Optical Properties of Ultra Low Absorption Silicon

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Introduction:

Silicon (Si) is a semiconductor that is commonly used for its ability to absorb energy in electronic and photovoltaic purposes, like solar cells. Crystal Silicon (c-Si) is mostly used for these purposes. However, there is also extensive interest in cultivating a different structure of silicon, amorphous silicon (a-Si) that has low absorption and a large energy band gap. This structure of silicon has a more disorganized structure as it is a non-crystalline, with dangling bonds. a-Si has more practical applications in optical coatings for infrared devices. Thin films of a-Si and hydrogenated a-Si (a-Si:H) are synthesized by magnetron sputtering onto a substrate, creating a silicon that has almost double the band gap of c-Si. Substrate temperature, thickness, and hydrogenation affect the band gap and absorption over a broad spectral range.

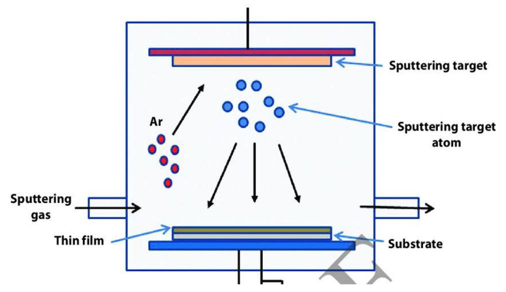
Motivation:

The goal is to use broad-band reflectance and transmittance to check if thin films of a-Si synthesized by magnetron sputtering have large energy band gaps and low absorption.

Method:

Magnetron Sputtering:

Electrons from Si target are sputtered onto substrate to grow thin films

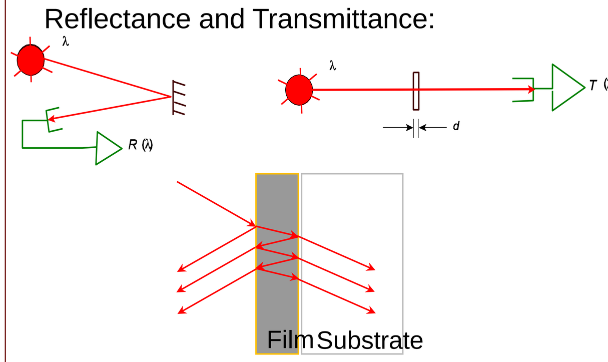


a-Si films:

a-Si:H films:

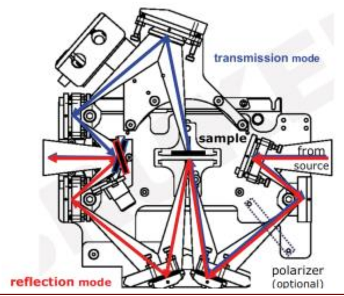
- T23-075( ) – grown at 50°C with thicknesses:
  (A) 60 nm
  (B) 120 nm
  (C) 240 nm
- T23-076( ) – grown at 425°C with thicknesses:
  (A) 60 nm
  (B) 120 nm
  (C) 240 nm
- C23-017A – grown at 50°C thickness 250 nm + 10nm Se capping
- 1 reference silica substrate

Reflectance and Transmittance:



When shining light onto the film substrate, the light will fractionally split between reflectance, transmittance and absorbance. Part of the light will bounce off the film and measure as the reflectance, while the rest goes into the film, refracts back as reflectance while also bouncing into the substrate, where it also refracts and reflects and transmits light through, seen by the representations to the left. Part of the light can be absorbed seen by the equation: $R + T + A = 1$, where R represent reflectance, T represents transmittance, and A represents absorbance.

