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Light Trapping for Silicon Solar Cells: Theory and Experiment

Hui Zhao

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Abstract

Crystalline silicon solar cells have been the mainstream technology for photovoltaic energy conversion since their invention in 1954. Since silicon is an indirect band gap material, its absorption coefficient is low for much of the solar spectrum, and the highest conversion efficiencies are achieved only in cells that are thicker than about 0.1 mm. Light trapping by total internal reflection is important to increase the optical absorption in silicon layers, and becomes increasingly important as the layers are thinned. Light trapping is typically characterized by the enhancement of the absorptance of a solar cell beyond the value for a single pass of the incident beam through an absorbing semiconductor layer. Using an equipartition argument, in 1982 Yablonovitch calculated an enhancement of $4n^2$, where $n$ is the refractive index. We have extracted effective light-trapping enhancements from published external quantum efficiency spectra in several dozen silicon solar cells. These results show that this “thermodynamic” enhancement has never been achieved experimentally. The reasons for incomplete light trapping could be poor anti-reflection coating, inefficient light scattering, and parasitic absorption.

We report the light-trapping properties of nanocrystalline silicon $\text{nip}$ solar cells deposited onto two types of Ag/ZnO backreflectors at United Solar Ovonic, LLC. We prepared the first type by first making silver nanoparticles onto a stainless steel substrate, and then overcoating the nanoparticles with a second silver layer. The second type was prepared at United Solar using a continuous silver film. Both types were then overcoated with a ZnO film. The root mean square roughness varied from 27 to 61 nm, and diffuse reflectance at 1000 nm wavelength varied from 0.4 to 0.8. The finished cells have a thin, indium-tin oxide layer on the top that acts as an antireflection coating. For both back reflector types, the short-circuit photocurrent densities $J_{sc}$...
for solar illumination were about 25 mA/cm$^2$ for 1.5 micron cells. We also measured external quantum efficiency spectra and optical reflectance spectra, which were only slightly affected by the back reflector morphology.

We performed a thermodynamic calculation for the optical absorptance in the silicon layer and the top oxide layer to explain the experimental results; the calculation is an extension of previous work by Stuart and Hall that incorporates the antireflection properties and absorption in the top oxide film. From our calculations and experimental measurements, we concluded that parasitic absorption in this film is the prominent reason for incomplete light trapping in these cells. To reduce the optical parasitic loss in the top oxide layer, we propose a bilayer design, and show the possible benefits to the photocurrent density.
Light Trapping for Silicon Solar Cells:

Theory and Experiment

By

Hui Zhao

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Isc: Photocurrent
Jsc: Short circuit current density
EQE: External quantum efficiency
IQE: Internal quantum efficiency
$\alpha$: Absorption coefficient
$\rho_0$: Energy density in air
$\sigma_{tot}$: Modes intensity in the semiconductor
$\omega$: Optical frequency for incoming beam
$\beta$: Propagating constant of waveguide
$\Gamma$: Confinement factor
$\sigma_r$: Radiative modes intensity
$\sigma_m$: Waveguide modes intensity
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Chapter 1. Silicon Photovoltaics and Light Trapping

Chapter 1 gives a short introduction to photovoltaic technology and provides the reason for why light trapping is important in silicon solar cell. We will illustrate light trapping ideas and show the corresponding enhanced absorption.

1.1. Photovoltaic Effect and Silicon solar cell

The photovoltaic effect refers to the creation of an electromotive force when light shines on an inhomogeneous semiconductor or a metal-semiconductor contact. The photovoltaic effect was reported initially in 1839 by French physicist Edmond Becquerel, who observed that “electrical currents arose from certain light induced chemical reactions” [1]. In his experiment, AgCl and AgBr coated platinum electrodes were immersed in an aqueous nitric acid electrolyte solution. A voltage was created when shined by light. The photovoltaic effect in a solid system was first observed in 1876 in selenium [2]. This experiment had a palladium wire that inserted into a vitreous selenium bar, forming a metal-semiconductor interface. The working solid state solar cell devices using silicon crystals were developed in 1950s by Chapin, Fuller and Pearson [3]. Later on, the development was driven by the application of power source in extra-terrestrial missions. The dates of relevance to photovoltaic solar energy conversion were listed by L. EI Chaar [4], whose timeline is reproduced in Table 1:

In the mid-seventies, efforts were initiated to make solar cells for terrestrial applications. Within the last three decades, technology has significantly improved cell efficiency and reduced cost for large scale commercial applications.

As shown by Shockley and Queisser [5], the best semiconductor to reach the highest efficiency should have a 1.4eV band gap, which is the minimum energy required to excite an
Table 1. Dates of relevance to photovoltaic solar energy conversion [4].

<table>
<thead>
<tr>
<th>Scientist and innovation</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>Becquerel discover the photovoltaic effect</td>
<td>1839</td>
</tr>
<tr>
<td>Adams and Day notice photovoltaic effect in selenium</td>
<td>1876</td>
</tr>
<tr>
<td>Planck claims the quantum nature of light</td>
<td>1900</td>
</tr>
<tr>
<td>Bose discovered selective conductivity [6]</td>
<td>1927</td>
</tr>
<tr>
<td>Wilson proposes quantum theory of solids</td>
<td>1930</td>
</tr>
<tr>
<td>Mott and Schottky develop the theory of solid-state rectifier (diode)</td>
<td>1940</td>
</tr>
<tr>
<td>Bardeen, Brattain and Shockley invent the transistor</td>
<td>1949</td>
</tr>
<tr>
<td>Chapin, Fuller and Pearson announce 6% efficient silicon solar cell</td>
<td>1954</td>
</tr>
<tr>
<td>Reynolds et al, highlight solar cell based on cadmium sulfide</td>
<td>1954</td>
</tr>
<tr>
<td>First use of solar cell on an orbiting satellite “Vanguard”</td>
<td>1958</td>
</tr>
</tbody>
</table>

electron that is in bound state into a free state where it can participate in conduction[7]. The ideal solar cell materials should have a “direct” band gap between 1.1eV and 1.7 eV, consisting of readily available, nontoxic materials; an easily reproduced deposition technique, suitable for large area production; good photovoltaic conversion efficiency; long term stability[8]. Silicon is one material that meets most of those requirements.

Since their invention in 1954, silicon solar cells have been the dominant product on the market. Single crystal and “ multicrystalline” silicon solar cells are used by about 80% of the market [9], and will continue to be the leading technology until more cost effective PV technologies are developed. Single crystal silicon solar cells are used for the highest efficiency commercial modules. They use a crystalline silicon wafer as the main body to make a p-n junction, which is a boundary or interface between silicon materials doped to produce lower (p-
type) or higher (n-type) Fermi levels. Usually the thickness of the wafer is about 300 µm sliced by a fine saw from a silicon ingot. Then a heavily doped p layer (n layer) is made on top of the thick n type (or p type) substrate of very low doping concentration. Photo carriers generated inside the thick substrate will diffuse into the depletion region at the junction interface, where electrons and hole are separated and collected by two electrodes.

The thickness is required for conversion efficiency since the energy production by photons is decreased at higher wavelength. The use of high quality crystal material has the benefit of long diffusion times and long diffusion lengths of photo generated carriers. The highest energy conversion efficiency from lab cells of this type is 24.7%, with approximately 35mA/cm² and an open circuit voltage of 0.55V at full illumination [10]. The limit of energy conversion efficiency is set at 34% by Shockley and Queisser [5], they neglect the non radiative recombination process and assume a step function of optical absorption, i.e. all the photon above $E_g$ will be absorbed, none will be absorbed below. The resulted open circuit voltage is equal to the separation of the quasi-fermi level between the photo generated electrons and photo generated holes. Under AM 1.5 solar illumination, the open circuit voltage is about 0.25V below $E_g/q$, where $E_g$ is the band gap, and $q$ is the electron charge. This limit was later modified by M.A. Green to be 31%, when considering the Auger recombination effect which would convert the recombined energy into an electron instead of giving off a photon [11]. SunPower, Inc., currently provides the highest commercially available module efficiency of silicon solar cells at 24% [12].

There are several reasons why crystalline silicon solar cell is dominating over the market. Silicon is an abundant earth element, non-toxic, and there is a low cost of reconditioning at the end of the module’s life cycle. The life time of c-Si module is as long as 25 years, it does not
have a significant degradation effect over the years. The processes to make c-Si solar cell can be
adapted from Si semiconductor industry, which is a huge advantage. [13]

The disadvantage of c-Si is the cost of high quality silicon. Since the cost of material is
about 50% of the total cost [14]. Thus, there is a current drive to reduce the thickness of the
silicon layer.

Another silicon technology uses thin film hydrogenated amorphous silicon or nc-Si as the
active absorber layer. The material quality in these cells is worse than for crystalline silicon, it
needs hydrogenation to passivate defect states to keep material quality at device level. Due to the
high density of defect states, the carrier drift mobility in these cells is very slow,[15] thus the
typical thickness of active absorber layer is about 300 nm for amorphous silicon and about 3.0
microns for nc-Si, thus the material cost is lower.

The basic structure of thin film silicon cell is an intrinsic silicon layer sandwiched in
between a thin p layer and thin n layer. The most economical way of making amorphous silicon
and nc-Si films is plasma enhanced chemical vapor deposition (PECVD), which is widely used
in the solar cell industry. Silane (SiH₄) gas is used as precursor, and dopant gases can be added to
control the film’s carrier type at certain concentrations. The films can be deposited on ordinary
window glass and on flexible substrates (stainless steel or polyimide). These cells can be used in
building windows or roofs, as well as in solar fields.

The main disadvantage of thin film silicon solar cells is the modest efficiencies that have
been achieved to date, and the uncertain durability. Economically, lower efficiency will lead to
bigger land use and assembly cost. The thin film materials will degrade over time. Also, the
material used in the fabrication line are toxic, and the depositing techniques are rather
complicated. Those makes the technology economically unfavorable comparing to crystalline silicon [16].

1.2. I-V property of solar cell devices

Different types of solar cells have different structure designs, and material composition. The photo carriers inside the cells are also different between different types of cells. However, despite the differences in photo carrier transport in different type of cells, we can do a standard general current-voltage test to characterize the cells, which is termed the I-V curve spectra.

![Diagram of an I-V setup](image)

**Figure 1.** Illustration of an I-V setup.

In Figure 1, we show an illustration of an I-V test system. \( I \) is the current generated in the device, \( V \) is the voltage applied onto the p side of the cell. If \( V \) is positive, the cell is positive biased; if \( V \) is negative, the cell is negative biased. I-V measurement can be performed at different illumination levels. In the dark, for an ideal p-n junction, the I-V relation is [17]:

\[
I = I_0(\exp\left(\frac{qV}{kT}\right) - 1)
\]

Here, \( I_0 \) is the “reverse saturation current”, \( q \) is the electron charge, \( k \) is the Boltzmann constant, and \( T \) is the temperature.
When a p-n junction is under illumination, the optical absorption in the semiconductor will generate charge carriers. The photo generated electrons and holes will move to different electrodes to be collected in the external circuit. Then the $I-V$ relation is:

$$I = I_0 \left( \exp \left( \frac{qV}{kT} \right) - 1 \right) - I_{sc}$$ \hspace{1cm} 1-2

$I_{sc}$ is called short circuit current, which is related to the rate of photo carrier generation.

In Figure 2, we show ideal $I-V$ curves for a p-n junction calculated from equation 1-2.

![Figure 2: $I-V$ curve of an ideal p-n junction in the dark and under illumination at room temperature. The reverse saturation current is $2e^{-24}$ A; the photogenerated current is 40 mA.](image)

1.3. **Characterization methods for solar cell device: $J_{sc}$, EQE, and IQE**

1.3.1 **Short Circuit Density ($J_{sc}$)**

Experimentally, the areal photocurrent density $J_{sc}$ can be derived from $I-V$ curve under illumination when the external bias voltage is zero. From an $I-V$ curve, we can find the short circuit $I_{sc}$ from the intersection with $V$ axis. Suppose the illuminated device area is $A$, then short circuit current density is derived as:
For a finished solar cell device, $I_{SC}$ is determined by the intensity of the illumination, stronger illumination will give higher $I_{SC}$, thus higher $J_{SC}$. The expected working condition is the regular solar illumination. Since the solar radianc e on earth is not a steady spectrum and depends on many factors like time of day, weather, air quality, etc., usually a standard averaged spectrum is used. A good average spectrum is AM1.5 spectrum for the average photon flux in the sunlight that incidents on the earth surface at an angle of 38 degree.

![Figure 3. The incoming photon flux for an AM1.5 solar radiation spectrum.](image)

The solar spectrum is usually in the unit of power per area per wavelength ($\text{Wm}^{-2}\text{nm}^{-1}$), however since we are interested in the current from a cell generated from solar radiation, and solar cells usually generate at most one quantum of charge per absorbed photon, we plot the photon flux instead, denote as $F(\lambda)$, (photon intensity per area per wavelength), as shown in Figure 3.

In a real solar cell, an incoming photon does not always contribute a quantum of charge; photons are some wavelengths may be weakly absorbed, or the cell may not deliver one quantum
of charge for every absorbed photon. The “external quantum efficiency” $EQE(\lambda, V)$ accounts for these two effects; at zero bias the short circuit current density could be calculated as:

$$J_{sc} = q \int F(\lambda)EQE(\lambda, 0)d\lambda$$

$F(\lambda)$ is the photon flux. For silicon, we are interested in the region between 300 nm and 1200 nm. We will use this equation to calculate for $J_{sc}$ from $EQE$ spectra in the following chapters.

### 1.3.2 External Quantum Efficiency ($EQE$)

As defined above, the short circuit photocurrent density $J_{sc}$ is directly dependent on the optical absorption and the related external quantum efficiency ($EQE$) spectra, which is defined as the fraction of the incident photon flux that is converted to an electric current. If all photons of a certain wavelength are absorbed, if each absorbed carrier generates an electron-hole pair, and if the resulting carriers are collected in the circuit, then the $EQE$ is unity. Because the absorption in the cell is highly related to the absorption coefficient of the material, which is dependent on incident beam wavelength, $EQE$ is also mostly expressed a function of photon wavelength or energy. At different wavelengths the effectiveness of absorption is different, so measuring $EQE$ curve would give the clue for which part of wavelength should be improved.

$EQE$ is also dependent on bias voltages, which have an effect on the collection of photo generated carriers. This effect is more profound in devices that are not optimized. For devices with good collection efficiency, photo carriers could be collected efficiently.

In Figure 4 we show an $EQE$ spectrum for a nc-Si: H thin film solar cell. The layers of this cell are also illustrated; the light is incident from the top. In this cell, light may pass through layers of ITO (indium tin oxide, which is a transparent conducting material), a microcrystalline Si p-type layer, the intrinsic nc-Si:H (i) layer, the n-type layer, and finally reach a composite back reflector (100 nm of ZnO on a textured Ag layer). In the short wavelength region before
500 nm, the $E_QE$ is low. The absorption coefficient of the microcrystalline silicon p-layer in that region is very high, so light is mostly absorbed in the p layer. The recombination lifetime of electrons in microcrystalline p-layers is very short, so the electron-hole pairs generated in this layer recombine without contributing to the photocurrent. The $E_QE$ nearly reaches unity at about 550 nm. At longer wavelengths above 700 nm, the $E_QE$ again starts dropping. One of the reasons for the low $E_QE$ at long wavelengths is that the absorption coefficient of silicon is low in this region. This is also the region where light trapping is important. In this thesis, we will look at the long wavelength part of $E_QE$ spectrum to study the light trapping enhanced absorption.

![EQE spectrum](image)

Figure 4. An example of $E_QE$ of a thin film silicon solar cell. The layers in the solar cell structure and the way light enters are illustrated.

We built a setup to measure $E_QE$, which will be illustrated in Chapter 2.

1.3.3 Internal quantum efficiency (IQE)

$E_QE$ measurements will give the probability of an incoming photon’s contributing an electronic charge $q$ to the current in the external circuit. However, the optical design of a real solar cell always has an anti-reflection (AR) layer. Ideally, such layers have zero reflectance at all significant wavelengths, but real AR layers (the ITO layer in Figure 6) reflect some of the
incident light. Also, when light comes into the cell propagating through the layers there is a chance it will not be absorbed, but will be reflected or scattered back out instead. \textit{EQE} is a good indicator of silicon absorption. However, information from \textit{EQE} curve is not enough to learn the entire processes of absorption occurred inside the device. To look at the fraction of absorption in the active silicon layer compared to the total absorption in the device, the internal quantum efficiency (\textit{IQE}) is defined as:

\[ \text{IQE} \equiv \frac{\text{EQE}}{1 - R} \]

Here, \( R \) is the total reflectance, including both specular and diffuse parts. Of course \( 1 - R \) gives the total absorptance in the cell structure.

