

Project 2A – Building A Solar Cell (1): Band Gap and Anti-Reflection Coating of Solar Material

In Lab 4 we have investigated the absorption spectrum of Si and the effect of optical coating on the surface reflectance by PC1D simulation. In this project we are going to experimentally measure the transmittance spectrum of Si and derive its band gap, as well as observe the effect of thin Si_3N_4 and SiO_2 films on reducing the surface reflectance.

Objective:

- (1) Measure the band gap of silicon using the transmittance spectrum.
- (2) Study the effect of optical coating layers on the reflectance spectra. Understand the interference in thin film coating and estimate the thickness of the Si_3N_4 and SiO_2 layers from the reflectance spectra.

Experimental Instrument

Monochromators are often used for spectrum analysis (<http://en.wikipedia.org/wiki/Monochromator>). Fig. 1 schematically shows the components of a monochromator. A broad band light source (A), such as an incandescent lamp, is focused onto an entrance slit (B) and is collimated by a concave mirror (C). The collimated beam is diffracted from a rotatable reflection grating (D) (http://en.wikipedia.org/wiki/Diffraction_grating) and the dispersed beam is re-focused by a second mirror (E) at the exit slit (F). Since the grating diffracts light of different colors (i.e., wavelengths) into different angles, each wavelength of light is focused to a different position at the slit, and the wavelength that is transmitted through the slit (G) depends on the rotation angle of the grating. Therefore, by rotating the grating we can observe monochromatic light of different wavelengths at the exit slit and obtain transmission or reflection spectrum.

Diagram of a [Czerny-Turner monochromator](#) removed due to copyright restrictions.

1. Qualitative understanding of a monochromator

We have an antique monochromator opened for you to play with. As you can see, the core part is a rotatable grating, as we mentioned in the previous session. Now either fix your eyes on the grating at a certain angle and slowly turn the knob to rotate the grating, or simply look at the grating from different angles. Do you see a change in the color? Do you understand better how a grating helps to select a beam of monochromatic light?

2: Measure the transmittance of a silicon chip

We are going to measure the transmittance spectrum of a piece of double-side polished silicon wafer to observe the band gap experimentally using Cary 5E UV-Vis-NIR Dual-Beam Spectrophotometer at the Center for Materials Science and Engineering (CMSE).

1. Log onto the computer next to Cary 5E, and open the file “Scan” under “Cary WinUV”
2. Open the method file “Jifeng” under folder “3.003” of “Cary Data”
3. Click on “Set up” and set the scan wavelength range from 300 to 1300 nm
4. Now click on the button “Baseline”. This step measures the transmitted optical signal when no sample is mounted. We will use this data as a reference for 100% transmittance
5. After this step is finished, open the chamber and block the light with black paper board. Then click “zero” on the screen. This step defines 0 transmittance.
6. Now insert the sample into the sample holder such that it covers the hole in the middle. Click on “Start”. Enter the file name “SiTrans” when prompted, followed by sample name “Si wafer”
7. After taking the spectrum, click “finish”, and save the document as a “.CSV” file. This ASCII file records the transmittance vs. wavelength of the Si wafer:

Questions:

1. Why do we use a double-side polished silicon chip? If one or both sides of the wafer are rough how will it affect the measurement result?
2. Can you calculate the band gap of silicon using the transmittance spectrum? Is silicon transparent to visible light? How about near infrared spectrum at wavelengths >1200 nm?
3. Now let us look at the transmittance of Si beyond the band gap (wavelengths >1200 nm). Do you expect any significant absorption in this wavelength range? If not, why is the transmittance much less than 100%? Can you calculate the transmittance in this wavelength range and explain this result? (hint: refractive index of Si is 3.5. Note there is reflection on both the top and bottom surface of Si. Reflectivity $R = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2}$)

3: Measure the reflectance spectrum of Si wafers with and without optical thin film coating

Now let us measure the reflectance spectrum of (a) a piece silicon wafer, (b) a piece of silicon with Si₃N₄ coating, and (c) a piece of silicon with SiO₂ layer using Cary 500i UV-Vis-NIR Dual-Beam Spectrophotometer at the Center for Materials Science and Engineering (CMSE).