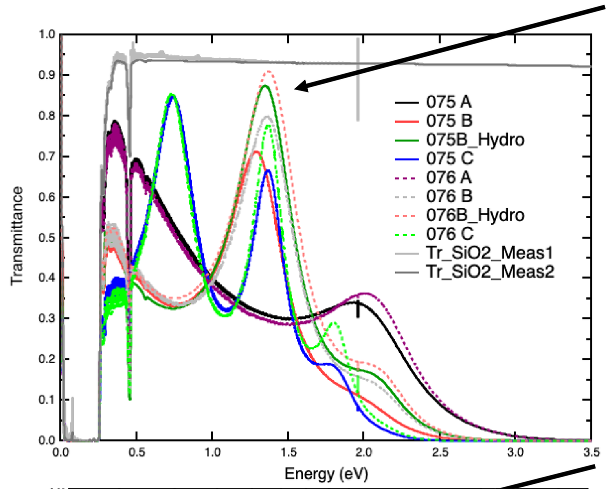
Vertex 70:

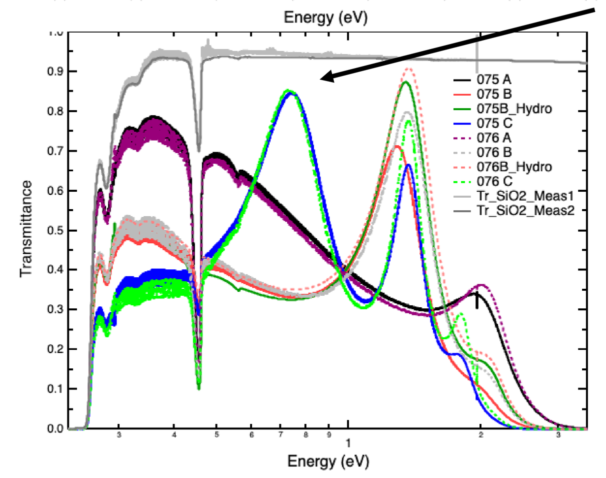


Using the Vertex 70 Spectrometer, we performed combined measurements of broadband optical reflectance and transmittance of the samples (10 meV to 4 eV). Depictions of the reflectance stage can be seen with the red line while the transmittance is highlighted by the blue.

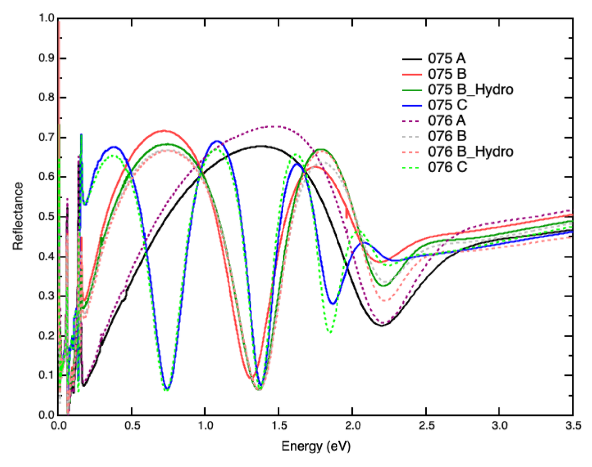
Reflectance and Transmittance:

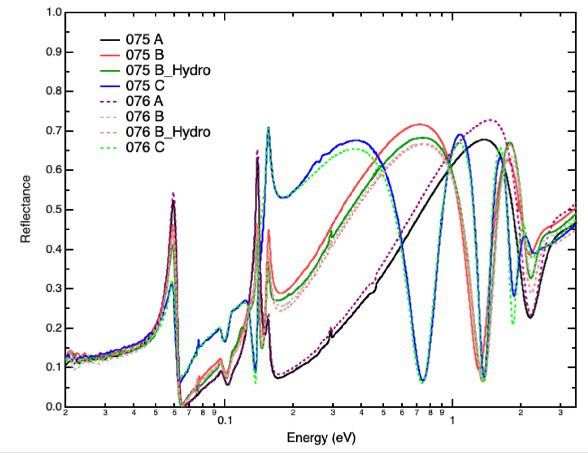
The transmittance of 075B_H and 076B_H seem have the highest transmittance levels relative to silica substrate at higher energies.