If silicon were the only absorbing layer, and if all photons absorbed there generate photocarriers that are collected and contribute to the photocurrent, then \( \text{IQE} = 1 \). Even neglecting imperfect collection, this ideal case is not what we will see in the real experiments. There is always “parasitic loss” in layers like the transparent conducting oxide (TCO), the doped layers, and the back reflector. Any of these effects will cause \( \text{IQE} < 1 \).

![Diagram](image_url)

**Figure 5.** Example of the \textit{IQE} spectrum for a 260 µm monocrystalline silicon solar cell.
In Figure 5 we show an example of an experimental IQE spectrum for a monocrystalline silicon cell, with corresponding EQE and R curves [18]. We can see that the EQE curve at long wavelength is dropping; the reasons could be that the light is not absorbed or that the light is absorbed but not in silicon. From the IQE curve, which drops a lot from unity, we see that the silicon absorption is low. Light is mainly absorbed in other layers besides silicon, or by interface defects, which leads to the conclusion that parasitic loss is substantial in this cell beyond 1100 nm. Since the 1.12 eV bandgap of silicon corresponds to a wavelength of 1100 nm, this cell is fairly well optimized.

1.4. Light trapping for silicon solar cells

Silicon satisfies all requirements except that it is an indirect band gap material. For nc-Si and c-Si, the absorption coefficient drops below 1000 cm\(^{-1}\) quickly for the wavelengths above 800nm [19,20], as shown in Figure 6. Since the absorption of photons to produce electron-hole pairs is one of the three essential steps, light trapping technique becomes crucial for silicon solar cell.

![Absorption coefficient spectra of hydrogenated amorphous silicon and nc-Si](image)

Figure 6. Absorption coefficient spectra of hydrogenated amorphous silicon and nc-Si
The rudiments of light-trapping are illustrated in Figure 7. On the left, a highly idealized solar cell is shown which has a perfect antireflection coating on its front and back, and no back reflector, and no parasitic absorption. A light beam is incident on the cell that is very weakly absorbed. The path length of the beam in the layer (thickness $h$) is evidently about $h$ shown in the bottom graph. The absorptance $A$ of this structure can be written $A = \alpha h$, where $\alpha$ is the absorption coefficient of the semiconductor, and $\alpha h \ll 1$. If the AR coating on the back is replaced by a simple mirror, the path length doubles and the absorptance is $A = 2\alpha h$, which corresponds to an enhancement factor $Y = 2$.

Larger light-trapping enhancements can be realized by coupling the incident sunlight into internally reflected rays in the thin film. This mechanism for light-trapping is illustrated at the right of the figure; light propagating to the right or left within the film is confined by total internal reflection at the top interface, and metallic reflection at the bottom. In order to get coupling of the incident light into these internal modes, there is usually some geometrical "texturing" at the top or bottom interfaces of the semiconductor film that scatters incident light. Structures such as grain boundaries within a film also create such coupling.

Structures that couple incident sunlight into the internal modes also couple light from those modes into outgoing waves that leave the film altogether. Of course the detailed dynamics of such couplings could be very intricate. An important approximation, proposed in 1982 by Yablonovitch [21], is to assume "ergodicity" or equipartition, which says that the energy stored in each electromagnetic mode of the film is the same.
We now illustrate ideal thermodynamic light-trapping by considering equipartition of the energy density for all the possible photon modes in a thick film ($h \gg \lambda/n$). In $k$-space, these modes are distributed evenly over the spherical shell shown in the figure. The film has a...
backreflector and an antireflection coating on the top. The small “cap” of the sphere corresponds
to photons traveling up at sufficiently small angles ($\theta < 1/n$) that they leave the film without
being internally reflected by the top interface.

Equipartition can be established by roughening the backreflector; as we show subsequently,
as little as 30 nm of rms roughness appears to be sufficient to establish equipartition. Neglecting
corrections of order $n^{-2}$, the energy density and absorption associated with the “radiative” cap of
the mode distribution is the same as previously calculated for a simple beam: $u = nI/c$.
However, by equipartition, the total energy density in the film is increased by the ratio of the
total area of the sphere to the area of this cap. When $n^2 \gg 1$, this ratio is $4n^2$, which is about 50
for silicon. The total energy density, and also the total absorption per unit volume, in the film is
thus $4n^2$ larger than it is for a ray that simply passes once through the film at normal incidence.

This is the well-known $4n^2$ enhancement for ideal thermodynamic light trapping. The
absorptance of the thin film without a back reflector and without light-trapping is $A = ah$; with
light-trapping the absorptance increases to $A = 4n^2 ah$. Both expressions are valid only for small
absorptance, which means $4n^2 ah \ll 1$ with enhancement.

More general treatments that are valid up to $ah \approx 1$ lead to the form first proposed by
Tiedje, et al., and rederived more rigorously by Stuart and Hall:[22,23]

$$A_{cl} = \frac{4n^2 ah}{4n^2 ah + 1}$$ 1-6

When $4n^2 ah \ll 1$, this expression reduces to the result $A \approx 4n^2 ah$, indicating an
“enhancement factor” of $4n^2$ for the absorptance relative to its value when a beam passes directly
through the film. When $4n^2 ah \gg 1$, the absorptance is unity, and the details of light-trapping
have little effect.
For the most general case, the light trapping enhanced absorptance is less than $4n^2$, with an “enhancement factor” $Y$. We plot the absorption curves for different values of $Y$ in an ideal 2.5 µm nc-Si solar cell in Figure 8. We also show the absorptance by substituting a variable $Y$ for $4n^2$ in equation 1-6:

$$A_Y = \frac{\alpha h}{\alpha h + 1/Y} \tag{1-7}$$

For $Y = 1$, the absorption is very low over a broad range of wavelengths that are shorter than the 1100 nm that corresponds to the bandgap of crystalline silicon. This reflects the fact that silicon is an indirect band gap material and silicon layer is thin. When $Y$ increases, the absorption curve is increased substantially; “thermodynamic” behavior is realized when $Y = 50$, corresponding to $4n^2$ enhancement and an index of refraction $n = 3.5$.

![Absorptance graph](image)

Figure 8. Illustration of the absorptance for an ideal thin film silicon solar cell (2.5 µm) with different degrees of light-trapping enhancement $Y$. $Y = 1$ corresponds to light that enters the layer and exits through the back; increasing values of $Y$ correspond to increased scattering into rays that are internally reflected by the interface, reaching $Y = 50$ when equipartition applies and the cell has a backreflector.
Figure 9. Short-circuit current densities $J_{SC}$ under solar illumination as a function of the light trapping factor $Y$ for different thicknesses of a silicon layer. The layer is assumed to be incorporated in an ideal cells with perfect antireflection coatings and backreflectors.

The enhanced light absorption in the cell will boost the short circuit current density $J_{SC}$ under solar illumination $J_{SC}$ is calculated by integrating the product of the solar photon flux spectrum and the absorptance for varying degrees $Y$ of light trapping. In Figure 9, we plot results as a function of the thickness of the silicon layer. We use equation 1-4 with AM1.5 illumination.

For a 1 µm thick silicon layer, $J_{SC}$ is only 12 mA/cm$^2$ with no light trapping. With complete 4$n^2$ light trapping, $J_{SC}$ goes to 32 mA/cm$^2$. For a 100 µm silicon layer, the light trapping effect is not as profound as for the thin film, but is still significant. $J_{SC}$ can be boosted from 35mA/cm$^2$ to 43 mA/cm$^2$.

Since $J_{SC}$ is one of the key parameters for conversion efficiency, Figure 9 illustrates the importance of light trapping for silicon solar cell.
1.5. **Outline of this dissertation.**

This dissertation will focus on experiment results for light trapping in silicon solar cells. The light trapping theories we show above are based on the assumptions of perfect antireflection (AR) coatings, perfect backreflectors, efficient scattering, and no parasitic absorption. However, in an experiment result, the photons that come into the cell will undergo different processes other than silicon absorption. In Figure 10, we show an illustration of the photon management that we’ve calculated for a particular thin-film silicon solar cell made by our collaborators at United Solar Ovonic, LLC. The band at the bottom of the figure corresponds to the measured EQE spectrum for this cell; the dashed line indicates the absorptance of a cell with the same thickness based on the classical $4n^2$ calculation.

![Figure 10. Photon management calculations corresponding to a nc-Si:H silicon substrate solar cell with 1.0 µm silicon and a 70 nm ITO coating on top. The coating serves both as a quarter-wavelength antireflection coating and as an electrical conductor.](image)

The width of the top region of the diagram indicates the specular reflectance from the front of the cell; the 70 nm thickness of the ITO layer has zero reflectance for incident wavelengths near 0.6 µm, and is increasingly reflective at longer wavelengths. The photons that are not
specularly reflected will go into the semiconductor layers, and then be either absorbed or radiated out as diffuse reflectance. The photon absorption could occur in silicon layer and other layers like the top ITO layer. Only the silicon absorption would generate photo carriers which will be collected by electrodes and contribute to external quantum efficiency. By definition, parasitic absorption will not contribute to the external quantum efficiency.

Due to the optical processes illustrated above, experimental EQE spectra are always lower than the $4n^2$ absorptance, which assumes a perfect antireflection coating and neglects parasitic absorption processes.

We develop a metric in Chapter 2 to summarize the light trapping enhancement from experimental EQE spectra, and then we apply the metric to many experiment results in the past decades for various Si solar cells. The empirical enhancement factors we derive are much lower than $4n^2$. We discussed the possible reasons for inefficient light trapping; as can be seen in the figure above, we think that parasitic absorption by the top TCO is very important in the particular cells we’ve studied.

In Chapter 3, we study the EQE and IQE spectra of a set of substrate nc-Si solar cells fabricated on different types back reflectors. We performed optical and electrical measurements for those cells. We developed a thermodynamic calculation method for the internal quantum efficiency. Our thermodynamic calculation of cell absorptance to incorporate parasitic losses by a top oxide coating and an imperfect antireflection coating, which suggests that top oxide is the major source of optical loss. In 2008 Berginski, *et al* [24], followed a somewhat similar program for “superstrate” nc-Si:H cells deposited onto texture oxides on glass. They also assumed thermodynamic light trapping, and reached the conclusion that the absorption by the top conducting oxide reduced the quantum efficiency at longer wavelengths. Their thermodynamic
calculations used the approximation developed in the 1980s by Deckman, et al.[25], which essentially uses the property of a single waveguide mode to approximate the sum over modes in the treatment that we have done in our calculation. They fitted the small effects of an imperfect back reflector to gain agreement between calculation and measurement; it may be that the more complete treatment of modes that we have used here would offer an alternate explanation.

To reduce the parasitic loss in oxide layer, we propose an idea of introducing an intrinsic oxide layer as a buffer before putting the heavily doped oxide layer. This design have been used in commercial solar cells however for different purpose, we show the optical benefit from bilayer transparent conducting oxide in Chapter 4.
Chapter 2. Empirical enhancement factor metric

According to the classical $4n^2$ light trapping theory shown in Chapter 1, silicon absorption should be very efficient even for a relatively thin layer. This $4n^2$ absorption limit thus provides motivation for solar cell fabrications. To achieve $4n^2$ absorption limit, a set of requirements must be satisfied: perfect anti-reflecting coating, efficient scattering, and no absorption other than in the silicon layer. It is difficult to meet all requirements in an experiment. In experimental calibration sense, it is helpful to see how an experimental result compares to this $4n^2$ limit. In this chapter, we will develop a metric to derive the empirical light trapping enhancement factor $Y$. In principal, the value of $Y$ is between 0 and $4n^2 = 50$ for silicon.

An experimental EQE spectrum is used to calculate the enhancement factor $Y$. For a specific silicon thickness, we calculate “benchmark wavelength” at which $4n^2$ light-trapping would yield an EQE of 50%. For silicon, the benchmark wavelength lies above 900nm for practical silicon solar cell thicknesses.

We have calculated this metric both for many solar cells with published EQE spectra and also for the cells that were measured as part of this thesis. As part of this work, we built an experimental EQE setup to measure the EQE spectrum. Besides deriving the empirical enhancement factor $Y$, we will also show a thermodynamic light trapping analysis based on both spectra, which we shall describe more in Chapter 3. For the cells we surveyed in the literature, we look into EQE curves and cell thicknesses provided in their publication, then show heir empirical enhancement factor $Y$. An estimation of parasitic loss is also given if the cell reflectance is provided as well.

The empirical light trapping enhancement factor $Y$ for all studied solar cells are plotted against cell thickness. Surprisingly, most of $Y$s are well below the classical $4n^2$, even for those
cells with advanced light scattering structure. An in-depth quantitative study to explain the low empirical enhancement factor in thin film nc-Si:H solar cells will be shown in Chapter 3.

2.1 Review of models to characterizing light trapping effect

There is a need to characterize the efficiency of a light trapping structure and compared to the classical $4n^2$ limit. In this section we will show that a metric we developed can characterize the effectiveness of a light trapping experiment, using the empirical light trapping enhancement factor “Y”. Before we introduce our metric, we will first review different models people use to study their light trapping results.

J.A. Rand and P. A. Basore [26] introduced an experimental approach to quantify the level of light trapping in their crystalline solar cells by finding out the “effective optical path length” that could be used as part of a complete model for internal quantum efficiency(IQE) spectra. Their procedures require detailed understanding of the optical and electrical properties of the cell, and were applied to thick crystal silicon cells. For example, they distinguish between the reflectance of the front interface, $R_{front}$, and the light that ultimately escapes from the cell having once been transmitted into it. Thus their procedures aren’t generally usable with other cells.

A similar idea to effective optical path lengths was used by D. Zhou and R. Biswas [27] in their simulation work. For their device under simulation, the thickness of the active silicon is defined as $d$ and the absorption under rigorous calculation for solving Maxwell equation gives absorption as $A(\lambda)$. The conceptual one path absorption is calculated by Beer’s Law:

$$A_0 = 1 - e^{-ah}$$
where $\alpha$ is the absorption coefficient for silicon and $h$ is the thickness of the semiconductor layer. This is not true in experiment for weakly absorption light that $\alpha d \ll 1$. However, $A_0$ is generally used as a reference for the amount of weak absorption without light trapping. They derived an effective path length $L(\lambda)$ to give the absorption:

$$A(\lambda) = 1 - e^{-\alpha L(\lambda)}$$

The enhancement factor is then given by the ratio: $L(\lambda)/h$, also depending on wavelength. At the weak absorption limit, $\alpha d \ll 1$, $\frac{L(\lambda)}{d} = \frac{A(\lambda)}{A_0}$. They then plotted $\frac{A(\lambda)}{A_0}$ as an indicator for their light trapping enhancement.

The same idea of getting effective optical path length from absorptance is used by Daniel Lockau [28], which he termed the “light path enhancement factor” (LPEF) in simulation work. For a silicon layer with thickness $h$, the absorption in the silicon layer was calculated as $A(\lambda)$ for the amount of light $I(\lambda)$ transmitted into the silicon layer. Note $I(\lambda)$ is less than unity due to front specular reflection.

$$LPEF(\lambda) = \frac{-\ln \left( 1 - \frac{A(\lambda)}{I(\lambda)} \right)}{ah}$$

$LPEF(\lambda)$ is also wavelength dependent, so in order to get a simple number to describe light trapping, Lockau did an average of $LPEF(\lambda)$ for the interval between 1000nm and 1100nm where the absorption is weak. The averaged number lies between of 0 and 50 in the examples he showed.

The effective absorption length approach is inconsistent with the thermodynamic light-trapping calculations of Tiedje, et al., in the important intermediate angle of wavelengths where $1 < 4n^2\alpha h < 4n^2$. H.W. Deckman et al. calculated a light trapping factor based on statistical
ray optics and ergodicity [29]. In a real structure, they assumed that only a fraction of the incoming light, $\beta$, is scattered into oblique angles that are large enough for total internal reflection. The rest of the light ($1-\beta$) will travel non-ergodically for only one path length of layer thickness. In the absence of parasitic loss at the electrodes, the absorption enhancement factor $E_{\text{exp}}$, is then simply given by $E_{\text{exp}} = \beta \times 4n^2$. They also studied light trapping with complete ergodicity ($\beta=1$), however there was parasitic absorption, $\eta$, at the back electrode which would reduce the light trapping enhancement factor.

