Development of a Multi-layer Anti-reflective Coating for Gallium Arsenide/Aluminum Gallium Arsenide Solar Cells

by Kimberley A Olver

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# Development of a Multi-layer Anti-reflective Coating for Gallium Arsenide (GaAs)/Aluminum Gallium Arsenide (AlGaAs) Solar Cells

A process for calculating the true refractive index of an as-deposited dielectric for use as an anti-reflective (AR) coating was established. Yttrium oxide and tantalum oxide were used in the design of multi-layer AR coatings for use with gallium arsenide (GaAs) solar cell devices. These AR coatings were found to greatly reduce the reflective losses from the surface of the GaAs, therefore increasing the external quantum efficiency of the device.

**Subject Terms**
- anti-reflective, gallium arsenide, GaAs solar
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Acknowledgments

The author would like to acknowledge Mr Fred Towner, formerly of Maxion Technologies, for growing the gallium arsenide wafer from which the test solar cells were made, and Dr Eric DeCuir, Jr, of the US Army Research Laboratory (ARL) for his support in writing this report.
1. Introduction

The Army has been developing new types of photovoltaic (PV) devices – solar cells – for use in its efforts to more efficiently functionalize the Army warfighter. Gallium arsenide (GaAs) solar cells as well as other III-V semiconductors are currently being studied for their advantages over silicon solar cells. Because GaAs is a direct bandgap material, its conversion of light into power is more efficient than silicon. This gives GaAs solar cells the advantage in low-light conditions. Further, with their multi-junction architecture, GaAs solar cells are able to respond to multiple wavelengths of light, also increasing their efficiency.

Solar cells work by converting sunlight (electromagnetic radiation) into electricity. Reflection of incident light falling on to the surface of a solar cell is a major optical loss mechanism, which limits the efficiency of the PV device.\(^1\) Photon absorption needs to occur inside the solar cell active region (near the bandgap) (where photon energy \(\geq\) material bandgap) for a PV conversion to occur. However, only a certain percentage of photons incident on the surface of the solar cell actually end up in the active region able to convert photon energy into electrical energy. Several mechanisms contribute to energy losses in solar cells, including heat loss, recombination loss, and reflection loss. This study focuses on reducing reflective losses from the surface of single junction GaAs solar cells, where typical reflection losses are shown to be on the order of 30–35\%, as seen in Fig. 1.

![GaAs Substrate Reflectivity](image)

**Fig. 1** Measured reflectivity of a bare GaAs wafer with no anti-reflective (AR) coating

To overcome this reflective loss and increase the photo conversion efficiency, one method is to design an anti-reflective (AR) coating, which will lower the surface reflectivity. AR coatings enhance absorption of the light into the PV cell by
decreasing the reflection off of the semiconductor surface. AR coatings work by creating a 2 reflective wave scenario, one from the surface of the coating and the other from the surface of the substrate. The AR coating is designed so that these 2 waves destructively interfere with each other when reflected, cancelling each other out (Fig. 2).

![Illustration of a quarter-wavelength AR coating, which causes destructive interference by creating a 180° phase change in light reflected from the substrate](Diagram)

Typical AR coatings consist of dielectric materials with calculated thicknesses and refractive indices that closely match the optimal refractive index of the solar cell material for a given wavelength. The refractive index \( n \) of a material is defined as the ratio of the speed of light in a vacuum and the speed of light in a material or

\[
 n = \frac{\text{Velocity of light in vacuum}}{\text{Velocity of light in material}}
\]  

By lowering the reflectivity of the surface, more light particles (photons) are able to be absorbed, and therefore, generate more photocurrent in the solar cell. As the photon having energy equal to or greater than the bandgap travels into the material, a conversion (photon absorption) occurs. For GaAs, a photon of energy 1.424 eV (or greater) transfers its energy to an electron in the valence band, which enables the electron to overcome the bandgap energy and move into the conduction band, leaving a hole behind in the valence band. This combination is known as an electron-hole pair and is responsible for charge moving through the PV device. These electron-hole pairs are also known as charge carriers. A measure of the photon to electron conversion efficiency in the material is referred to as the quantum efficiency \( (QE) \) and is basically the measure of the solar cell’s sensitivity.
to light. \(QE\) is the ratio of the number of carriers collected by the solar cell to the number of photons of a given energy incident on the solar cell.\(^1\) It is the ratio of electrons out versus photons in:

\[
QE = \frac{\text{Electrons out/second}}{\text{Photons in/second}}
\]

\[\text{(2)}\]

A single layer AR coating reduces reflectance in a narrow wavelength area, however a 2 (or more) layer AR coating of the correct dielectric materials can broaden out the wavelength area where the reflections are at a minimum. Our GaAs solar cells operate in the 400–900 nm spectral range. Because of this broad spectral range, a multilayer AR coating was designed and fabricated to lower the reflectivity in the 600 to 900 nm wavelength range. This wavelength range also aligns with the peak power of the solar spectrum, thus the most power (solar radiation) available to our devices (Fig. 3).