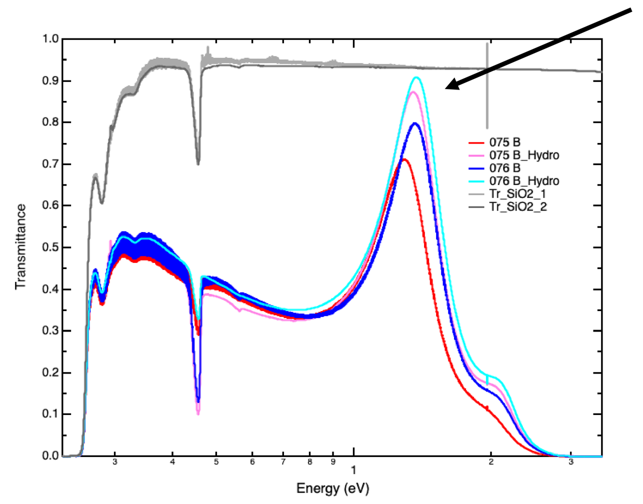
075C and 076C perform decently relative to substrate, but performance drops when it reaches higher energy levels.

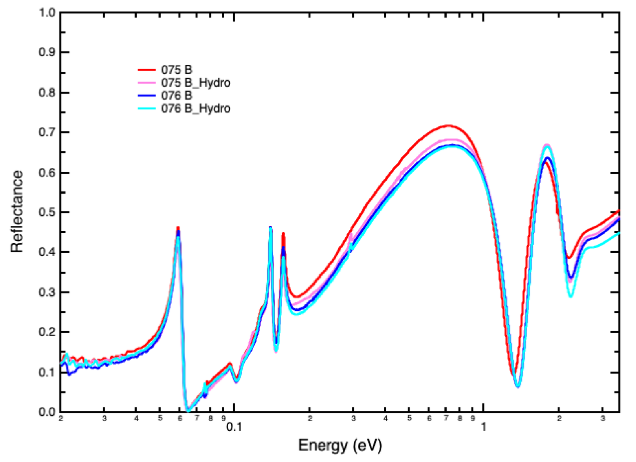


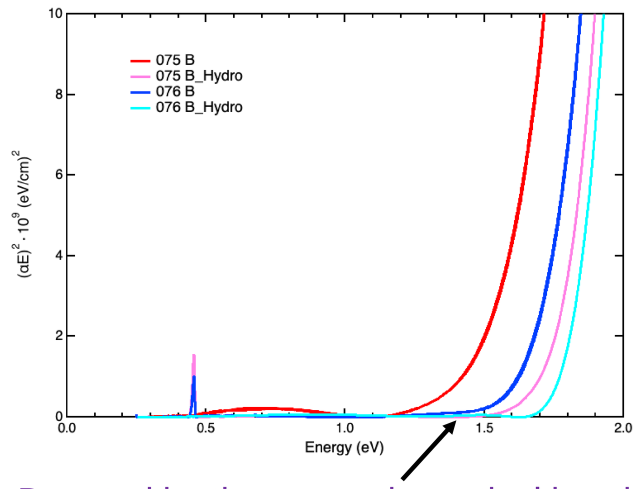


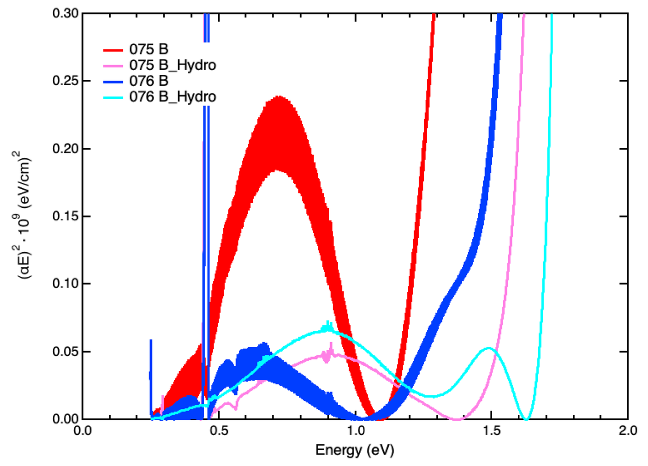
Hydrogenated films:

Denoted by the arrow, transmittance of 075B_H and 076B_H are enhanced and reach the closest to the transmittance of the silica substrate.