From this point of view, they assumes that incident light will get randomized at the front interface to have a Lambertian angular distribution (the radiant intensity is directly proportional to the cosine of the angle $\theta$ between the surface normal and the light traveling direction). The averaged travelling angle for Lambertian distribution is $60^\circ$, giving a path length which is twice the thickness of the film. The absorption $A$ from this path would give:

$$A \equiv \frac{1 - \eta e^{-2\alpha h} - (1 - \eta)e^{-4\alpha h}}{1 - (1 - \eta)e^{-4\alpha h} + \frac{1-\eta}{n^2} e^{-4\alpha h}}$$ \hspace{1cm} 2-4

Here, $\alpha$ is the absorption coefficient, $h$ is film thickness, $n$ is the refractive index of silicon, $\eta$ is reflection loss at the electrode interfaces for each internal reflection. Then the enhancement factor is given by:

$$E_{\text{exp}}(\eta) = A/(1 - e^{-\alpha h})$$ \hspace{1cm} 2-5

They then use equation 2-4 to fit their experimental EQE to get $\eta$, and the corresponding enhancement factor $E_{\text{exp}}(\eta)$.

An effective optical path length is used in first three models. However, the relation of the enhanced absorption and effective optical path is not trivial, since it requires good knowledge of
the optical process in the device. Basore’s model studies the ray pattern in crystalline silicon solar cell. In thin film cells, absorption is more complicated. The fact that the effective optical path length is wavelength dependent makes it hard to compare between different light trapping experiments.

Deckman’s model looks at the portion of scattered light from silicon absorptance, and then the enhancement factor is the same portion of the classical $4\pi^2$ limit. Under full scattering, he studied the electrodes’ parasitic loss for an averaged optical path length angle (single mode).

### 2.2 Proposed light trapping metric

To compare the light trapping effect from experiment to experiment, we explore a simple procedure for benchmarking the light-trapping in solar cells based on experimental $EQE$ curves. First, we need to find out the thickness of the medium layer $h$, and the absorption coefficient spectra for the material, then plug into equation 2-6, which is the best possible upper absorption limit for a layer of material with that thickness; we call it classical absorptance:

$$A_{cl} = \frac{4n^2ah}{4n^2ah + 1} \quad 2-6$$

As far as the effectiveness of light-trapping for improving a solar cell’s efficiency is concerned, the wavelength at which the classical absorptance $A_{cl}$ is 0.5 is arguably the most significant. We’ll call this the “benchmark wavelength” $\lambda_b$. When $\lambda > \lambda_b$, $A_{cl}$ is smaller than 0.5, and incident sunlight generates relatively little photocurrent. When $\lambda < \lambda_b$, $A_{cl}$ approaches 1, and light-trapping plays fairly little role in determining the $EQE$.

In Figure 11, we present the graph for the benchmark wavelength $\lambda_b$ of thin-film silicon solar cells as a function of the absorber layer thickness; the wavelength is defined implicitly through $A_{cl}(\lambda_b) = 0.5$. To prepare Figure 11, we have used the absorption coefficient and index
of refraction spectra for crystalline silicon [30]. Absorption coefficient measurement in nc-Si:H are somewhat difficult because of the need to correct for internal optical scattering in the films. The net result is that the absorption coefficient is somewhat larger than for c-Si, but otherwise varied fairly little for one series of samples [31]. For nc-Si:H, we used the index of refraction spectrum of monocristalline silicon.

![Benchmark wavelength vs. film thickness for crystalline silicon and nc-Si:H.](image)

Figure 11. Benchmark wavelength $\lambda_b$ vs. film thickness for crystalline silicon and nc-Si:H.

Silicon is an indirect band gap material, and the absorption coefficient is low for a broad region above 600nm. As a consequence the benchmark wavelength depends strongly on thickness.

In Figure 12, we present a comparison of the classical absorptance for a 1 micron film with a published external quantum efficiency spectrum from an experiment on a nc-Si:H cell [32]. As can be seen, at benchmark wavelength of 930 nm, the measured quantum efficiency is about 0.2, which is well below the classical absorptance of 0.5. In principle, part of the difference could be due to a failure to collect some of the photo carriers that were generated by the light in the silicon; we shall be ignoring the possibility for the cells we study, and more generally the better nc-Si:H solar cells do have collection efficiencies close to 1.0 [33]. One approach to the difference is to
use equation 2-6 for calculating the \( EQE \) spectrum, but with an “empirical enhancement factor" \( Y \) that is less than \( 4n^2 \):

\[
\frac{E QE(\lambda_b)}{Y ah + 1} = \frac{Y / 4n^2}{Y / 4n^2 + 1}
\]

Figure 12. Comparison of classical absorptance \( A_{ct} \) spectrum to the external quantum efficiency spectrum measured in a typical nc-Si:H solar cell. The graph also shows the benchmark wavelength for a 1.0 micron film, at which this particular cell had a \( EQE \) of 0.20, this gives the enhancement factor of 13 according to equation 2-8.

We can then calculate \( Y \) from \( E QE(\lambda_b) \):

\[
Y = 4n^2 \frac{E QE(\lambda_b)}{1 - E QE(\lambda_b)}
\]

For the cell in Figure 12, the value of \( Y \) is about 13. This is well below the classical absorptance \( 4n^2 = 50 \).

We choose a benchmark wavelength to calculate the empirical enhancement factor \( Y \).

However, the \( E QE \) or absorption spectrum covers a broad band region. From our metric, we can retrace the experimental spectra from the empirical \( Y \):
Figure 13. Test of light trapping metric. We get the empirical enhancement factor $Y$ at the benchmark wavelength, and then apply this $Y$ in the retrace procedure using equation 2-9. We show the retrace results for two solar cells. One is a 1 µm thin film nc-Si:H solar cell ($Y=13$); the other is a 100 µm HIT cell ($Y=33$). The open squares are from the measured EQE spectrum, and the dashed blue curve is the classical $4n^2$ absorptance. We derive the $Y$ factor from those two curves, then retrace it back as the orange curve shown. The retrace curve agrees with the experiment EQE well for wavelengths above 600 nm.

It is nice to have a good agreement between trace-back curves and experiment EQE spectra; In Figure 13, we show the test result for our light trapping metric for two samples: one is a 1 µm thick thin film nc-Si cell [32], the other is a 100 µm thick HIT cell [34] (“heterojunction with intrinsic thin film”, which is a type of monocrystalline silicon solar cell). The blue curves are absorption curves representing the classical $4n^2$ absorptance, the open squares are experimental EQE spectra, and the orange curves are retrace curves from equation 2-9 with empirical
enhancement factors $Y$ which we calculated. The retrace curves agree with the experiment $EQE$ well.

However, this agreement is not always as precise in all cells. We derive the light trapping enhancement factor $Y$ from the benchmark wavelength $\lambda_b$ which is in the weak absorption region. This behavior is also seen by Basore [26], who found in thick monocrystalline cells at the enhancement factor was essentially constant in the weak absorption region ($ah < 1$). So it is not surprising that the trace-back curves calculated from $Y$ can describe the experimental $EQE$ spectrum that we measured at longer wavelengths. For the shorter wavelength region, the agreement is more incidental; it is no longer valid by relating the number of optical modes to the absorption behavior. Since the strong absorption is not our focus, we will leave it as it is without discussion.

2.3 Experiment $EQE$ set up.

To get the empirical light trapping enhancement factor, we have to measure the $EQE$ spectrum experimentally. Standard $EQE$ measurement kits can be purchased from Newport Corporation (QE/IPCE Measurement Kit) [35], Oriel Instruments (Model: Oriel IQE-200) [36], etc. In a typical EQE measurement setup, the components in a kit include:

1) A light source for broad band spectrum covering the region between 350nm to 1100nm;

2) Monochromator unit to select single wavelength beam from the broad band radiation of the light source;

3) Optical chopper to chop the light at controlled frequency, the same frequency is used for phase synchronization in LIA;

4) Lock In amplifier (LIA) to get the photocurrent generated from alternating illumination at high resolution;
5) a well calibrated detector with known spectral response (SR, in the unit of A/W, the current generated per watt of incident power) to measure intensity of the beam;

6) Optics unit to direct the light onto solar cell sample and reference detector;

7) Computer program to drive the motor unit in the monochromator for wavelength scan, usually written in Labview.

The wavelength resolution of an EQE measured is determined by the wavelength resolution of the monochromator. Usually, a commercial set up has a resolution of 5nm or 10nm. The measurement error is about 2 to 5 percent.

Here, we will show the EQE measurement set up we built in our lab using our own equipement. We illustrate our set up in Figure 14:

The light source is a tungsten halogen lamp (300W) mounted at the back compartment of a monochromator (Horiba Jobin-Yvon model H20). The spectrum of the halogen lamp covers the wavelength region from 400nm to 2500nm [37]. The collimated light incident on a diffraction grating (600 cm⁻¹). The angle of the grating is adjusted by a motor unit which is controlled by a computer program, so that the first order diffraction for the selected beam wavelength will be in the direction of the output slit of the monochromator. In H20, the slit width is changeable, smaller slit widths give higher resolution at the cost of less intensity. We set the slit width as 2mm, which corresponds to a wavelength resolution of 2 nm. For short wavelengths, the output from the monochromator is then approximately single wavelength beam. For long wavelengths, the output from the monochromator has a mixture from higher order diffraction of relevant short wavelengths. In order to get single wavelength beam, a filter is placed in the beam path, which would not transmit the part of the short wavelength beam.
After passing through the monochromator, the beam then passes through an optical chopper (Stanford Research System, model SR540) with rotating disk. The chopping ratio is 50/50, which means that beam is transmitted for half of the time in each period. The chopping frequency can be adjusted from 10 Hz to 4000Hz. We picked a chopping frequency at 1000Hz, which is low enough not to affect photocarrier transport in our cell.

After passing through the chopper, the incident beam goes through a set of lenses and mirrors to be directed to an optical microscope (Zeiss, 46-03-9901). The microscope is designed for optical lithography; however, we use it for a different purpose here for three reasons. First, it has a beam splitter on the top. One branch of light is directed onto a reference photodetector, and the other branch is directed to the objective lens system to become the eventual illumination spot on our solar cell sample. Second, the illumination spot size can be adjusted by different objective lenses, so that we can measure a variety of samples with even very small areas. Third, the microscope sample platform can move smoothly in all three directions, making it very easy for sample positioning.

The beam splitter inside the microscope is a semi-transparent film deposited on glass slide, placed at 45° to the incident beam, as shown in Figure 14. The incident beam will be partially reflected and partially transmitted.

The transmitted beam reaches a reference detector, which is a calibrated silicon photodetector (OSI optoelectronics model PIN-10DP-SB) with a known spectral response (SR, the ratio of current generated to the power incident on the photodetector, in the unit of amperes per watt (A/W)) [38]. The photocurrent measurement of the reference detector thus yields the number of photon incident per second of the beam transmitted by beam splitter. The reflected beam will go through an objective lens system and part of it reaches our solar cell sample.
Supposing the two branches of light that reach reference detector and solar cell sample have a ratio M/1, this ratio can be measured by putting identical detectors at both the sample stage and the detector stage. The ratio of the resulting current will be the ratio of beam intensities of the two branches. In our setup, once the objective lens is chosen, the ratio M is measured and stored for later use until the next calibration.

Figure 14. Illustration of EQE measurement set up in our lab.

We will measure the beam intensity using a reference detector, and then calculate the photon current (number of photons per second) that shines on the sample solar cell.

The photocurrent generated in our measurements is at the nA scale. Because the beam is very weak, the direct measurement of current through a regular amplifier would not give good accuracy since the noise level is always too high, and the real signal would be buried, thus, the accuracy would be reduced. We use lock in amplifier (LIA) for current measurement. LIA is working at current mode; the lockin phase is synchronized to the optical chopper.

The photocurrent from our sample is \( I_{\text{Sample}} \) under the illumination of light reaching the sample stage; the corresponding particle current of electrons is \( I_{\text{Sample}}/e \).

31
The photodetector gives a photocurrent that is \( I_{\text{detector}} \) by another LIA. From this photocurrent and the spectral response (SR, in the unit of A/W) of the photodetector, we can calculate the beam intensity \( N \) (number of photons incident on the cell per second),

\[
N = \frac{I_{\text{detector}} \lambda}{SR \ h c}
\]  \hspace{1cm} 2-10

Here \( \lambda \) is the beam wavelength, \( h \) is the reduced planck constant, \( c \) the speed of light. Then the photon current incident on the sample is \( N/M \). The EQE will be derived as:

\[
EQE(\lambda) = \frac{I_{\text{Sample}}}{N/M} = \frac{I_{\text{Sample}}}{I_{\text{detector}}} \frac{hc}{\lambda e} SR \star M
\]  \hspace{1cm} 2-11

In equation 2-11, the beam splitting ratio \( M \) is an input which we measured in advance. After building up the EQE set up, we placed an identical photodetector both at sample stage and photodetector stage (as shown in Figure 14), and then measured the corresponding photocurrent \( I_1 \) and \( I_2 \). The generated current will be proportional to the beam intensity (number of incident photons per second), so we have: \( M = I_2/I_1 \). Once \( M \) is known, we will fix the optics of the system and keep it until the next maintenance calibration.

Since EQE is a spectrum dependent on wavelength, the diffraction grating in the monochromator is rotated by a step motor driver which can be controlled by a computer program written in Labview[39].

The **EQE** set up is now ready for measurement. We test the setup by a second reference photodetector (PIN-10DP-SB) since its **EQE** is calculated from SR by: \( = SR * \frac{hc}{\lambda e} \). In Figure 15 we show the test result:
Figure 15. Test of our $EQE$ set up. The reference sample is PIN-10DP-SB silicon diode. The black curve is calculated from the known SR, and the red dashed curve is the measurement of our set up. Our error range is about 3%.

The sample we use for testing is another PIN-10DP-SB silicon diode; the $EQE$ can be calculated from SR, given by the black curve. The red curve is the measured $EQE$ from our setup. The curves are in good agreement for two regions: 400nm to 800nm and 1000nm to 1100nm. Between 800nm to 1000nm, the measured value is around 2% lower than calculated value, which occurs after we apply the low pass filter. The error in our setup is then estimated to be roughly 3%.

2.4. Reflectance measurement

Optical reflectance is measured by a commercial UV-VIS spectrometer (Perkin Elmer, model Lambda 950), where the spectral region ranges from UV to near infrared. The sample is located the center of an integrating sphere. The beam comes from the front side of the integrating sphere, and incidents on the sample surface at a small angle off to the normal direction.
Generally, the reflected beam is divided into two parts: specular reflection and diffuse reflection. The diffuse reflected beam will be bouncing on the inner wall of the integrating sphere. The curvature of the inner wall is carefully designed so that the diffused beam will be directed to the spot where the detector is. There is a small window on the integrating sphere that permits specularly reflected light to leave the sphere. When the window is open, the detector will only detect the light from diffuse reflection $R_{\text{diff}}$. When the window is closed, the specular reflection will also be directed to the detector, giving the total reflection $R_{\text{tot}}$. By measuring $R_{\text{diff}}$ and $R_{\text{tot}}$, we also get $R_{\text{spec}} = R_{\text{tot}} - R_{\text{diff}}$.

![Integrating sphere diagram](image)

Figure 16. Integrating sphere for optical reflectance measurement.

### 2.5. Empirical $Y$ factor for various silicon solar cells

We have applied the proposed metric to many experimental thin film nc-Si:H solar cells. We used published results incorporating both $EQE$ spectra and film thickness data. We also incorporate our own measurements on cells provided to us by United Solar Ovonic LLC. For these cells we have access to, we measured the $EQE$, diffuse and specular reflectance, and film thickness with profilometer [40]. We also looked into literatures for published results with EQE spectra and film thickness data.
There have been many light trapping techniques developed so far, for both thick wafer and thin film cell. The cells we studied cover a wide range of thickness, and different light trapping techniques are used. We will review the techniques used in those cells, and then show the empirical enhancement factor $Y$ vs. thickness.

For crystalline silicon, surface texturing is the most popular approach to increasing light trapping. By developing the surface structure on a Si substrate, the following effects can be observed: a reduction of surface reflection, an increase in the amount of internal reflection which in turn reduces the amount of light escaping from the cell, and an increase in the optical path length which leads to an increase in the optical absorption [41].

