity $I_0$.

Using $R$ to denote the reflectance of the sample surface, in accordance with P. Bouguer’s law, the intensity of infrared at a depth $x$ below the sample surface is given by [4]

$$I = I_0 (1-R) \exp(-\alpha x)$$

(1)
where $\alpha$ is the absorption coefficient.

$$\alpha = \frac{4\pi n \kappa}{\lambda}$$  \hspace{1cm} (2)

$$R = \frac{(1-n)^2 + \kappa^2}{(1+n)^2 + \kappa^2}$$  \hspace{1cm} (3)

where $n$ is the refractive index of the sample, $\kappa$ is extinction coefficient, $\lambda$ is the wavelength in vacuum.

For near-normal incidence, according to Equation (1) and considering the multiple reflections in the plate as a sample with the thickness of $w$, using $R = I_r/I_0$ and $T = I_t/I_0$ to denote the reflectance and the transmittance of the plate, therefore, there are

$$R = R \left[ 1 + \frac{(1-R)^2 \exp(-2\alpha \omega)}{1-R^2 \exp(-2\alpha \omega)} \right]$$  \hspace{1cm} (4)

and

$$T = \frac{(1-R)^2 \exp(-\alpha \omega)}{1-R^2 \exp(-2\alpha \omega)}$$  \hspace{1cm} (5)

In accordance with Equations (2)-(5) and the measured dates of $R$ and $T$, the value of the refractive index $n$ and the extinction coefficient $\kappa$ of the silicon substrate can be obtained by using calculation.

3.2.2. Multilayer material

The scheme of multilayer films is shown as Fig. 3.

![Multilayer films diagram](image)

Figure 3. Multilayer films

According to the electromagnetic theory, the equations used for describing the relationship of the reflectance $R_\Sigma$ and the transmittance $T_\Sigma$ of multilayer materials is given by [5]

$$R_\Sigma = \left[ (\eta_0 B - C) \cdot (\eta_0 B + C)^{-1} \right]\left[ (\eta_0 B - C) \cdot (\eta_0 B + C)^{-1} \right]$$  \hspace{1cm} (6)

$$T_\Sigma = (1 - R_\Sigma) \frac{\eta_{k+1}}{\Re(BC')} = \frac{4\eta_0 \eta_{k+1}}{(\eta_0 B + C)(\eta_0 B + C)}$$  \hspace{1cm} (7)

$$\begin{bmatrix} B \\ C \end{bmatrix} = \prod_{j=1}^{k} \begin{bmatrix} \cos \delta_j & i \cos \delta_j \cdot \eta_j^{-1} \\ i \eta_j \sin \delta_j & \cos \delta_j \end{bmatrix} \begin{bmatrix} 1 \\ \eta_{k+1} \end{bmatrix}$$  \hspace{1cm} (8)

$$\delta_j = \frac{2\pi}{\lambda} d_j (n_j^2 - k_j^2 - n_0^2 \sin^2 \theta_0 - i 2 n_j k_j)^{1/2}$$  \hspace{1cm} (9)
where $j$ is the number of the film layer (shown as figure 3); $n_j$ and $k_j$ are the refractive index and the extinction coefficient of the film layer respectively; $d_j$ is the thickness of the film layer; $\theta_0$ is the incident angle. For near-normal incidence, $\eta_0 = n_0$ and $\eta_j = n_j$.

Using Equations (6)-(9), and according to the measured value of $R_\Sigma$ and $T_\Sigma$, the value of the refractive index $n$ and the extinction coefficient $k$ of films can be obtained by using Matlab software based on the inverse calculation.