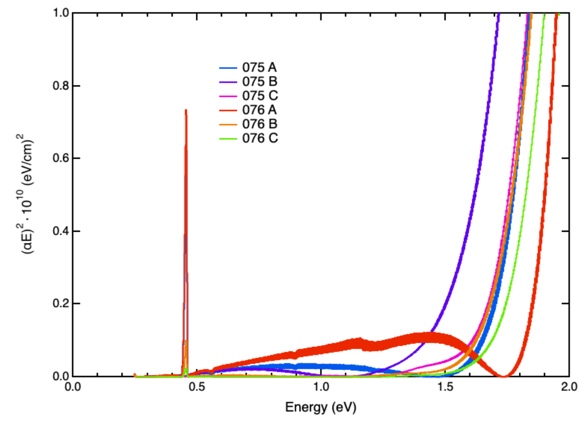
Denoted by the arrow, the optical band gaps for 075B and 076B increase significantly after hydrogenation, leaving a ~0.2 to 0.4 eV increase.

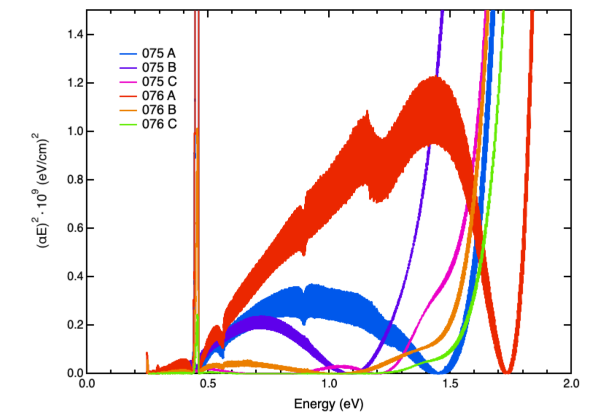
Optical band gap (E_g):

The threshold for a material in which a photon is absorbed is called the optical band gap. Once energy matches or exceeds the band gap, the energy is absorbed. To reach as low absorption as possible, the energy band gap must extend to higher energies. To calculate the absorption coefficient we used the equation,

$$\propto = \frac{1}{\mathrm{d}} \ln\left(\frac{1-R}{T}\right)$$

E_g can be determined as the intercept of the plots (αE)2 vs. Energy (E), shown below for samples: 075 A, B, C and 076 A, B, C (hydrogenated samples not included).





The optical band gap for Si is 1.1 eV. As seen in the graphs, the non-hydrogenated samples exhibit a-Si with optical band gaps of 1.1 to 1.75 eV, which indicate a general increase in the band gap.

Conclusion:

- a-Si and a-Si:H films can be grown in different conditions to obtain higher levels of transmittance and reflectance
  - Leads to lower levels of absorption at higher energies
  - Indicates an increase in the optical band gap
- Hydrogenation of a-Si enhances the advantages of a-Si
  - the transmission and reflectance levels increase
  - reduce the dangling bonds in a-Si
  - reduces mechanical loss
  - Increases optical band gap threshold
  - Lower absorption at higher energies

Overall, hydrogenating the samples does output results that signify an enhancement in transmittance and in the optical band gap, which can suggest further research into growing conditions and hydrogenation.

References:

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- Zhou, R. (2023). Development of Amorphous-silicon-based Optical Coatings for Gravitational-wave detectors. *UC Berkeley*
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