Single c-Si solar cells are generally textured with random pyramids, which are produced by anisotropic wet chemical etching solutions such as those of KOH and NaOH [42]. In most of the cases the random pyramids have feature sizes in the range of several microns. For less graded silicon material, e.g., mc-Si, the crystal sizes are smaller and less ordered. The random nature of mc-Si makes such a technique less effective, surface texturing by dry processes such as reactive ion etching (RIE) have been investigated and applied to mc-Si solar cells [43,44,45].

When the thickness of the layer is on the order of a few microns, the depth of the texturing is comparable with the thickness and anisotropic wet chemical etching method is less feasible. Instead, texturing is incorporated into the substrate or superstrate first, and then followed by conformal deposition of a silicon layer. The texture will be transferred during the deposition. We show the typical substrate and superstrate structure in Figure 17.
Figure 17. Illustration of superstrate and substrate thin film cells. A substrate cell is a bottom up structure which starts with a back reflector (BR) fabricated on a substrate like stainless steel. For thin film silicon cells, efficiencies are highest when light enters through the p-type layer. The n, i, and p layers are deposited in sequence, and finished with a transparent conducting oxide (TCO) coating on top; the TCO acts both as an electrical contact as well as anti-reflection layer.

A superstrate cell is a top down structure which usually starts with a transparent conducting layer made on top of glass. Then the p, i, and n layers are deposited; the cell is finished with a metal back reflector. The texture is usually made on the superstrate or substrate, which then transfers to the subsequent layers.

For example, a n-i-p cell deposited onto a Ag/ZnO layers that has previously been applied to the substrate. The silver layer can be textured by elevating the silver deposition temperature [46]. In p-i-n cells, which are made on TCO-coated glass, a texture aluminum doped zinc oxide (AZO) is made first due to the crystal growth of AZO itself. Different methods are used for crystal growth: it could either be direct growth of zinc oxide film by low pressure chemical vapor deposition. Alternatively, a sputtered zinc oxide film can be etched to create a texture [47,48].
The sputtered zinc oxide film was etched for 10s in a 0.5% diluted hydrochloric acid (HCL) solution. Surface texturing of the film leads to a surface morphology that very closely resembles a pyramid-like structure, albeit not perfectly symmetrical ones [49].

Figure 18. Scatter plot of the light trapping enhancement factor for many nc-Si:H and crystalline Si solar cells of varying thickness. For most of the thin film cells, enhancement factor $Y$ is well below $4n^2=50$, the best one is for a 2.5 $\mu$m cell, with $Y$ about 25. For thick crystalline silicon cells, the best ones have $Y=33$ from 47 $\mu$m and 100 $\mu$m HIT cells.
Applying the metric to the published results we found, we calculated the empirical enhancement factors and plotted them versus the silicon absorber layer thickness in Figure 18 [50-72].

Most of the cells have $Y < 20$. The best one is a 2.5 $\mu$m nc-Si substrate cell made by USO, $Y \approx 25$, which is only half of the classical $4n^2$ absorptance. We will discuss the possible reasons for this discrepancy.

Table 2. Reference and Symbol for Figure 18 c-Si solar cells.

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<td>♦</td>
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<tr>
<td>100</td>
<td>33.3</td>
<td>×</td>
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Table 3. Reference and Symbol for Figure 18 thin film nc-Si solar cells.

<table>
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<tr>
<td>2.0</td>
<td>2.5</td>
<td>—</td>
<td>72</td>
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2.6 Discussion: the possible reasons for low Y factor

Knowledge of the effective enhancement factor $Y$ does not address the mechanisms that reduce light-trapping below classical $4n^2$. The classical value of $4n^2$ has several minor limitations. It applies to a film embedded in air, without other encapsulation or superstrate. It is
only strictly valid for weakly absorbed light ($\alpha h \ll 1$) for thick cells $h \gg \lambda$. Under thick cell limit, the mode density in the silicon layer could be quite precisely estimated from radiation theorem. And in the weak absorption regime, absorption behavior will not affect the mode calculation profile. To fill the full mode spectrum in the cell, strong scattering is needed so that photons can be scattered to occupy all the possible states. The absence of parasitic loss is also required, in order to make sure that the occupant photons will only damp their energy into silicon absorption channel.

However, it is hard to satisfy all the requirements listed above in one cell. The structure of the device itself may have intrinsic limitation, limited thickness, encapsulation superstrate, etc. Besides the effect from the cell structures, there are several general reasons for low empirical enhancement factor in experiments. For example, one possibility is inefficient scattering of the incident sunlight into all trapped modes of the cell; another possibility is parasitic absorption by layers in the cell that do not contribute to photocurrent. The mechanism of incomplete light trapping can be distinguished experimentally to some degree if the total reflectance spectrum of the cell is reported as well as its quantum efficiency spectrum.

We will talk about different categories of reasons for incomplete light trapping.

### 2.6.1 Encapsulation and film thickness effect

For superstrate cells fabricated on glass, after corrected for the effect from glass substrate, the classical absorptance that could be achieved in ergodicity is reduced to $4(n/n_s)^2$, where $n_s$ is the refractive index of glass or encapsulation layer. The high index encapsulation could reduce light trapping is a direct consequence of ergodicity. With higher refractive index, the possible optical modes outside the cell are larger than 1 unit which is corresponding to air medium. Thus, in ergodicity, photons have a higher tendency to fill the optical modes that is not in the cell. For
the same incident beam, there will be less number of photons occupying the states in the semiconductor layer. Thus, the absorption will be lowered.

For thin film layers, however, the supported modes in the device are no longer continuous but discrete. It is not quite valid to use radiance theorem to estimate the total modes density. This effect is more severe when the film thickness is quite thin. In this thesis, we will use wave form radiance theorem [73] for thermodynamic calculation of nc-Si:H thin film silicon solar cells.

2.6.2 Poor Anti-Reflecting Coating.

In substrate n-i-p thin film solar cells, the typical an anti-reflecting layer is designed by quarter wavelength thin film optics with \( d = \lambda / 2n \), to have a minimum or zero reflecting loss around \( \lambda \) usually around 500nm to 600nm, thus, the absorption in this region would be maximized. However, reflection at longer wavelengths is not zero, for example, the quarter wavelength design gives about 20% reflection at those wavelengths.

We show a reflectance curve by an ITO layer on top of silicon substrate. The dashed orange curve is calculated value for a 70nm dielectric film with refractive index \( n=2 \) sitting on top of infinite thick substrate with refractive index \( n=3.5 \), at \( \lambda = 560\text{nm} \), reflection reaches minimum of zero and all the light transmits through to the other layers; After passing the minimum, reflection keeps increasing and reaches about 20% at \( \lambda = 1100\text{nm} \).

Overall, the specular reflected light does not involve in light trapping, reducing the light trapping enhancement factor from \( 4n^2 \).

There is a new design of AR coating by silver nanowire network [74], or incorporating a 2-D photonic dielectric grating [75]. These new designs have already achieved very low reflectance around 4% for the full range from 400nm to 1200nm, which will bring it closer to the assumption of perfect anti-reflection coating.
Figure 19. Specular reflectance from a virtual design with 70 nm ITO (refractive index n=2.0) on top of an infinite silicon substrate (n=3.5).

### 2.6.3 Inefficient light scattering:

Accessing as many modes as possible is crucial for light trapping, the simplest way of accessing optical modes is scattering. The full classical $4n^2$ light trapping requires strong scattering so that all the modes would be populated with equal amount of energy. For inefficient scattering, only a fraction of the modes can be excited and the number of modes populated is dependent on how strong the scattering is. It has been shown that Lambertian scattering [76] is strong enough for populating all the modes. In reference 71, a solar cell is fabricated on a 260µm silicon wafer without etching for texture, the resulting $EQE$ and reflectance spectrum is provided in the paper as shown in Figure 20. The critical wavelength for 260µm thick silicon is 1140nm, according to our calculation in Figure 11, at this wavelength, $EQE(\lambda_b) = 0.03$ $R(\lambda_b) = 0.9$, the enhancement factor is equal to 1.5, which is extremely low. $EQE(\lambda_b)$ is lower than the classical absorption $A_{ct}(\lambda_b) = 0.5$ by 0.47.
Figure 20. $EQE$ and $R$ for planar cell, the thickness of the cell is 260 $\mu$m; the benchmark wavelength for this thickness is 1140nm. At the benchmark wavelength, the $EQE$ is measured as 0.03 and the reflectance is about 90%. Measurements are from reference 71.

The sum of $EQE(\lambda_b)$ and $R(\lambda_b)$ at critical wavelength gives 0.93 which is very close to unity, the parasitic loss absorptance is only about 0.07, which is not large enough to explain the inefficiency of 0.47. Above all, the reason for poor silicon absorption at the critical wavelength is due to inefficient scattering, which is consistent with the preparation of the sample: it is not textured. For this cell, texturing is the most important things to do to achieve classical absorption limit.

2.6.4 Parasitic loss:

In a real cell, silicon is not the only active absorbing layer. TCO layers and interfaces can lead to sizable contribution to the absorption and it is impossible to completely avoid the absorption in those layers. Assuming perfect photo carrier collection, if the sum of the quantum efficiency and the reflectance at a given wavelength is less than unity, the difference is due to parasitic absorption.

In the sample with pyramids’ texture in reference 71, pyramids were etched on top of a 260$\mu$m silicon wafer. Light scattering by those pyramids is very strong; which is evidenced by a
specific ray tracing study [77]. However, from the $EQE$ spectrum, at $\lambda_b = 1140\text{nm}, EQE(\lambda_b) = 0.34$. This gives us an enhancement factor of $Y=26$. From the reflectance spectrum $R(\lambda_b) = 0.34$, the sum of $EQE(\lambda_b) + R(\lambda_b) = 0.68$, which tells us that the parasitic loss is around 0.32 at benchmark wavelength.

![Figure 21. EQE and $R$ for a pyramidally textured monocrystalline silicon cell. The thickness of the cell is 260 $\mu$m, and the benchmark wavelength for this thickness is 1140 nm. The empirical enhancement factor is $Y=26$ for this cell. Note that at the even longer wavelength $\lambda=1200\text{nm}$, where $R=0.5$, the silicon’s absorptance goes to zero and all the cells’s absorption is parasitic. The bar chart illustrates the budget for incident illumination at $\lambda_b$. Measurements are taken from reference 71.](image)

Since $EQE(\lambda_b)$ is only 0.16 lower than classical absorption $A_{cl}(\lambda_b)$ of 0.5, a 0.32 parasitic loss is considered to be very strong. It is reasonable to assume that the scattering is strong enough so that all the modes are in thermodynamic equilibrium. The total number of modes accessible is $4\pi^2$. We will show that thermodynamic calculation with parasitic loss leading to an agreement between $EQE$ and $R$ curves in Figure 21.
We propose an approximate treatment of parasitic absorption that appears to be useful in analyzing combined reflectance and quantum efficiency measurements. In particular we replace the bulk absorptance term \( ah \) in equation 2-6 by \( ah + a_p \), where \( a_p \) is an effective parasitic absorptance; we are assuming that, in the absence of parasitic absorption, the cell would have classical light-trapping.

When parasitic absorption in a cell is incorporated, we distinguish between the total absorptance and the absorptance in the semiconductor layer. Of course, only the semiconductor absorptance contributes to the quantum efficiency. The total and semiconductor absorptance in this approximation are:

\[
A^e = \frac{4n^2(ah + a_p)}{1 + 4n^2(ah + a_p)}
\]

\[
A_s^e = \frac{4n^2ah}{1 + 4n^2(ah + a_p)} = \frac{4n^2}{1 + 4n^2a_p} ah
\]

So, in this expression, the parasitic absorption yields a subclassical enhancement:

\[
Y = \frac{4n^2}{1 + 4n^2a_p}.
\]

In the cell we illustrate in Figure 21, \( Y \) is 26. At strong scattering limit, it corresponds to a parasitic loss of \( a_p = 0.02 \) according to equation 2-14.

In order to check the value of parasitic loss \( a_p \), we further study the reflectance curve at long wavelengths. If \( a_p \) depends weakly on wavelength, it can be measured using the long wavelength reflectance. At long wavelengths, where \( ah \approx 0 \), the total reflectance of the film is
\[ R_p^e = 1 - A^e \approx 1 - \frac{4n^2a_p}{1 + 4n^2a_p} = \frac{1}{1 + 4n^2a_p} \]

\[ Y = \frac{4n^2}{1 + 4n^2a_p} \approx R_p \cdot 4n^2 \]

At \( \lambda = 1200\text{nm} \), silicon absorption is negligible, \( R \approx 0.5 \), then by equation 2-15, \( a_p = 0.02 \), which agrees with the value we calculated from equation 2-14.

The parasitic loss in each mode is as small as 0.02, however, the parasitic absorption at critical wavelength is significant, that is because parasitic absorption also gets enhanced when multiple modes are launched.

This parasitic loss is related to the material property of various layers and quality of each interface. We show absorption coefficients for typical materials in a solar cell device in Figure 22. Since the light trapping regime is at long wavelength above 800nm, we will only look at the part above 800nm. In this region, amorphous silicon is non-dispersive with an extremely low absorption coefficient, so that the n type doped layer and p type doped layer (in amorphous phase) are negligible in terms of optical absorption. The TCO absorption coefficient is about 1 or 2 orders of magnitude higher than nc-Si/c-Si, thus TCO absorption could be very large, becoming a major source for parasitic loss, especially when we consider light trapping enhanced TCO absorption since it is in close vicinity to high index material silicon(n=3.5).

\( EQE \) indicates the absorption in silicon (we assume one absorbed photon can only generate one electron hole pair which is true for conventional cells). The total cell absorptance (1-R) is higher than \( EQE \), the difference between the two is a measure of how much parasitic absorption there is. In the cell, parasitic losses are pretty significant. At different wavelength regions, the mechanisms of parasitic absorption are different. In the short wavelengths, \( \lambda < 500\text{nm} \), parasitic
Figure 22. Absorption coefficient of different materials. TCO is much more absorptive than silicon at long wavelengths, thus be a source of parasitic loss.

loss is due the p type doped layer, light will travel through p layer first to reach active silicon layer. Even a thin p layer would has a noticeable amount of absorption, the photo carriers generated by this layer would not contribute to photocurrent or $EQE$, because of the high defects states: photo carriers recombine immediately and dissipate energy into heat.

For long wavelengths, especially for $\lambda > 900\text{nm}$, silicon absorption is weak. However, the TCO absorption is strong at these wavelengths as shown in Figure 22.

Parasitic loss by TCO at long wavelengths is carefully studied in Chapter 3.
Chapter 3. Parasitic Loss Analysis for Incomplete Light Trapping in Substrate nc-Si Solar Cells

As can be seen in Figure 18, all the light trapping enhancement factors are well below $4n^2 = 50$. To identify the reason for incomplete light trapping requires a careful study of the $EQE$ and reflectance spectra. In this chapter, we show an experiment result of a set of nc-Si:H substrate (n-i-p) cells, and the thermodynamic calculation we developed to explain the parasitic loss in front ITO layer.

The nc-Si:H thin film solar cells were fabricated by our collaborators at United Solar Ovonic (USO) using their cutting edge technology. We first created a set of back reflectors including both single-stage and 2-stage designs, in which their light scattering properties vary greatly. Solar cells made on top of both types of back reflectors give very similar results in $EQE$ and reflectance spectra. We find the empirical light trapping enhancement factors from those cells are around 13, which is much less than 50. The near-independence of $EQE$ on the back reflector morphologies suggests that inadequate light scattering is not likely to be the major reason for incomplete light trapping. The absorption could also occur in oxide layers beside silicon layer. In order to show the amount of absorption in silicon, we measured internal quantum efficiency ($IQE$) spectra, which shows a strong parasitic behavior inside the cell.

We developed a model to calculate the light absorption in both the silicon layer and the front TCO (ITO in our cells). This “thermodynamic” calculation invokes equipartition of the optical energy density stored in each of the electromagnetic modes of the cell. Using real material properties as input, we find that it gives a reasonable explanation for the parasitic loss. We then conclude that scattering at both types of back reflectors are strong enough to reach
thermodynamic ergodicity, and that the major reason for the low $Y$ is due to the ITO parasitic loss.

### 3.1. Preparation of Ag/ZnO Back Reflector

Our collaborators at United Solar LLC prepared nc-Si:H $nip$ solar cells on stainless steel substrates with the deposition sequence Ag / ZnO /n / i / p / ITO. Ag / ZnO layers are deposited first onto stainless steel by different methods, as we explain shortly. The n, i, and p layers are deposited in sequence, which were then using radio-frequency glow discharge with different hydrogen profiling and gas composition [78,79]. The cells were finished by depositing with a transparent conducting oxide (TCO) coating on top; the TCO acts both as an electrical contact as well as anti-reflection layer. In the cells we studied, the 70 nm top TCO is made of tin doped indium oxide (ITO). This film was sputtered at 170 C. The plasma deposition and sputtering processes for the nc-Si:H and ITO layers have been reported previously [80].