4. Samples and fabrication processes
There are many factors affecting the material parameters of thin films, such as fabrication environment temperate, crystallite dimension and arranged direction, the doped dosages and the uniformity of the film and so on.
In the sample preparation, the n-type silicon wafer of crystal orientation (100), with thickness of 500 μm and resistivity of 2-4 Ω·cm, is selected as the substrate. The size of the samples is 3.5cm×3.5cm. The prepared samples are as follows:
I. 1# sample is the substrate with parameters above.
II. 2# sample is that a layer of SiO$_2$ film with 300nm thickness is grown on the substrate at temperature of 1000°C by thermal oxidation, which is used for the implanting isolation in order to control the doped concentration of within the Poly-Si film.
III. 3# series samples are that a layer of Poly-Si film of 1 μm thickness is deposited on 300nm thickness SiO$_2$ film with the substrate at temperature of 610°C by low pressure chemical vapour deposition (LPCVD). Then, phosphorus-doped is implanted in a certain dosage, and annealing at temperature of 1000°C. The dosages of sample 3#-1, 3#-2, 3#-3 and 3#-4 are 1.0×10$^{14}$cm$^{-2}$, 6.0×10$^{14}$cm$^{-2}$, 1.6×10$^{15}$cm$^{-2}$ and 5.1×10$^{15}$cm$^{-2}$, respectively.

5. Test, Data Processing and Result Analysis

5.1. Test and Data Processing
The Fourier transform infrared spectrometer (Section 2) is used for measuring the spectral reflectance and transmittance of each sample at the room temperature in a given infrared spectral window in the air.
Data Processing is as follows:
I. Use Equations (2)-(5), in accordance with the value of the measured reflectance $R_\Sigma$ and the transmittance $T_\Sigma$ of the Si substrate for a given wavelength, the refractive index and the extinction coefficient of the Si substrate are obtained by using 1st Opt software based on Powell Optimization.
II. Appling Equations (6)-(9) to 2# sample, according to the refractive index and the extinction coefficient of the Si substrate, and the value of the measured reflectance and the transmittance of 2# sample, base on inverse calculation, the refractive index and the extinction coefficient of SiO$_2$ film for a given wavelength is obtained by means of Matlab software.
III. Appling Equations (6)-(9) to each of 3# series samples, utilizing the refractive indexes and the extinction coefficients of Si and SiO$_2$ above, and the value of the measured reflectance $R_\Sigma$ and the transmittance $T_\Sigma$ of 3# series samples for a given wavelength, base on the inverse calculation, the refractive index and the extinction coefficient of each of 3# series samples are obtained by using Matlab software.

5.2. Results Analysis
The calculation results and the related parameters of samples are tabulated for a given wavelength of 10μm in Table 1.
Table 1. Sample parameters

| Sample number | Implanted dosages cm$^{-2}$ | Refractive index n | Extinction coefficient $\kappa$ |
|---------------|-----------------------------|--------------------|------------------------------|
| 3#-1          | $1.0 \times 10^{14}$        | 3.30               | $3.48 \times 10^{-3}$       |
| 3#-2          | $6.0 \times 10^{14}$        | 3.27               | $1.09 \times 10^{-2}$       |
| 3#-3          | $1.6 \times 10^{15}$        | 3.14               | $2.23 \times 10^{-2}$       |
| 3#-4          | $5.1 \times 10^{15}$        | 2.67               | $2.04 \times 10^{-1}$       |

The calculation results show that the refractive index and extinction coefficient in infrared spectrum of doped Poly-Si films are related to the doped dosages for a given wavelength. The refractive index decreases with the doped dosages increasing, whereas, the extinction coefficient increases with the doped dosages increasing, i.e., the increases in the infrared absorbance of the Poly-Si film depending of the increase in doped dosage in it.

6. Conclusion
The method is effective that refractive index and extinction coefficient of the Poly-Si films with different doped dosages are obtained by the inverse calculation. This determination of film parameters has the advantage of that samples are fabricated simply. In addition, the calculation results demonstrate that the refractive index and extinction coefficient in infrared spectrum of doped Poly-Si films are related to the doped dosages for a given wavelength. This paper only explores an approach to obtain the refractive index and extinction coefficient of films. There is still a lot of result analysis and film optimization work to be done.

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