1. Log onto the computer next two Cary 500i, and open the file “Scan” under “Cary

WinUV”

2. Load the method file “Jifeng” under folder “3.003”
3. Click on “Set up” and set the scan wavelength range from 300 to 1300 nm
4. Place the mirror into the optical path as a reference for reflectance measurement. Click on the button “Baseline”. This step measures the reflected spectrum with the mirror.
5. After this step is finished, open the chamber and block the light with black paper board. Then click “zero” on the screen. This step defines 0 reflectance.
6. Now mount the double-side polished Si wafer sample onto the sample holder, and move the mirror from the back of the sample holder to the front. **Note that this configuration will let the light beam reflect twice on the Si surface. Therefore, the measured data is actually R^2 (where R is the reflectance). We will need to convert it back to R during data processing.** Click on “Start”. Enter the file name “Reflectance” when prompted, followed by sample name “Si wafer”.
7. When finished, change to the sample with a Si_3N_4 film. Record the color of the sample when looking from the top. Then enter sample name “SiN” and click “Start”
8. Change to the sample with SiO_2 film. Record the color of the sample when looking from the top. Then enter sample name “SiO2” and click “Start”
9. After taking the spectrum, click “finish”, and save the document as a “.CSV” file. This ASCII file records all the reflectance data.

Questions:

1. Derive the reflectance spectra of the three samples from the raw data (note that this data is R^2) and plot them in the same figure. Comment on the effect of Si_3N_4 and SiO_2 thin film coating on the reflectance compared to the bare Si wafer. Will it help to enhance the efficiency of solar cells?
2. Calculate and plot the absorbance spectrum of the Si wafer by using the following equation:

$$\text{Absorbance} = 1 - \text{Transmittance} - \text{Reflectance}$$

and the measured the transmittance and reflectance spectra. What is the absorbance at wavelengths > 1200 nm? Is it consistent with your expectation considering the band gap of Si?

3. Can you explain why there is a step in the reflectance spectrum of the double-side polished Si wafer at wavelengths near 1100 nm? (hint: at wavelengths transparent to Si you be able to see reflected light from the back surface of the sample...)
4. Looking at the reflectance spectrum of the Si_3N_4 and SiO_2 thin film samples, can you explain the color of the surface that you observed?
5. As you have learnt in class, reflectance reaches minimum at wavelengths λ that satisfies $d = (2N + 1)[\lambda/(4n)]$, where d and n are the thickness and refractive index of the thin film coating, respectively, and N is an integer. This is because the light reflected at the air/thin film interface and the thin film/substrate interface has a π degree phase shift and destructively interfere with each other. If $n = \sqrt{n_{\text{air}} n_{\text{substrate}}}$, this destructive interference will completely cancel out the reflection since the magnitude of reflectance at the two interfaces are also equal. On the contrary, if $d = (2N)\lambda/(4n)$ then the phase shift would be 2π for the reflected waves at the two interfaces, and the reflectance reaches maximum due to constructive interference. Therefore, we can use the maxima and minima in the reflectance spectra to estimate the film thickness.

- (1) The refractive index of Si_3N_4 is ~ 2.05 in the wavelength range of 400-600 nm (<http://www.ioffe.ru/SVA/NSM/nk/Nitrides/Gif/si3n4.gif>). Use the reflectance minimum near 600 nm and the maximum near 450 nm to estimate the thickness of the Si_3N_4 film. Input your estimated film thickness and refractive index of Si_3N_4 into PC1D5 to calculate the reflectance spectrum and compare it to the experimental data on the same plot. Are they consistent? What could be the reasons for the small differences?

From what you learnt in Lab 4, would you use a thinner or thicker film for a better anti-reflection coating?

- (2) Do the same for the SiO_2 film. The refractive index of SiO_2 is ~ 1.46 in this wavelength range (<http://www.ioffe.ru/SVA/NSM/nk/Oxides/Gif/sio2.gif>). Note that in this spectrum you have multiple maxima and minima to choose for the calculation and verification.

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