An ideal back reflector is assumed to have low reflection loss and high diffuse reflectance. United Solar had previously reported total and diffuse reflection spectra for four representative back reflectors [80]. Flat and textured Ag layers were deposited, and thin and thick ZnO layers had thicknesses of 0.12 $\mu$m and 2.0 $\mu$m were sputtered on top of those Ag layers. The best performance of those back reflectors used a combination of textured silver and thin ZnO. This combination will be used in our Ag/ZnO back reflectors design.

In our experiments, the Ag/ZnO back reflectors were prepared with single-stage and “two-stages” of silver deposition and annealing.

The conventional way of making Ag/ZnO back reflector as developed at United Solar by an elevated temperature magnetron sputtering, the back reflectors fabricated in this way were noted as single-stage back reflectors. The standard process carried out in USO is heating stainless steel
substrate to about 500 C first, then sputtering a layer of silver for about 500 nm. Sputtering at this elevated temperature create texture in the resulting silver films. The texture is thus used as a source for scattering.

Figure 23. Illustration of substrate solar cells made by United Solar Ovonic, LLC. Ag/ZnO back reflectors are sputtered on to a stainless steel substrate, followed by a thin layer of n type amorphous silicon and then intrinsic nc-Si:H layer of device quality. Then a p type amorphous silicon is deposited, and finally the last step is the top coating of ITO layer. The interfaces have an rms roughness of about 30-60 nm, or about 2-4% of the thickness of the cell.

After the deposition of silver layer, a thin ZnO layer with thickness about120 nm is sputtered on top of the rough silver surface at 200 C. An atomic force microscopy (AFM) image of typical single-stage back reflector is shown in Figure 24.

An alternative way of preparing a Ag/ZnO back reflector is to intentionally incorporate silver nanoparticles into the back reflectors, with the goals of intentionally launching surface plasmon polariton modes at the metal/insulator interface and of increasing the scattering of incident light into the waveguide modes of the cell. Metal gratings could be arranged at the back
to launch surface plasmon polariton modes [81] [93]; or metal nanoparticles can be buried in the oxide of the back reflector to be used as scattering centers [82]. In our study, we made silver nanostructure in the metal at the back reflectors by a 2-step fabrication process. We call these back reflectors “2-stage” back reflectors.

Figure 24. AFM image of a "single stage" back reflector. Imaging by employees of United Solar Ovonic LLC; used with permission.

As previously reported [83,84], silver nanoparticles were created by depositing a very thin silver film, typically 20 nm, and then annealing the film, which “balls up” into individual nanoparticles. The size distribution of the nanoparticles varies with the temperature, substrate, and ambient. We will use this annealing process as the first step for our 2-stage back reflectors.

First, a layer of thin Ag film is thermally evaporated onto the stainless steel substrate at room temperature; the substrates were provided by United Solar so that they’d be identical to those used for the single-stage process. Then the as deposited film is continuous, and it is transferred to an oven to be annealed for 2 hours at temperatures around 220°C. In ref 83 and 84,
annealing was taking place in furnace flew with dry nitrogen. However, in our experiment, annealing is taking place in an oven which is filled with air. Keeping the annealing time and temperature the same, we changed the thickness of the original continuous silver film as a way of controlling the sizes of silver nanoparticles.

Scanning electron microscopy (SEM) showed that the original continuous silver film had agglomerated into islands after annealing.

Figure 25. (top row) Silver nanoparticles annealed from different Ag film thicknesses. (bottom row) The same sample after coating by a 100 nm continuous Ag film. The islands from first step of annealing get more round and bigger after the second step of 100 nm silver film coating.

The thin layer of film breaks into an island layer at high temperature. For example, after annealing the 17 nm silver thin films, the mean island area was $2.5 \times 10^4 \text{ nm}^2$ with 28% coverage of the substrate. Usually, thicker films will create bigger islands after annealing. Using magnetron sputtering, we next deposited a second layer of silver 100 nm thick onto these silver islands to obtain a structured but continuous silver film. In the second step of coating 100nm
silver film, the substrate was in mechanical contact with a cooling stage at 10°C during the sputtering. The second Ag layer modified the morphology; the islands grew larger (mean island area $4.5 \times 10^4 \text{ nm}^2$), and became rounder and smoother than before. We show SEM images for our 2-stage back reflectors with different annealing film thickness in Figure 25.

Backreflectors were then shipped to United Solar to finish the cells. 120nm ZnO layers was sputtered on top of the silver layer at 200°C, heated by infrared heaters. The configuration for ZnO sputtering is the same for both single-stage and 2-stage back reflectors, as described before [80].

Figure 26. AFM image for a set of 2-stage back reflectors with different annealing layer thicknesses, and 100 nm continuous silver film coating. Images taken by employees of United Solar Ovonic LLC; used with permission.
Comparing single-stage and 2-stage back reflectors, we found a big difference in surface roughness, as shown by AFM measurement. A typical AFM image of single-stage back reflector was shown in Figure 24, and a set of 2-stage back reflectors are shown here in Figure 26. The four 2-stage back reflectors have different thicknesses for the original silver thin film before annealing.

The root mean square (RMS) roughnesses of the surfaces for one set of back reflectors are listed in Table 4. The roughness of the 2-stage back reflectors are higher than the single-stage back reflector. Before and after ZnO deposition for each back reflector, the roughness is qualitatively the same.

<table>
<thead>
<tr>
<th>Sample</th>
<th>RMS before ZnO (nm)</th>
<th>RMS after ZnO (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-stage-15nm</td>
<td>46.5</td>
<td>40.5</td>
</tr>
<tr>
<td>2-stage-17nm</td>
<td>49.7</td>
<td>43.4</td>
</tr>
<tr>
<td>2-stage-20nm</td>
<td>51.6</td>
<td>49.7</td>
</tr>
<tr>
<td>2-stage-25nm</td>
<td>56.9</td>
<td>60.8</td>
</tr>
<tr>
<td>single-stage</td>
<td>--</td>
<td>26.9</td>
</tr>
</tbody>
</table>

Table 4. The RMS roughness of the front surface of both single-stage and 2-stage back reflectors on stainless steel. For the 2-stage back reflectors, the thickness of the initial silver layer is indicated. The layer was annealed and then a second 100 nm layer was applied at 10 C. Roughnesses are shown before and after sputtering a 120 nm ZnO layer. Measured by United Solar employee, used with permission.
3.2. Optical properties of the back reflector

Besides the difference in roughness, single-stage and 2-stage back reflectors have very different optical properties. We performed optical measurement for both kinds of back reflectors. For each back reflector, we measured both before and after the deposition of ZnO.

In Figure 27, we first show atomic force microscopy images and reflectance measurements for a single-stage and a two-stage back reflector including the ZnO films. The histogram below the images indicates the depth distributions for the scans; as can be seen, the single-stage backreflectors are about half as rough as the two-stage backreflectors.

At the bottom of the figure we present diffuse and total reflectance spectra at normal incidence for these backreflectors before and after sputtering the 120 nm ZnO layer. As is evident, the two backreflectors have quite different properties; with the ZnO over layer, the two-stage back reflector has substantially greater diffuse reflection, but is also lossier than the single-stage back reflector. The most prominent feature is the bottoming out at 320 nm that is present for both backreflectors. This is the interband transition of silver that is seen even for specular films [85,86].

For the single-stage deposition of smoother films, there is only a modest effect of applying the ZnO layer. Since dielectric over layers strongly affect the frequency of a surface plasmon polariton [87], we conclude that there is little plasmonic effect on these spectra. The two-stage backreflectors are intentionally plasmonic. We attribute the secondary minimum in the reflectance at 360 nm (without ZnO) to the main surface plasmon resonance; this agrees fairly well with the resonance measured in planar films [86]. There is a well-defined maximum in the diffuse reflectance at 500 nm. The addition of the 120 nm ZnO layer shifted the 360 nm
minimum to 520 nm, which is reasonably consistent with the known effects of dielectric over
layers on surface plasmon resonance.

Figure 27. The top AFM graphs show the profile of the two typical back reflectors wth ZnO
layer deposited. The histogram below the images indicates the depth distributions for the scans;
as can be seen, the single-stage backreflectors are about half as rough as the two-stage
backreflectors. At the bottom we present diffuse and total reflectance spectra at normal incidence
for these backreflectors before and after sputtering the 120 nm ZnO layer.

The conclusion of those two back reflectors is that they have very different scattering
property, the scattering intensity from 800nm to 1200nm changes by a factor of 2 from single-
stage BR to 2-stage BR. AFM imaging by employees of United Solar Ovonic LLC; used with
permission.
For later use, we note the specular reflectance of the back reflectors. At 1200 nm, the specular reflectances are 0.3 and 0.6 for the 2-stage and single-stage backreflectors, respectively.

### 3.3 Device fabrication and characterization.

The subsequent fabrication of n, i, p, and ITO layers are the same for both type of back reflectors. After a device is finished, we performed AFM, I-V, EQE, and cell reflectance measurements.

#### 3.3.1. AFM on finished devices.

The devices are made on back reflectors with different roughnesses. The final texture of the ITO is determined by nc-Si:H layer with a few microns thickness, as will be shown by AFM later. We performed AFM measurements for finished cells made on both types of back reflector. The AFM tip is scanning on top of the ITO layer directly. The rms roughness from AFM measurement were typically 29 nm for the samples made on single-stage back reflector and 33nm for two-stage back reflectors.

#### 3.3.2. Device parameters.

The cell properties are summarized in Table 5 from I-V measurements under the solar simulator. The I-V measurements were carried out at USO. In our experiments, different batches of samples with varying silicon layer thickness were made. Within each batch, the silicon layer thickness varies slightly within 3% from cell to cell, measured by profilometry [88].
Table 5. Device characterization for different cells made in two batches. Samples a-e are in first batch, samples f-k are in second batch. Thickness of the cells are measured by profilometry.

Within each batch, the thickness changes slightly within 3%. The short circuit current from two BRs are very close to each other with a short range span. $V_{oc}$ from the 2-stage BR is generally slight smaller than the single-stage BR. The biggest difference is the fill factor (FF). single-stage BRs are smoother, leading to better fill factors (FF).

<table>
<thead>
<tr>
<th>BR</th>
<th>RMS (nm)</th>
<th>$L$ (µm)</th>
<th>$V_{oc}$ (V)</th>
<th>FF</th>
<th>$J_{sc}$ (mA/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>single</td>
<td>-</td>
<td>1.64</td>
<td>0.510</td>
<td>0.61</td>
</tr>
<tr>
<td>b</td>
<td>25</td>
<td>-</td>
<td>1.55</td>
<td>0.499</td>
<td>0.56</td>
</tr>
<tr>
<td>c</td>
<td>21</td>
<td>-</td>
<td>1.59</td>
<td>0.473</td>
<td>0.55</td>
</tr>
<tr>
<td>d</td>
<td>20</td>
<td>-</td>
<td>1.65</td>
<td>0.508</td>
<td>0.50</td>
</tr>
<tr>
<td>e</td>
<td>19</td>
<td>-</td>
<td>1.60</td>
<td>0.477</td>
<td>0.54</td>
</tr>
<tr>
<td>f</td>
<td>single</td>
<td>27</td>
<td>1.50</td>
<td>0.516</td>
<td>0.63</td>
</tr>
<tr>
<td>g</td>
<td>15</td>
<td>41</td>
<td>1.47</td>
<td>0.525</td>
<td>0.60</td>
</tr>
<tr>
<td>h</td>
<td>17</td>
<td>43</td>
<td>1.49</td>
<td>0.521</td>
<td>0.61</td>
</tr>
<tr>
<td>i</td>
<td>20</td>
<td>50</td>
<td>1.52</td>
<td>0.511</td>
<td>0.56</td>
</tr>
<tr>
<td>j</td>
<td>25</td>
<td>61</td>
<td>1.46</td>
<td>0.516</td>
<td>0.57</td>
</tr>
<tr>
<td>k</td>
<td>single</td>
<td>27</td>
<td>1.50</td>
<td>0.514</td>
<td>0.17</td>
</tr>
</tbody>
</table>

We listed both batches of samples that we studied. The open-circuit voltage $V_{oc}$ changes slightly between single-stage samples and 2-stage samples. In the first batch, 2-stage samples have slightly lower $V_{oc}$, but in the second batch 2-stage samples have slightly higher $V_{oc}$. $J_{sc}$ is also very similar between single-stage samples and two stage samples: in the first batch they are almost the same, in the second batch 2-stage samples are slightly lower. The difference in $V_{oc}$ and $J_{sc}$ are both very small. The most noticeable difference is in FF. single-stage BR has a higher FF. In this thesis, we are mainly interested in $J_{sc}$. What we learned from the $J_{sc}$
measurement is that even though the two types of back reflectors are very different, the resulting $J_{sc}$ are very similar.

The $J_{sc}$ we showed in Table 5 is calculated from equation 1-4 using the experimental $EQE$ spectra [89]. We will talk about our experimentally measured $EQE$ spectra in the next section.

3.3.3 $EQE$, Reflectance, and $IQE$

We show $EQE$ spectra for both batches and show them in Figure 28 and Figure 29. The $EQE$ spectra were measured by United Solar Ovonic, LLC, and agreed with the $EQE$ measurement carried out by our setup.

Figure 28. $EQE$ measurement for samples in the first batch with silicon layer thicknesses around 1.64 $\mu$m; the measurements are done at -2 V bias to ensure complete collection of photocarriers generated in the intrinsic layer. There are 6 samples in this batch. Two of them are made on single-stage back reflectors, and the rest four are made on “2 stage” back reflectors. The thicknesses of the first silver films before annealing in the 2-stage back reflectors are 19 nm, 20 nm 21 nm, 25 nm (see Table 5).
Figure 29. \( EQE \) measurements for samples in the second batch with silicon thicknesses around 1.5\( \mu \)m. There are 6 samples in this batch, two are made on single-stage back reflectors, and four are made on “2 stage” back reflectors. The thicknesses of the first silver layer before annealing in 2-stage back reflectors are 15 nm, 17 nm, 20 nm, 25 nm. Measurements done by employees of United Solar Ovonic LLC.

For both of the batches, \( EQE \) spectra are close to each other with a little variation. Here we will take the best curve from both type of design as the optimized data, then perform our analysis on the optimized data.

We take the best \( EQE \) spectra from both batches and compare with the corresponding classical \( 4n^2 \) absorptance, as shown in 1-6. What we can see is that the optimized curves are almost overlapping on each other, and both of them are lower than the classical \( 4n^2 \) absorptance.

Cells made on very different back reflectors have very different optical scattering properties. It is expected that the difference in light scattering shall lead to differences in \( EQE \) spectra. However, the measured \( EQE \) spectra are almost the same between the two types of samples. It is quite puzzling at the first look.
Figure 30. $EQE$ spectra for the highest $J_{SC}$ samples from both batches. We also show the $4n^2$ absorptance spectra for the same silicon thicknesses. Within both batches, optimized $EQE$ spectra are very similar to each other, and both are lower than the classical $4n^2$ absorptance. The empirical enhancement factors for both batches are about $Y=13$.

We consider two possible situations for the light trapping result in our experiments, in the absence of parasitic loss. When light scattering in the cell is weak, the corresponding $EQE$ should be lower than $4n^2$ absorptance. In this circumstance, an improvement over light scattering would then result in an increase in silicon absorption. When light scattering in the cell is strong enough to populate all the modes, then an increase in diffuse scattering would not help, because the modes are already fully populated in the cell. In this circumstance, the corresponding silicon absorption reaches the $4n^2$ absorptance, and it cannot be increased by an improvement over optical scattering.

However, either of the hypotheses above would explain our experiment $EQE$ spectra. If the light scattering is weak in cells made on “single-stage” back reflector, it can explain that $EQE$
spectra are lower than classical absorptance. However, the cells made on 2-stage back reflectors in the same batch, which has a higher diffuse reflectance, do not give higher $EQE$. The silicon absorption is the same for both types of samples.

If the scattering is strong enough in the cells made on “single-stage” back reflectors, then the absorptance for both types of cells should be the same: classical $4n^2$ absorptance. This is not consistent with experimental $EQE$ spectra, which are much lower than classical $4n^2$ absorptance spectrum.