![Solar Radiation Spectrum](https://www.commons.wikimedia.org)

Fig. 3  Solar radiation spectrum graph (from [www.commons.wikimedia.org](https://www.commons.wikimedia.org))

Ideally, for an AR coating to create a completely reflective-free interface with the solar cell material, it will have an optimal refractive index matched to the semiconductor material used for the solar cell, in this case, GaAs. In addition to matching the optimal refractive index, a quarter-wavelength coating thickness is chosen to ensure reflected light from the coating surface as well as the reflection from the AR coating/substrate interface are 180° out of phase (see Fig. 2). We calculate the optimal refractive index \((n)\) from the following equation:

\[
n_{\lambda/4} = \sqrt{n_{\text{air}} \times n_{\text{semi}}},
\]

\[\text{(3)}\]
where \( n_{\lambda/4} \) is the optimal refractive index of the AR material for a wavelength \( \lambda \), \( n_{\text{air}} \) is the refractive index of air (equal to 1), and \( n_{\text{semi}} \) is the refractive index of the semiconductor material (Fig. 4). Solving the equation for the optimal refractive index of GaAs at 880 nm \((n = 3.6 \text{ at } 880 \text{ nm})\), the calculated optimal index of refraction of GaAs at 880 nm is 1.89.

![Graph of wavelength vs. refractive index for GaAs](image)

**Fig. 4**  Graph of wavelength vs. refractive index for GaAs

## 2. Methodology and Results

Reported refractive indices of several dielectric materials were evaluated, and 2 were chosen as being close to the square root of the refractive index of GaAs at 880 nm, also known as the optimal index for GaAs (1.89). After evaluating several dielectric materials, yttrium oxide (\( \text{Y}_2\text{O}_3 \)) and tantalum pentoxide (\( \text{Ta}_2\text{O}_5 \)) were chosen due to their reported refractive indices at 880 nm being very close to this optimal refractive index. Refractive indices reported in the literature for \( \text{Y}_2\text{O}_3 \) and \( \text{Ta}_2\text{O}_5 \) were 1.91 and 2.11, respectfully,\(^{3,4}\) but to find the actual index of the material that would be used, each material was first evaporated onto an individual GaAs wafer and characterized. Reported and actual refractive indices of materials vary due to several factors including material density and deposition processes.

### 2.1 AR Deposition

The AR depositions were performed on an Evatec BAK 641 electron-beam evaporator with a chamber pressure of \( 2 \times 10^{-6} \text{ Torr} \), and an oxygen (\( \text{O}_2 \)) back pressure of \( 3 \times 10^{-4} \text{ Torr} \). The \( \text{O}_2 \) back pressure was used to keep the stoichiometry of the dielectric materials constant while the depositions took place. The deposition
rate was 1.3 Å/s for each material. Thicknesses of 105 nm of Y$_2$O$_3$ and 105 nm of Ta$_2$O$_5$ were evaporated onto individual GaAs wafers. Characterization took place using a Perkin Elmer Lambda 950 UV/VIS Spectrophotometer. A measurement of reflectivity ($R$) versus wavelength was performed on both evaporated films as well as a control sample GaAs substrate (Fig. 5).

