On refractive index of optical radiation of polycrystalline silicon films

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Abstract. Transmission spectra of layers of polycrystalline silicon on sapphire with a thickness of 0.1 ... 0.8 µm were investigated. The refractive indices were determined in the range of 0.5 ... 2.7 µm. An increase in the refractive index with decreasing wavelength was established. An increase in the film thickness from 0.1 to 0.8 µm led to a decrease in the refractive index from 3.2 to 2.8 at λ = 1.5 µm. Compared to single crystals, the refractive indices of polycrystalline films were lower. The data obtained can be used to build models for calculating the optical characteristics of complex compositions.

1. Introduction

Polycrystalline silicon layers are widely used in semiconductor device technology. This is associated with the use of thin films as elements of integrated circuits, as conductive, resistive and sacrificial layers, as well as with their various applications for the manufacture of sensor devices, solar energy converters, etc. [1–4]. Technological processes for the deposition of polysilicon on various substrates have been well developed [5–7]. The widespread use of polycrystalline silicon films requires knowledge of their properties. At the same time, a high sensitivity of the properties of nano- and polycrystalline silicon to the technology of their production has been noted [8]. In addition to traditional use, it is of interest to use thin polycrystalline layers as optical elements, for example, as integral filters for photodetectors. In this case, one of the most important characteristics of the filter is the refractive index of optical radiation. Its value may depend on the deposition method and film growth conditions. Because of the disordering of the structure, silicon in thin layers can differ significantly in optical properties from crystalline silicon. This makes the development and application of methods for monitoring the electrical and other physical properties of nano- and polycrystalline silicon films urgent. In this regard, we determined the values and investigated the effect of the thickness of the deposited polysilicon film on the value of the optical refractive index. The study was carried out for the most commonly used range of film thicknesses from 0.1 to 0.8 µm.

2. Description of samples and research methods

The refractive index of polysilicon should not differ much in magnitude from the refractive index of monocrystalline silicon. This can cause problems in its experimental determination if silicon wafers are used as a substrate, and the layers under study are thin. In this regard, we used sapphire plates as a substrate, the refractive index of which significantly differed from the refractive index of polysilicon layers. Sapphire substrates are characterized by high surface quality and are widely used in...
nanotechnology [9]. Sapphire has good transmission in the spectral range of 0.17 ... 5.5 μm [10]. This made it possible to observe the interference pattern in the transmission spectra of experimental samples and to determine the refractive index of polysilicon layers in a fairly wide spectral range.

The sapphire plates were 20 mm in diameter and 0.8 mm thick. The deposition of polysilicon was carried out by pyrolysis of monosilane at a temperature of 630 °C in a reactor with a reduced pressure (10–2 mm Hg). In the technological process, a mixture of monosilane with argon (5% SiH4 / Ar) was used. Before the operation of deposition of polysilicon, the sapphire substrates were cleaned twice: in a mixture of sulfuric acid with hydrogen peroxide and in a peroxide-ammonia solution.

To measure the thicknesses of the obtained polysilicon films, we used an automatic spectroscopic ellipsometer "Senduro" manufactured by SENTECH Instruments GmbH (Germany). The transmission spectra were measured on a V670 UF-VID-BLIK JASCO spectrophotometer. In a number of cases, for a more accurate quantitative determination of the transmittance, measurements at fixed wavelengths were carried out using an MDR 21 monochromator by the sample replacement method.

3. Conclusion
The values of the thicknesses of the obtained coatings are presented in table 1.

| Sample number | 1   | 2   | 3   | 4   |
|---------------|-----|-----|-----|-----|
| Film thickness, μm | 0.103 | 0.330 | 0.464 | 0.794 |

Microscopic studies have shown that the resulting films are fairly uniform. Figures 1-2 show surface images obtained with AFM. The polysilicon films consisted of single-crystal grains misoriented relative to each other and separated by amorphous silicon. The surface quality of the film is determined by the roughness and grain size. For each film, the average grain size was estimated and the surface roughness was calculated using the formula:

\[ R_a = \frac{1}{n} \sum_{i=1}^{n} |y_i|, \]

where \( y_i \) is a profile deviation from the centerline.

The surface roughness and standard deviation were determined for three profiles of each film and then averaged. The results are shown in table 2. As seen, with an increase in the coating thickness, an increase in the grain size was observed and the films became less prominent. Surface roughness value \( R_a \) and its standard deviation had significantly lower values compared to the film thickness. This could serve as a basis for confident observation of the interference spectra.

To determine the characteristics of the layers under study, it is necessary to know the refractive index of the optical radiation of the substrate. Such data can be taken from literary sources. However, we considered it expedient to carry out a confirmatory measurement of the refractive index of sapphire, which makes it possible to assess the performance of the experimental models and the validity of the chosen techniques. The data on the measured transmittance of the substrate (T) in the range from 0.4 to 2.5 μm are presented in table 3.

| Film thickness, μm | Average grain size, nm | Average surface roughness, \( R_a \), nm | Standard deviation \( R_a \), nm |
|-------------------|------------------------|----------------------------------------|-------------------------------|
| 0.103             | 10                     | 8.8                                    | 6.4                           |
| 0.330             | 100                    | 5.9                                    | 4.0                           |
| 0.464             | 200                    | 7.1                                    | 4.9                           |
| 0.794             | 400                    | 5.3                                    | 4.2                           |
Figure 1. AFM image of deposited polysilicon films with a thickness of 0.103 μm and 0.33 μm.