Without considering the parasitic loss, it is hard to explain the $EQE$ spectra we measured from two very different back reflectors. So, we will take into account the parasitic loss. Parasitic losses in the cell are particularly clear in internal quantum efficiency measurements, which were defined in equation 1-5:

$$IQE \equiv \frac{EQE}{1 - R}$$

$IQE$ spectra show the probability that an absorbed photon generates photocurrent, and they require measurement of both the $EQE$ and the total hemispherical reflectance $R$.

$EQE$ spectra are shown in

Figure 30 for typical cells from both batches. In Figure 31, we show the total and specular reflectance measurements for single-stage and 2-stage samples with 1.5 $\mu$m silicon thickness. The dashed orange curve is the calculated specular reflectance for a 70 nm ITO film on an infinite silicon substrate.

The wiggles in the specular reflectance spectra are interference fringes indicating that there is some specular reflection both from the front interfaces of the cell (ITO/air and Si/ITO) and also from the back (Ag/ZnO and ZnO/Si). The specular reflection in the device is significant, suggesting inadequate diffuse scattering from the backreflector. We analyzed the fringes to
calculate the specular reflectance from the back. The calculation indicates only modest specular reflection at the back; diffuse scattering is still dominating in the back reflectors.

Figure 31. Reflectance measurements for cells made on both types of back reflectors, with 1.5 μm silicon layers. Dashed gray lines are total reflectances, and solid lines are specular reflectances. The orange line is the calculated value for a 70 nm ITO ($n = 2$) film sitting on top of an infinite silicon substrate ($n = 3.5$).

The complex amplitude reflectance $r_{AR}$ of an ITO layer (thickness $\Omega$) on top of a silicon substrate is given by:

$$r_{AR} = \frac{r_1 + r_2 \exp \left(-\frac{4\pi n_{ITO}\Omega}{\lambda}i\right)}{1 + r_1 r_2 \exp \left(-\frac{4\pi n_{ITO}\Omega}{\lambda}i\right)}$$

3-1

here $r_1 = \frac{1-n_{ITO}}{1+n_{ITO}}$ is the amplitude reflectance at the top air/ITO interface, $r_2 = \frac{n_{ITO} - n_{Si}}{n_{Si} + n_{ITO}}$ is the amplitude reflectance at the bottom ITO/Si interface, where $n_{ITO}$ and $n_{Si}$ are the indices of refraction of the ITO and the Si, respectively, $\lambda$ is free space wavelength. We used this result to calculate the dashed orange curves in Figure 31.
To calculate the fringe amplitudes, we used the simplest approximation by assuming that the specular reflectance of the back reflector is weak and that we can neglect the absorption of the silicon. For a structure with specular amplitude reflectances $r_{AR}$ and $r_{BR}$ from the top and bottom interfaces, respectively, the maximum and minimum specular intensity reflectances $R_{mx}$ and $R_{mn}$ for the fringes are approximately:

$$R_{mx} = \left| |r_{AR}| + |1 - r_{AR}^2||r_{BR}| \right|^2$$  \hspace{1cm} 3-2$$

and

$$R_{mn} = \left| |r_{AR}| - |1 - r_{AR}^2||r_{BR}| \right|^2$$  \hspace{1cm} 3-3$$

Note that we are neglecting diffuse reflection by the top interfaces, and we have again assumed that absorption processes in the film are negligible: $\alpha h \ll 1$. The expressions are simplified ones that assume $|r_{AR}| \gg |(1 - r_{AR}^2)r_{BR}|$, so that amplitude contributions from waves that are reflected from the back more than once can be neglected. It is also worth noting that the phase shifts in $r_{AR}$ and $r_{BR}$ may be substantial. This would lead to anomalous fringe positions but would not affect the fringe maxima and minima.

Near 800 nm, the maximum and minimum fringe reflectance corresponds to back reflector intensity reflectances $r_{BR}^2 = 0.015$ for the single-stage back reflector and 0.0004 for the 2-stage back reflector. At 1200 nm the fringes correspond to specular reflectances of $r_{BR}^2 = 0.09$ for the single-stage BR and 0.03 for the 2-stage BR; it is interesting that these fairly small specular reflectances lead to quite noticeable interference fringes. These specular reflectances that are inferred from interference fringes are several times smaller than the corresponding specular reflectances in Figure 27, which were measured prior to deposition of the nc-Si:H. This fact suggests that the nc-Si:H over layer significantly increases the diffuse reflectance of the back reflector. One reason is that the sign of the amplitude reflectance by a ZnO/nc-Si:H interface is
opposite from that of a ZnO/air interface and interference between this amplitude and amplitude reflected by the Ag/ZnO interface will be very different. Indeed, one can roughly describe the ZnO as a coating that suppresses specular reflection in favor of diffuse.

The study of cell specular reflectance supports the hypothesis that the diffuse scattering at the back reflectors inside the cell is strong. Now it is puzzling to us why a strong scattering does not end up with $EQE$ curves as same as the classical $4n^2$ absorptance. We will look for clue in $IQE$ spectra. We show the $IQE$ spectra for $1.5 \, \mu m$ cells in Figure 32.

![Figure 32. IQE measurements of cells made on two types of back reflector. The silicon thickness is $1.5 \, \mu m$ in these cells. The solid blue is a single-stage sample and solid gray is a 2 stage sample. With no parasitic loss, the $IQE$ should be unity as shown by the dashed line. However, parasitic loss reduces it. Especially above 900 nm, the $IQE$ falls below 50%, and silicon is no longer the major absorber layer in the cell.

The dashed curve shows a perfect $IQE$ curve when there is no parasitic loss at all. However in our cells, both types of cells have low $IQE$ for wavelengths longer than 600 nm. $IQE$ spectra keep falling when they go to longer wavelengths, suggesting that the parasitic loss is growing relatively stronger when silicon absorption becomes weaker. When the wavelengths go above
900nm, the value of $IQE$ drops down below 50%, which means that silicon is no longer the major absorber in the cell.

$EQE$ and $IQE$ spectra from both types of cells suggest that parasitic absorption in the cells should be considered, otherwise, it is hard to explain the experimental result. The places for parasitic loss at long wavelengths could come from either front ITO or back reflectors. The fact that back reflectors used in our experiments are very different without much affecting the $EQE$ spectra suggests that the major contribution of parasitic loss is coming from front interface instead of the back. Another clue that parasitic losses are becoming worse at longer wavelength also agrees with the property of ITO, which has stronger free carrier absorption at longer wavelengths.

### 3.4. The parasitic loss calculation of experiment data

The analysis in last section suggests that parasitic loss in ITO could be the reason for low $EQE$ and $IQE$. In this section, we will develop a method of thermodynamic calculation for silicon absorption and ITO parasitic loss absorption. Thermodynamic light trapping theories were first explained in the early 1980s by Yablonovitch [91]. His thermodynamic calculations assume equipartition, meaning that each electromagnetic mode of a cell with a given optical frequency has the same energy density under illumination, as is necessarily the case in thermal equilibrium. The calculations are independent of the detailed texturing or morphology of interfaces, as long as these don’t modify the mode densities significantly. Similar methods were also used however for different design in thin film slabs [92], thin film on surface plasmon polariton back reflector [93, 94]. In this section, we will compare our thermodynamic calculation results with experiment.
3.4.1 Thermodynamic calculation model for silicon absorption and oxide absorption

The two nearly identical quantum efficiency curves would be due to thermodynamic behavior, so we did a calculation under thermodynamics condition.

According to the theory model we showed in Chapter 1, under thermodynamic limit, all the modes that are supported by the layer structure will be equally populated. These modes can be divided into two categories: radiative modes and waveguide modes indexed by \( m \), each with mode density \( \sigma_r \) per area and \( \sigma_m \) per area, the total density of modes is summed up to be:

\[
\sigma_{tot} = \sigma_r + \sum_m \sigma_m \tag{3-4}
\]

Under perfect anti-reflection coating condition, the density of radiative modes \( \sigma_r \) for a semiconductor layer of thickness \( h \) and index \( n \) is approximately [92]:

\[
\sigma_r \approx \left(1 - \sqrt{1 - 1/n^2}\right) h \frac{\omega^2 n^3}{\pi c^3}. \tag{3-5}
\]

In each mode, the energy confinement (defined as the fraction of power that flows through that layer) in Si, Oxide and air, are denoted as \( \Gamma_{Si} \), \( \Gamma_{air} \), \( \Gamma_{O} \), \( \Gamma_{Si} + \Gamma_{air} + \Gamma_{O} = 1 \). When the propagating constant \( \beta \) of that mode is solved, the mode profile thus then confinement factors can be calculated by integrating the power [95]. Then, the partial absorptance in Silicon layer gives:

\[
f_{rad} = \frac{\frac{\Gamma_{Si} \alpha}{\overline{n}}}{\frac{\Gamma_{Si} \alpha}{\overline{n}} + \frac{1}{4 \left( \frac{\sigma_{tot}}{\rho_0} \right)}} \tag{3-6}
\]

for radiative modes, and

\[
f_m = \frac{\frac{\Gamma_{Si} \alpha}{\overline{n}}}{\frac{\Gamma_{Si} \alpha}{\overline{n}} + \frac{1}{4 \left( \frac{\sigma_{tot}}{\rho_0} \right)}} \tag{3-7}
\]

for waveguide modes. Here, \( \rho_0 \) is the mode density in the coming light before it goes to thermal dynamics scattering. \( \alpha \) is the absorption coefficient for silicon in that waveguide mode, according
to Dr. Schiff’s calculation [94], the absorption coefficient in a certain mode is the same for all
the modes, all equal to the bulk material absorption coefficient \( \alpha \). \( \alpha_o \) is the absorption
coefficient for oxide, \( n_o \) is the refractive index for oxide, \( n \) is refractive index for silicon.

Then, from equipartition assumption, the total absorptance in silicon (relates to experimental
EQE) can be derived from this partial absorptance by:

\[
a_{Si} = \frac{\sigma_{rad} f_{rad}}{\sigma_{tot}} + \sum_m \frac{\sigma_m}{\sigma_{tot}} f_m
\]

Thus the reflectance is:

\[
r = 1 - a_{Si}
\]

For thin-film solar cells, parasitic absorption by a top TCO, and potentially by the back reflector
as well, are not negligible at long wavelengths. We extend the thermodynamic treatment to
include the top oxide’s absorption as follows; the same approach was used previously to
incorporate surface plasmon polariton absorption in cells.[94] The thermodynamic absorptance
incorporating parasitic loss \( \alpha' \) is:

\[
\alpha' = \frac{\sigma_r}{\sigma_{tot}} (f'_{r} + f'_{r,o}) + \sum_m \frac{\sigma_m}{\sigma_{tot}} (f'_m + f'_m,o)
\]

where \( f'_{r,o} \) is the partial absorptance of the radiative modes by the oxide and \( f'_m,o \) is the partial
absorptance of a waveguide mode by the oxide. We are not considering possible surface plasmon
polariton modes in this calculation. Denoting the confinement factor for the TCO as \( \Gamma_{m,o} \), and
noting the fact that energy confined in air is negligible, the four partial absorptance terms are
now:

\[
f'_r = \frac{\Gamma_r \alpha / n}{\Gamma_r \alpha / n + (1 - \Gamma_r) \alpha_o / n_o + \rho_0 / 4 \sigma_{tot}}
\]

\[
f'_{r,o} = \frac{(1 - \Gamma_r) \alpha_o / n_o}{\Gamma_r \alpha / n + (1 - \Gamma_r) \alpha_o / n_o + \rho_0 / 4 \sigma_{tot}}
\]
\[
    f_m' = \frac{\Gamma_m \alpha / n}{\Gamma_m \alpha / n + \Gamma_m \alpha_o / n_o + \rho_o / 4 \sigma_{tot}} \tag{3-13}
\]

\[
    f_{m,o}' = \frac{\Gamma_m \alpha_o / n_o}{\Gamma_m \alpha_o / n_o + \rho_o / 4 \sigma_{tot}} \tag{3-14}
\]

where \(\alpha_o\) and \(n_o\) are the absorption coefficient and refractive index of the oxide. For later use, we note that the absorptance \(a'_s\) in the semiconductor film is:

\[
    a'_s = \frac{\sigma_r}{\sigma_{tot}} (f'_r) + \sum_m \frac{\sigma_m}{\sigma_{tot}} (f_m') \tag{3-15}
\]

The part of light not been absorbed in the cell will be radiated out, noticed as reflectance

\[
    r' = 1 - a'. \tag{3-16}
\]

Because the radiation pattern is random, so it contributes to the diffusive reflectance.

We assume perfect anti reflection coating in deriving equations above, which means that the specular reflection at the front surface is zero. In a real experiment, specular reflection \(R_{spec}\) at front will reduce the amount of light going to the cell, only the portion of \(1 - R_{spec}\) will go into the cell. The above waveguide mode analysis is only suitable to this part of non-specular reflected: \(1 - R_{spec}\).

**3.4.2. Mode calculation: waveguide mode profile and density of states in the device**

The first step in waveguide mode calculation is to solve for all the optical modes supported by the structure, the modes are distributed at certain mode densities, and each mode has different profile which gives different confinement of energy in different layers.

We summarize the calculation of the waveguide mode parameters needed to support the thermodynamic calculation of light-trapping. For each mode, the two parameters needed are the confinement factor \(\Gamma_m\) and areal mode density \(\sigma_m\). We used standard optical slab waveguide calculations.
Figure 33. Illustration of the structure we use for calculation. The left is the silicon solar cell in the experiment, which has a 70 nm ITO layer, a 1.5 µm silicon layer, and a back reflector. We approximate the back reflector to be a perfect metal mirror. Then, the waveguide modes in our device will be equivalent to the odd modes in a 5 layer symmetrical dielectric waveguide, with a core layer of 3 µm and a cladding layer 70nm on both sides.

The structure is illustrated in Figure 33. As discussed in the body of the paper, we did waveguide model calculations assuming that the back reflector is a perfect mirror, which neglects the effects of surface plasmon polariton at the back Ag/ZnO reflector.

At a given optical frequency $\omega$, each mode $m$ has a propagation constant $\beta_m$, and the electric field has the general form $\overrightarrow{E}(x) \exp( i(\beta_m z - \omega t))$, where $t$ the time. There are transverse electric (TE) and transverse magnetic (TM) modes. At a given optical frequency $\omega$, only a discrete set of values $\beta_m$ are compatible with the boundary conditions. TE modes have three nonzero components: $E_y$, $H_x$ and $H_z$, where $H_x = H_x = -\frac{\beta}{\sigma \mu_0} E_y$ and $H_z = -\frac{i}{\sigma \mu_0} \frac{\partial E_y}{\partial x}$. 
The TM modes have the three nonzero components $H_y, E_x$ and $E_z$ with $E_x = \frac{\beta}{\omega \mu_0} H_y$. So we only need to solve for $E_y$ for TE modes and $H_y$ for TM modes.

The modes of the structure with the metal reflector are the odd (anti symmetric) modes for an all-dielectric structure with a semiconductor layer of thickness $2w$, as illustrated in the figure. We will summarize the TE mode calculation for the dielectric structure from Adams’ monograph; the TM mode calculation, is similar [95]. Propagation constants in the range $n_3 k_0 < \beta \leq n_2 k_0$ correspond to waveguide modes that are evanescent in the air, but not in the ITO. For these modes, the electric field profile is (eq. 2.214 – 2.218)

$$E_y, H_y = \begin{cases} 
\sin(h_1 x) & , \quad 0 < x < h \\
\frac{\sin(h_1 w) \sin(h_2 x + \psi)}{\sin(h_2 w + \psi)} & , \quad h < x < h + \Omega \\
A \frac{\sin(h_1 w) \sin(h_2(x + w) + \psi)}{\sin(h_2 w + \psi)} \exp(h_3(w + \Omega - x)), x > h + \Omega 
\end{cases}$$

where the wavevector $k_0 = 2\pi/\lambda$ and $h_1^2 \equiv n_1^2 k_0^2 - \beta^2, h_2^2 \equiv n_2^2 k_0^2 - \beta^2, h_3^2 \equiv \beta^2 - n_3^2 k_0^2$. The phase parameter $\psi$ is determined implicitly by solution of the equation:

$$\tan(h_2 h + \psi) = \eta_{12} h_1 / h_2$$

Here, $\eta_{12}$ takes different value for TE and TM modes:

$$\eta_{ij} = \begin{cases} 
1 & \text{for TE modes} \\
\frac{n_i^2}{n_j^2} & \text{for TM modes}
\end{cases}$$

The eigenmode equation from which $\beta_m$ is calculated is (eq. 2.216 in ref.95):

$$h_3 h = m\pi + \tan^{-1}\left(\eta_{12} \frac{h_2}{h_1} \tan^{-1}\left(\eta_{23} \frac{h_3}{h_2} - h_2 \Omega\right)\right), (m = 1/2, 3/2, 5/2, ...)$$
\[
E_y = \begin{cases} 
A \sinh(h_1 x), & 0 < x < h \\
\frac{A \sinh(h_1 w) \sinh(h'_2 x + \psi')}{\sinh(h'_2 w + \psi')}, & h < x < h + \Omega \\
\frac{A \sinh(h_1 w) \sinh(h'_2 (w + \Omega) + \psi')}{\sinh(h'_2 w + \psi')} \exp(h_3 (w + \Omega - x)), & x > h + \Omega
\end{cases}
\]

where \((h'_2)^2 \equiv \beta^2 - n^2 k_0^2\), and the phase constant \(\psi'\) is calculated from the equation:

\[
\tanh(h_2 h + \psi') = \eta_{12} h_1 / h'_2
\]

The eigenmode equation from which \(\beta_m\) is calculated is (eq. 2.218 in ref. 95):

\[
h_1 h = m\pi + \tan^{-1}\left\{ \eta_{12} h'_2 h_1 \tan^{-1}\left[ \tanh^{-1}\left( \eta_{23} h'_3 / h'_2 - h'_2 \Omega \right) \right] \right\} \quad (m = 1/2, 3/2, \ldots)
\]

Figure 34. The two upper graphs show the TE and TM dispersion relations for a 1.5 µm device.