Figure 2. AFM image of deposited polysilicon films with a thickness of 0.464 μm and 0.794 μm.

Table 3. Transmittance of the sapphire substrate.

| λ, μm | 0.4  | 0.5  | 0.6  | 1.0  | 1.5  | 2.0  | 2.5  |
|-------|------|------|------|------|------|------|------|
| T     | 0.833| 0.837| 0.851| 0.853| 0.857| 0.859| 0.860|

The absorption coefficient of sapphire in the considered spectral range has a small value (α=1.4·10⁻³ cm⁻¹ at 300 C λ= 2.4 μm) [11]. Then the attenuation of the beam due to absorption at a distance equal to the thickness of the substrate (0.8 mm) will be hundredths of a percent. This makes it possible to take into account only reflection from the plate boundaries in energy calculations. The transmittance of the plate for the case of multiple reflections (figure 3) at normal incidence of the rays can be obtained as the sum of the intensities \( I_1 + I_2 + I_3 + \ldots \), related to the incident radiation intensity \( I_0 \). Since the intensity of each beam is:

\[
I_{n+1} = I_0 (1 - R^2)^2 R^{2n},
\]

the transmittance can be obtained as the sum of the terms of a geometric progression, where \( R \) is a reflectivity from the air-sapphire interface:
In turn, the reflection coefficient for natural light at normal incidence, in accordance with the Fresnel formulas [12], is determined by the refractive index:

\[ R = \left( \frac{n - 1}{n + 1} \right)^2. \]

These dependences make it possible to calculate the values of the refractive index from the experimental data on the transmission of the substrate. The results are shown in figure 4. For comparison, the same figure shows, in the form of a solid line, the dependence of the refractive index of leucosapphire according to work [13]. As can be seen, our data are in good agreement, which may indicate the reliability of the methods used and the efficiency of the experimental setup.

**Figure 3.** Transmission of radiation by a sapphire substrate.

**Figure 4.** Spectral dependence of the refractive index of a sapphire substrate. Points – experiment, line – work data [13].
The transmission spectra of test samples of thin polysilicon layers on sapphire substrates are shown in figures 5 and 6. As can be seen, pronounced interference spectra were observed in all samples. Since the thickness of the polysilicon layers is three orders of magnitude smaller than the substrate thickness, it is possible to associate the features of the spectral distribution with polysilicon. The condition for the interference maximum of radiation transmission for a film of thickness \( h \) is:

\[
2nh = k\lambda.
\]

For the interference minimum, respectively:

\[
2nh = (2k + 1)\frac{\lambda}{2}.
\]

These dependences can be used to determine the refractive index of thin films. The value of the refractive index can be determined from the value of the wavelengths corresponding to the extreme points of the transmission spectrum. For complex spectra, the value of the number \( k \) can be determined by two adjacent extrema \((\lambda_1 > \lambda_2)\) according to the dependence:

\[
k_1 = \frac{\lambda_2}{\lambda_1 - \lambda_2}.
\]

It should be noted that to reduce the error associated with radiation absorption, it is advisable to use data with small values of the number \( k \). Figure 7 shows the obtained spectral dependences of the refractive index for the range of 0.5 ... 2.7 μm. As seen, the refractive index determined by the proposed method was not constant. For each sample, an increase in the refractive index with decreasing wavelength was observed. An interesting fact is that with an increase in the thickness of the deposited layer, a decrease in the refractive index occurred. Thus, at \( \lambda = 1.5 \) μm, an increase in the film thickness from about 0.1 to 0.8 μm led to a noticeable decrease in the refractive index from 3.35 to 2.8. Comparison with the refractive index of monocrystalline silicon [14 - 16] (curve 5) shows lower values of \( n \) for polycrystalline layers. This can lead to the appearance of interference phenomena when a polycrystalline layer is deposited on a single crystal. However, the estimate of the reflection coefficient at the interface at \( \lambda = 1 \) μm is from 1.6% to 0.2% for the used range of polysilicon thicknesses. In many cases, this makes it possible to ignore the interference phenomena and gives rise to research for the practical use of polysilicon coatings as absorption filters for silicon photodetectors.

![Figure 5. Transmission spectra of samples 1 and 2.](image)
Based on the data obtained, for the region of weak absorption in the interference maximum, one should expect an increase in the transmittance for films with greater thickness. This can be indirectly confirmed by the following results of the measured values of the transmittance obtained by the sample replacement method: \( T = 0.79 \) (\( h=0.103 \ \mu m, \lambda=0.74 \ \mu m \)), \( T = 0.85 \) (\( h=0.33 \ \mu m, \lambda=1.087 \ \mu m \)), \( T = 0.86 \) (\( h=0.464 \ \mu m, \lambda=1.428 \ \mu m \)). However, here one should take into account the possible additional influence of the spectral dependence of the refractive index, since the positions of the interference maxima for different thicknesses did not coincide.

The data obtained can be used to build models for calculating the optical characteristics of complex compositions.

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