The lower graphs are the corresponding mode densities.
There are many sophisticated methods developed to solve for equation 3-20 and equation 3-23, including the finite-element method [96,97,98], the plane-wave method [99,100], the graphical method, etc. We used a simple graphical method, which gave results consistent with those for a numerical solver posted by researchers at the University of Twente [101]. In Figure 34 we illustrate the values for $\beta$ as a function of $\omega$ for a cell with a silicon thickness of 1.5 $\mu$m and an ITO thickness of 70 nm. The dashed line in the figure is $\beta = \omega / c$; for frequencies well above a mode cutoff we have $\beta = n_g \omega / c$. The corresponding mode profiles at a wavelength of 1000 nm were presented in Figure 35.

Once the mode propagation constant $\beta_m$ is obtained, we can readily calculate the mode confinement factor and the mode density by integration of the field profile. The TE mode confinement factors for each layer can be calculated considering only the electric field profile as (eq. 2.226 of ref.12):

$$
\Gamma_m = \frac{\int_0^h E_y^2 dx}{\int_0^h E_y^2 dx}, \Gamma_{m,o} = \frac{\int_0^{h+\delta} E_y^2 dx}{\int_0^{h+\delta} E_y^2 dx}, \text{ and } \Gamma_{m,air} = \frac{\int_0^\infty E_y^2 dx}{\int_0^\infty E_y^2 dx}
$$ 3-24

A similar expression applies for TM modes using integrals of the magnetic field profile $H_y^2 / n^2$.

$$
\Gamma_m = \frac{\int_0^h H_y^2 n_2^2 dx}{\int_0^h H_y^2 / n^2 dx}, \Gamma_{m,o} = \frac{\int_0^{h+\delta} H_y^2 n_2^2 dx}{\int_0^{h+\delta} H_y^2 / n^2 dx}, \Gamma_{m,air} = \frac{\int_0^\infty H_y^2 n_2^2 dx}{\int_0^\infty H_y^2 / n^2 dx}
$$ 3-25

We evaluated the confinement factors from numerical integration of the field profiles; the results at 1000 nm for $\Gamma_{m,o}$ are illustrated in Figure 37.

As shown in previous treatments, the mode density for the waveguide mode is conveniently written in terms of these confinement factors (equation A7 in ref. 92 and eq. 2.133 in ref. 95 give
The equation for 3 layer dielectric waveguide. We derived the relation between confinement factors and waveguide mode density for the 5 layer symmetrical waveguide, which is:

$$\sigma_m = \frac{\omega h}{2\pi c^2} [\Gamma_m n_1^2 + \Gamma_{m,o} n_2^2 + (1 - \Gamma_m - \Gamma_{m,o}) n_3^2]$$  

The proof of equation 3-26 is given here. For dielectric waveguides, the group velocity of a mode with propagating constant $\beta$ at frequency $\omega$ is given as $v_g = \frac{d\omega}{d\beta} = \frac{P}{W}[102,103]$ here $W$ is the stored energy in the and $P$ is the power flow, then $\frac{d\beta}{d\omega} = \frac{1}{v_g} = \frac{W}{P}$, the timed averaged power flow $P$ can be derived by the integral over the guide cross-section of the $y$- component of the Poynting vector $S_z[95]$, (equation 2.93):

$$P = \int_{-\infty}^{+\infty} S_z \, dy$$  

In TE modes, $S_z$ is given by $S_z = \frac{\beta}{2\omega \mu_0} E_y^2$, and in TM modes, $S_z = \frac{\beta}{2\omega \epsilon_0} H_y^2$. $j$ is an index for different layers.

The energy density in the mode is:

$$W = \int_{-\infty}^{+\infty} \left( \frac{d(\omega \epsilon)}{d\omega} E \cdot E^* + \frac{d(\omega \mu)}{d\omega} H \cdot H^* \right) \, dy$$  

Given that the materials in the structure are all nonmagnetic dielectric and we ignore the material dispersion, which means for each layer $j$, $\epsilon_j = \epsilon_0 n_j^2$, $\mu = \mu_0$, $\epsilon_0$ and $\mu_0$ are vacuum permittivity and magnetic permeability, $\epsilon_0 \mu_0 = \frac{1}{c^2}$. The time averaged energy density then gives:

$$W = \frac{1}{2} \epsilon_0 n^2 E^2 \, dy.$$  

Or
\[ W = \int_{-\infty}^{+\infty} \left( \frac{d(\omega \varepsilon)}{d\omega} \mathbf{E} \cdot \mathbf{E}^* \right) + \frac{d(\omega \mu)}{d\omega} \mathbf{H} \cdot \mathbf{H}^* dy = \int_{-\infty}^{+\infty} \frac{1}{2} \mu_0 H^2 dy. \]  

We use the top one for TE modes, then:

\[ \frac{d\beta}{d\omega} = \frac{W}{P} = \frac{\int_{0}^{+\infty} \frac{1}{2} \varepsilon_0 n^2 E^2 dy}{\int_{0}^{+\infty} \frac{\beta}{2\omega \mu_0} E_y^2 dy}. \]  

Then the mode density (per volume per frequency) for TE modes is:

\[ \rho_m = \frac{1}{2\pi} \frac{d\beta}{d\omega} = \frac{\omega}{2\pi c^2} \frac{\int_{0}^{+\infty} n^2 E_y^2 dy}{\int_{0}^{+\infty} E_y^2 dy}. \]

In our structure, we have Si, ITO layers and air, then plugging in equation 3-24 for confinement factors in TE modes:

\[ \sigma_m = \hbar \rho_m = \frac{\hbar}{2\pi} \frac{d\beta}{d\omega} \]

\[ = \frac{\omega h}{2\pi c^2} \frac{\int_{0}^{h} n^2 E_y^2 dy + \int_{h}^{h+t} n^2 E_y^2 dy + \int_{h+t}^{\infty} n^2 E_y^2 dy}{\int_{0}^{+\infty} E_y^2 dx}. \]  

\[ = \frac{\omega h}{2\pi c^2} (\Gamma_m n_1^2 + \Gamma_m,\sigma n_2^2 + \Gamma_m,air n_3^2) \]

The same relation could be derived for TM modes for using the expression of P and W with magnetic components:

\[ \frac{d\beta}{d\omega} = \frac{W}{P} = \frac{\int_{0}^{+\infty} \frac{1}{2} \mu_0 H^2 dy}{\int_{0}^{+\infty} \frac{\beta}{2\omega m^2_\mu} H_y^2 dy} = \frac{\omega}{\beta c^2} \frac{\int_{-\infty}^{+\infty} \frac{H^2}{n^2} dy}{\int_{-\infty}^{+\infty} \frac{H^2}{n^2} dy}. \]
Then:

\[
\sigma_m = h \rho_m = \frac{h}{2\pi} \beta \frac{d\beta}{d\omega} = \frac{\omega}{2\pi c^2} \int_0^{+\infty} \frac{n^2}{n^2} \frac{H^2}{n^2} dy
\]

\[
= \frac{\omega h}{2\pi c^2} \left[ \int_0^{w} \frac{n^2}{n^2} \frac{H^2}{n^2} dy + \int_w^{+\infty} \frac{n^2}{n^2} \frac{H^2}{n^2} dy + \int_{w+\alpha}^{+\infty} \frac{n^2}{n^2} \frac{H^2}{n^2} dy \right]
\]

\[
= \frac{\omega h}{2\pi c^2} \left( \Gamma_m n_1^2 + \Gamma_{m,o} n_2^2 + \Gamma_{m,ai} n_3^2 \right)
\]

The mode densities for our device are calculated and presented in Figure 34, along with the areal density of radiative modes. For each individual mode \( m \), the density increase with frequency is nearly proportional to the frequency, and is lower than the radiative mode density at higher frequencies. However, the sum of all the waveguide mode densities significantly exceeds the radiative mode density; at 1000 nm, the radiative mode density is about 5% of the total mode density.

### 3.4.3. Thermodynamic Calculation of Absorption in ITO and Si

When the modes are derived, we can plug in the material properties of nc-Si and ITO to figure out the partial absorptance in silicon and ITO for each of the modes. Thus the absorptance in silicon and ITO can be derived at each incident wavelengths. We show an example at \( \lambda = 1000 \text{nm} \) for one batch of the experiment samples with 1.5 \( \mu \text{m} \) nc-Si thickness and 70nm ITO. At \( \lambda = 1000 \text{nm} \), the TE and TM modes are shown in Figure 35:
Figure 35. TE modes and TM modes at 1000 nm for the device illustrated in Figure 33.

The modes profile for the TE and TM modes that are supported in the structure are shown above. Referring to equation 3-24, the confinement of energy in silicon and ITO are shown as:

Figure 36. Confinement factors for silicon and ITO for TE and TM modes at \( \lambda = 1000 \text{nm} \). There is also a small energy density in air that isn’t shown.
For most of the modes, the energy is tightly confined in silicon, and only a bit of energy is confined in ITO. For the rest of the modes, especially edge modes that penetrate into ITO layer, the confinement in ITO increases.

Now we can plug in equation 3-10-3-15 with the experimental absorption coefficients for Si and ITO at 1000 nm: $\alpha_{ITO} = 3000 \text{ cm}^{-1}$, $\alpha_{Si} = 50 \text{ cm}^{-1}$, to get the partial absorption. The large absorption coefficient of ITO makes the energy damping into ITO at a rate much higher than in silicon. Considering this effect, even though the energy confined in ITO is so little, the partial absorption in ITO is very high. Energy that is confined in silicon but not been absorbed will keep leaking into ITO to be absorbed. We show the partial absorption for each mode: $f_{m}'$, $f_{m,o}'$, both for ITO and Si.

![Graph](image)

Figure 37. Partial absorption in each mode at $\lambda = 1000$ nm. About half the modes are tightly confined, and silicon is the main absorber. The other half of the modes are loosely confined, and a noticeable amount of energy is confined in ITO. The ITO absorption dominates over silicon for the lower index modes.

The sum of all the partial absorption over the modes will give the absorptance in silicon, by equation 3-8.
At each wavelength, we can figure out the confinement factors of corresponding modes, thus and the absorptance in both silicon and ITO. Thus, the ratio of silicon absorption to the total absorption can be calculated, relevant to experiment IQE. We will compare the calculation result to IQE spectra in next section.

3.4.4 Simulation of IQE and thermodynamic reflectance.

We will show our simulation results for IQE and for the diffuse reflectance in this section. IQE shows the ratio of silicon absorption to the total absorption in both silicon and parasitic layers. IQE spectra will not be affected by the optical specular reflection. By measuring IQE, we can exclude the effect from imperfection in optical design and show both silicon absorption and parasitic absorption. As noted in Chapter 1, photons absorbed within the intrinsic layer contribute to the photocurrent collected assuming perfect collection efficiency. The collection efficiency in our cells is very close unity.

According to optical reflectance measurement of our devices shown in Figure 31, the specular reflectance from the cell is not zero. The waveguide modes analysis we developed is only valid for the light that goes into the cell, we need a procedure for managing the imperfect anti reflection coating.

The thermodynamic calculation just presented assumes perfect anti reflection coating, our cells had substantial specular reflectance at longer wavelength. We shall compare the thermodynamic reflectance calculation \( r' \), which is implicitly random, with the measured ratio:

\[
r' \approx \frac{R_{\text{diff}}}{1 - R_{\text{spec}}}
\]

where \( R_{\text{diff}} \) and \( R_{\text{spec}} \) are the measured diffusive and specular reflectances of the cell. We thus assume that the light which is not specularly reflected can be treated using the thermodynamic calculation.
Similarly, the partial absorptance \( \alpha_{Sl}' \) of the silicon calculated using thermodynamic approach is compared to the absorptance \( A_S \) of the semiconductor through \( \alpha_{sl}' \approx A_S/(1 - R_{spec}) \). For longer wavelengths, we anticipate that \( A_S \sim EQE \). It is convenient to use a variation of this expression. The fractional absorptance of the semiconductor film \( \alpha_{Sl}'/\alpha' \) can be identified with the measured internal quantum efficiency IQE over most of the wavelength range:

\[
\alpha_{Sl}'/\alpha' = \alpha_{Sl}'/(1 - r') \approx \frac{EQE}{1 - R_{spec}} \times \frac{1}{1 - R_{diff}/(1 - R_{spec})} = \frac{EQE}{1 - R_{diff} - R_{spec}} = IQE
\]

Evaluating the thermodynamic equations 3-37 and equation 3-38 requires calculation of the waveguide properties of the cell as well as knowledge of the optical absorption spectra of the component films.

We repeat the analysis above for the whole region from 600nm to 1200nm. The material properties in this region is shown in Figure 38 [104,105,106].

In Figure 32, we show IQE spectra for cells with 1.5\( \mu \)m silicon layer, the solid blue curve is for sample made on single-stage BR, the solid grey curve is sample made on 2-stage back reflectors in the same batch. They roughly follow the same trend, very similar to each other. In our thermodynamic calculation, if the ITO is lossless, then the calculated value is the purple line which is unity; when the ITO is lossy, the calculated IQE drops down significant as the wine curve shows, which agree with the experiment data very well up to 1000nm. The gap between the two dashed lines shows the part of absorption in ITO.

The good agreement between experiment and calculation in IQE suggests that the parasitic loss in front ITO is very significant. Light is efficiently trapped however due to ITO absorption; the absorption in silicon is greatly reduced from the classical \( 4n^2 \). At the back, parasitic loss is
much weaker than at the front ITO, thus they don’t show out in the experiment: two very
different back reflectors give the same $EQE$ and $IQE$.

![Graph](image.png)

Figure 38. Ratio of the absorption coefficient to the refractive index for nc-Si and ITO. We
calculated the absorption coefficient and index for our ITO by depositing a 60 nm ITO film on
glass and measuring the transmittance and reflectance at normal incidence. We also show the
spectrum from recently published data on an ITO film deposited under similar conditions [104].

It sounds contradictory to the conventional understanding of ITO layer absorptance. Usually,
ITO absorptance is simply measured by depositing ITO on top of glass slide, then shining a
plane wave and to get the optical absorptance, which gives only a few percent. However, when
the same ITO layer is deposited on top of silicon, the absorption regime is very different. Light
entering into the cell is scattered into waveguide modes, the electromagnetic field resulted from
waveguide modes is much higher than what plane wave can do. Thus, the electromagnetic field
in ITO is also greatly enhanced to give a larger absorptance.
Figure 39. The solid curves are measured IQE spectra from Figure 32. The dashed curves are calculations with the measured absorption of ITO (Figure 38) and with zero absorption. The ITO absorption accounts for most of the difference between the IQE measurements and unity.

The thermodynamic reflectance $r'$ calculation result is shown in Figure 40. Measurements are shown for two cells, one with a single-stage back reflector and one for a two-stage back reflector; they show that the normalized diffuse reflectances $R_{diff}/(1 - R_{spec})$ are very similar. The thermodynamic calculation of $r'$ gives a fair account for the measured ratios $R_{diff}/(1 - R_{spec})$. Up to about 1000 nm, the measured reflectance is as much as 0.1 larger than predicted by the thermodynamic calculation. Beyond 1000 nm, the measured reflectance ratio is less than predicted. Since the effects are nearly the same for both the single-stage and two-stage back reflectors, we don’t think they are related to the back reflector or to breakdown of the equipartition assumption. There is an approximation in equation 3-5 for the radiative modes that might be large enough to account excess reflectance below 1000 nm. Beyond 1000 nm, an additional effect might be our use of reference films on glass to infer the absorption coefficient of ITO; the optical properties of 70 nm films applied to the somewhat rough surface of the nc-Si:H solar cells can in principle differ from those applied to a smooth glass surface, and the IQE
is sufficiently low that it would not clearly show these effects diffusive reflectance simulation result from the same waveguide mode calculation is shown in Figure 40:

![Graph showing reflectance ratio vs wavelength for single and two stage backreflector cells](image)

Figure 40. The solids curves are the measured spectra of the normalized diffuse reflectance for the single and 2 stage backreflector cells (cf. Figure 39). The dashed curves are the thermodynamic calculation for the diffuse reflectance.

### 3.5. Discussion.

The central experimental conclusion is that quite different morphologies for Ag/ZnO back reflectors give very similar reflectances and quantum efficiencies for otherwise identical nc-Si:H solar cells. We are able to account for these measured properties fairly well by using (i) a thermodynamic calculation using waveguide modes of planar cells with essentially the same silicon and (slightly absorbing) ITO layers and an ideal back reflector, and (ii) correcting for the measured specular reflectance, which is assumed to be zero in standard thermodynamic calculations.

In 2008 Berginski, et al. [107], followed a somewhat similar program for “superstrate” type nc-Si:H cells deposited onto textured oxides on glass. They also assumed thermodynamic light trapping, and reached the conclusion that the absorption by the top conducting oxide reduced the
quantum efficiency at longer wavelengths. Their thermodynamic calculations used the
approximation developed in the 1980s by Deckman, et al. [108], which essentially uses the
properties of a single waveguide mode to approximate the sum over modes in the treatment that
we’ve done here. They fitted the (small) effects of an imperfect back reflector to gain agreement
between calculation and measurement; it may be that the more complete treatment of modes that
we’ve used here would offer an alternate explanation. Another recently experiment work also
report the study of the optical loss in front ITO in a HIT cell [109], ITO is found to be the reason
for major optical loss at long wavelength. An improvement is made by inserting a weak
absorbing buffer oxide layer in between ITO and silicon. In next chapter, we will show a bilayer
TCO design and propose the possible benefit in photocurrent.

The main oddity of our results is that the absorption that is plainly evident in direct
measurements on bare Ag/ZnO backreflectors is apparently negligible for the waveguide modes
of finished cells when compared to the ITO absorption. This small magnitude of the back
reflector absorptance is evidenced both by the fact that backreflectors with rather different losses
give nearly the same experimental results in cells, and by the success of the thermodynamic IQE
calculations in accounting for measurements with both backreflectors. Some insight into this
behavior can be gained from Figure 35, which shows the electric energy density of the
waveguide modes across the 70 nm thick ITO layer. The ITO is thick enough that the energy
density is small at the top, air interface. We speculate that the undoped 100 nm ZnO layer is
thick enough to suppress losses by surface plasmon polariton generation at the Ag/ZnO interface,
but the subject needs further study.
Chapter 4. Improvement of $J_{SC}$ by Bilayer TCO

In chapter 3, we studied the incomplete light trapping for thin film nc-Si:H solar cells. The conclusion from the experiment is that EQE spectra are independent on back reflector morphologies, when the ITO parasitic absorption is enhanced in thermodynamic equilibrium. The photocurrent density $J_{SC}$ is also limited by parasitic absorption.

Here we propose our bilayer design of TCO, in which a thin buffer is deposited onto silicon before the heavily doped layer. We perform thermodynamic calculation for bilayer design, and show the possible benefit in photocurrent.

4.1 Property of TCO in solar cells.

TCO layer is essential in solar cells to collect photo carriers. The sheet resistance of TCO layer is required to be at a low level in order to avoid the power loss by contact resistance. The low sheet resistance is usually achieved by heavily doping the semiconducting oxide layer. In the heavily doping layer, the free carrier density is very high. In long wavelengths region near infrared, those free carriers are able to move together in a collective mode, thus give a strong free carrier absorption. Thus, an incoming beam will lose its energy into free carrier absorption when transmitting the oxide layer, then the transparency of the oxide film is reduced. Free carrier absorption becomes stronger at longer wavelengths.

There is always a compromise between transparency and conductivity of TCO layer.

The most two popular TCO used in silicon solar cells are ITO and aluminum doped Zinc Oxide (AZO). For both of them, the optical absorption at long wavelengths is affecting the silicon absorption. Experiment work has shown that a 100nm ITO layer causes about 1mA/cm² loss in a 280μm crystalline silicon cell [110]. In thin film superstrate silicon solar cells, silicon layer is deposited on glass coated by about 500nm conducting AZO layer. The thick AZO layer
will have a significant effect optical absorption. In terms of waveguide modes, the energy confinement in silicon tends to become less and loose when waveguides are launched. As a result, the absorption loss in AZO is very high. Previous studies by different groups show the parasitic loss in their superstrate cells [111,112]. The amount of parasitic absorption in AZO is estimated to be equivalent to about 2mA/cm² drop in photocurrent.

### 4.2. Bilayer TCO

In conventional design, a single layer of TCO is deposited in the fabrication, shown in Figure 34 left. In order to get a good compromise between optical transmittance and electronic conductivity, the doping concentration and the film thickness are carefully optimized, so that the finished device will give the best efficiency.

For silicon solar cells, making light trapping structures is an essential step in fabrication. Under light trapping condition, the absorption in TCO is enhanced simultaneously. In thin film solar cells, light goes into the cells in waveform which gives non uniform absorption profiles at different depth of the device. In a waveguide mode, the absorption profile inside the TCO tends to be stronger when it is closer to the silicon interface. As illustrated in Figure 41 and Figure 42, the most part of the TCO absorption is coming from a small vicinity to the silicon/TCO interface. To reduce the total parasitic absorption, the close vicinity region to silicon is replaced by an optical buffer layer which has a very low absorption coefficient.

In Figure 41 right, we illustrate the design of bilayer TCO. Instead of depositing a heavily doped TCO layer for a certain thickness \(d\), we deposit the layer in two steps. First step is depositing an oxide layer of thickness \(d_1\), which is very lightly doped so that the mobility is low and the absorption coefficient is also low. The second step is depositing a heavily doped layer for thickness \(d_2\). This highly doped layer will function as the carrier collecting layer.
move across the first layer, they will flow laterally in the second layer and eventually will be collected by the external circuit. The total thickness of the two layers in bilayer is the same as the thickness of single layer TCO: $d = d_1 + d_2$.

![Figure 41. Single layer TCO and Bilayer TCO design](image)

For a waveguide mode propagating in the device, the energy confined in silicon is less than unity. We show the TE mode profiles in Figure 42 for the 1.5 $\mu$m silicon device with 70nm ITO. The energy confinement in ITO is not negligible, the electromagnetic field intensity in ITO layer decays in the direction away from the silicon/ITO interface. Higher intensity of electromagnetic field will give higher absorption rate. Thus, the absorption in ITO is mostly strong at the interface and it decays into ITO for bigger depth from the interface.

In bilayer design, as shown in the upper corner in Figure 42, in buffer layer region (light grey), the electromagnetic field does not contribute to absorption. The red region is the only place that energy can be absorbed by ITO. It is suppressed significantly.

One concern of the bilayer design is the carrier transportation across the buffer layer. Similar design of bilayer TCO are successfully used in thin film CdTe and CIGS solar cell, which show good properties of carrier transportation. We believe that a proper oxide will not affect carrier transportation. In this thesis, we will look into optical property rather than electrical properties,
and show the optical benefit by our thermodynamic calculation. The experiment work to prove the optical benefit will be the future plan.

Figure 42. The mode profile and confinement of energy in TCO. The bilayer TCO has a buffer layer which is lossless, so the energy confined in the buffer would not contribute to absorption. In the lossy TCO which is farther from the silicon/TCO interface, the electromagnetic field intensity drops quickly, thus it would greatly reduce the amount of energy confined in lossy TCO. When the absorption in TCO is dropped, the competition with silicon absorption will be weakened.

4.3. Benefit of bilayer design

4.3.1. Substrate cells.

The energy confinement in lossy ITO layer in bilayer design, which is the source of parasitic absorption, is shown in Figure 43. Here, we shown an example of bilayer ITO structure, which
has half of the 70nm ITO replaced by intrinsic oxide, thus the optical modes will stay the same for both single layer case and bilayer case.

Figure 43. Energy confinement in ITO to be absorbed. Bilayer design reduce the amount of energy confinement in lossy ITO. Beam wavelength is 1.5 µm, 70nm ITO total thickness. the bilayer contains 35nm intrinsic oxide and 35nm heavily doped oxide.

Since the amount of energy confined in lossy ITO is dropped, then the absorption in ITO is also dropped. We show the partial absorption in silicon and ITO for each mode, both in single layer and in bilayer design. The partial absorption is referring to the equation (3-11,3-14) in Chapter 3.

Silicon and ITO are competing in absorption. In Figure 44, single layer ITO receives a good amount of energy and has a strong absorption in each mode. Even silicon confines most of the energy, its absorption is still low (black curve) because of low absorption coefficient. In bilayer, ITO receives less energy and absorption drops, the competing with silicon absorption becomes weaker thus silicon absorption increases (up triangles). Here, even though the amount of energy confined in silicon does not change, silicon absorption increases in bilayer design. This is because we are working in equipartition condition, which means the lifetime of each modes is
sufficiently long. Therefore, the energy that has not been absorbed in ITO will be contained in the mode, and it will be eventually absorbed by silicon even though silicon absorption rate is low.

Figure 44. Partial absorption in Si and ITO for each mode, when the beam wavelength is 1000nm. For single layer, the energy confined in lossy ITO is big, so the absorption is very strong as the red curve shows, which also suppress the silicon absorption (black square curve). In bilayer design, the lossy ITO can only absorb less confined energy, thus the partial absorption drops. Since ITO is competing with silicon in absorption, the drop in ITO absorption would boost the silicon absorption, as shown by the up triangles.

The thickness of buffer layer can be adjusted in experiment to get the best cell performance; it can be made as thick as possible as long as the carrier transport is not affected. The reduction of ITO absorption would increase the absolutely amount of silicon absorption, also increases IQE. We repeat the above step for the spectrum range from 600nm to 1200nm, the IQE calculated as shown in Figure 45, for different buffer layer thickness (0 < d₁ < 70nm).

The silicon absorptance related to those curves under perfect ARC condition can also be calculated as well.
Figure 45. IQE from bilayer design. The buffer layer in bilayer design would reduce the ITO absorption thus boost the IQE. Thicker buffers will give higher IQE.

We can also figure out the short circuit current benefit from the bilayer design:

Figure 46. Absorption of silicon in bilayer oxide device at perfect AR coating condition.

The possible short circuit current is then derived by:
\[ J_{sc} = \int A_{Si}(\lambda) \times F(\lambda) d\lambda \]

Plugging in the different Si absorptance curve, the short circuit current under perfect ARC conditions are:

Table 6. Short current density benefit from bilayer design for substrate cell with 1.0 µm silicon layer and 70nm ITO on top.

<table>
<thead>
<tr>
<th>Bilayer/ nm</th>
<th>0</th>
<th>10</th>
<th>20</th>
<th>30</th>
<th>40</th>
<th>50</th>
<th>60</th>
</tr>
</thead>
<tbody>
<tr>
<td>( J_{sc} ) (mA/cm(^2))</td>
<td>25.6</td>
<td>25.8</td>
<td>26.3</td>
<td>26.7</td>
<td>27.1</td>
<td>27.5</td>
<td>27.9</td>
</tr>
</tbody>
</table>

### 4.3.2 Bilayer for superstrate cell.

We perform the same calculation for a superstrate thin film silicon cells made on AZO glass. Usually AZO layer has a big thickness that is comparable to the active layer thickness, the parasitic loss in silicon is more profound. We show a typical dimension of the cell structure in Figure 48.

The Aluminum doped ZnO property is depending on the deposition method, different depositions give different morphology, carrier mobility and absorption coefficient. Here, as a demonstration, we take the absorption coefficient of an sputtered Al: ZnO thin film from Z.C Jin [113]. The Al doping has a weight percentage of 2.14%, and the optical measurement was derived with variable-angle reflectance measurement. We take the absorption spectrum as a typical value of AZO in order to get the qualitative behavior in the device.

The AZO absorption coefficient is shown in Figure 47.
Figure 47. A typical absorption coefficient spectra of AZO. From Lin’s measurement [113].

Figure 48. Dimensions of a virtual superstrate cell made on AZO glass. The AZO layer is 500nm, nc-Si is 1.0 μm. In bilayer design, the buffer thickness d out of 500nm touching silicon.
We will calculate for a superstrate device made on 500nm AZO glass, refractive index for glass is 1.33 and for AZO layer it is around $n=2$, active layer of nc-Si is 1um, $n\sim 3.5$. There is a perfect back metal reflector.

In bilayer AZO, the buffer layer thickness is $d$: $0 < d < 500\text{nm}$.

Since the AZO layer is thick, the confinement in single layer AZO is relatively bigger than that in substrate cell (below 100nm). We show the confinement factors at 1000nm in Figure 49. We show the confinement factors in silicon and AZO layer. For half of the modes, confinement factor is about unity, those modes are tightly confined. For the rest of the modes energy leaks out of silicon for a noticeable amount. Especially for modes at the edge, silicon can only loosely confine the electromagnetic field, the rest of the energy is mostly in oxide layer. In single layer, all the energy in AZO is subject to energy dissipation; in bilayer design, the buffer layer is not active for damping since it is intrinsic, the amount of energy subject to dissipation is only in the AZO. For thicker buffer layer, the energy confinement in AZO is smaller.

![Figure 49. Confinement factors in silicon and AZO layer are shown with different thicknesses of buffer layer.](image-url)
Bilayer design has a big effect in AZO absorption, as shown in Figure 50. For the tightly confined mode, single layer AZO only confines very little energy, however, it is not negligible. The absorption in those modes are mostly from the region in close vicinity to the silicon/AZO interface. The buffer layer would eliminate this absorption. For the loosely confined modes, AZO absorption dominates and reaches the value of above 50% in single layer design. The field intensity goes deep into oxide layer, the buffer layer only covers part of this region. The AZO absorption is also reduced for those modes, however, less than tightly confined modes.

For the silicon partial absorption in each mode, bilayer has a stronger effect on the loosely confined modes than tightly modes. In tight modes, silicon already dominates in absorption, thus the improvement of AZO absorption wouldn’t have much consequence on silicon absorption. For loosely confined modes, silicon absorption is not dominating, thus the improvement would be more profound. The potential benefit on Jsc is also shown in Table 7.

Figure 50. At λ=1000 nm, the left figure shows the energy confined in AZO for different TE modes in the structure (cf. Fig. 48), with different buffer layer thicknesses. The right figure shows the corresponding partial absorption in silicon.
Table 7. Short current density benefit from bilayer design for superstrate cell with 1.0 µm silicon layer and 500nm AZO.

<table>
<thead>
<tr>
<th>Bilayer/nm</th>
<th>0</th>
<th>10</th>
<th>20</th>
<th>50</th>
<th>100</th>
<th>200</th>
<th>300</th>
</tr>
</thead>
<tbody>
<tr>
<td>J_{SC} (mA/cm^2)</td>
<td>21.6</td>
<td>21.7</td>
<td>21.76</td>
<td>21.88</td>
<td>22.08</td>
<td>22.1</td>
<td>22.2</td>
</tr>
</tbody>
</table>
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88 Film thickness was measured by profilometer. Silicon layer was etched by dipping in 0.05 mol HCl solution for about 1 minute. The etching stops at ZnO layer. An edge is produced at the of HCl/air interface. The height of the edge is measured by profilometer and used as the silicon layer thickness.

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Curriculum Vitae

The author was born in China on December 20\textsuperscript{th}, 1984. He grew up in China and went to University of Science and Technology of China (Anhui), where he received Bachelor of Science degree in physics major, in July 2006. Then he came to Syracuse University and enrolled in physics Ph.D program. Under the guidance of his advisor, Professor Eric. A. Schiff, he pursued research in light trapping for thin film solar cell