As the graphs show, a 2.0% minimum reflectance at the 732-nm wavelength for Y$_2$O$_3$, and a 0.2% minimum reflectance at the 870-nm wavelength for Ta$_2$O$_5$ were measured for these deposited films. Using the measured thickness of the 2 coatings, the empirical refractive index at these minima were calculated using the following equation:

$$d = (\lambda)/4 \times n,$$

where $d$ is the thickness of the original film (105 nm) and $\lambda$ is the wavelength of the measured minimum reflection for each dielectric. We calculate the actual index of

![Graphs showing reflectivity of Y$_2$O$_3$ and Ta$_2$O$_5$ films on GaAs substrates.](image)

**Fig. 5**  a) Reflectivity of 105-nm Y$_2$O$_3$ on GaAs and b) reflectivity of 105-nm Ta$_2$O$_5$ on GaAs
refraction for our materials as 1.74 for Y₂O₃, and 2.07 for Ta₂O₅. These measured refractive indices match quite well with the indices reported in literature, and deviations from the reported indices could be attributed to deposition techniques, which may have produced slight density variations in the film. Using these new refractive indices and the wavelength of interest, the calculations were repeated for the correct thicknesses needed for our AR coatings at the 800-nm wavelength. From these new thickness calculations, 2-layer multilayer structures were designed and deposited onto fabricated GaAs solar cells.

2.2 GaAs Solar Cell Fabrication

GaAs solar cells were fabricated using standard photolithographic techniques. A wafer was grown using molecular beam epitaxial (MBE) technology. The simple device design consisted of a single p-n junction of GaAs/aluminum gallium arsenide (AlGaAs) structure with a p-type top contact, an absorbing layer of AlGaAs, and an n-type bottom contact. Three solar cell devices were fabricated from this wafer. First, individual 5x5 mm² device mesas were etched into the substrate. Next, a blanket contact of gold/tin/gold (Au/Sn/Au) was e-beam vacuum evaporated onto the backside of the substrate. This contact metal was rapid thermally annealed at 350 °C for 60 s. Next, using photolithographic patterning techniques, a top metal contact (the collector) of chromium/gold (Cr/Au) was e-beam vacuum evaporated onto the top surface of the mesas, and a metal liftoff was performed. The wafer was then diced into individual solar cell devices (Fig. 6).

To address the ordering of the dielectric layers, a typical structure for a multilayer AR coating is to place the higher indexed material next to the solar cell, and the lower indexed material on top of this layer, a method known as high-low layering. Snell’s Law states
where $n_1$ is the refractive index of medium 1, $\sin \theta_1$ is the angle of refraction relative to normal incidence for medium 1, $n_2$ is the refractive index of medium 2, and $\sin \theta_2$ is the angle of refraction for medium 2. As the refractive index increases, the angle of refraction relative to normal incidence decreases. Therefore, placing the higher indexed material next to the solar cell surface allows more light to enter the solar cell.

To see if the ordering of these dielectrics would perform as Snell’s Law said they should, 2 different structure orderings were tested (Fig. 7). Dielectric evaporations were performed as before in the Evatec deposition tool using the parameters from before. One of the three solar cells acted as the control in that no AR coating was used. The second solar cell (sample A) was coated with a multilayer AR coating consisting of 65 nm of Y$_2$O$_3$ on top of 65-nm Ta$_2$O$_5$, and the third solar cell (sample B) was coated with a multilayer AR coating of 60 nm of Ta$_2$O$_5$ on top of 70-nm Y$_2$O$_3$. Sample A and sample B are shown in Fig. 8.

![Fig. 7 Explanation of Snell’s Law](image)

![Fig. 8 Sample A and sample B solar cells](image)

All 3 solar cell devices were wirebonded into packages for testing purposes. The 3 solar cells were evaluated using an Oriel IQE 200 Quantum Efficiency.
Measurement System, and percent reflectivity ($R$) and external quantum efficiency ($EQE$) were measured. GaAs has a 35% reflectivity minimum at 880-nm wavelength. Comparing the 2 solar cells with AR coatings to this typical reflectivity loss for GaAs, both of the AR coating structures demonstrated a much reduced reflection in the wavelength range of 700 to 900 nm. At 880 nm, the reflectivity value for sample A was 1.82% with sample B giving a reflectivity of 2.65%.

Of the 2 dielectric materials used, Ta$_2$O$_5$ had the higher index of refraction. Comparison of reflectivity for the 3 solar cells confirmed that the higher dielectric material used as the first layer to interface the GaAs (sample A) gave a slightly lower measured response for reflectivity in the 600 to 900 nm wavelength range (Fig. 9).

![Fig. 9 Results of reflectivity measurements for GaAs control, sample A and sample B](image)

As mentioned, the $QE$ is the ratio of the number of carriers collected by the solar cell to the number of photons of a given energy incident on the solar cell.$^1$ The $EQE$ of a solar cell includes the effect of optical losses such as transmission and reflection. Internal quantum efficiency ($IQE$) refers to the efficiency with which photons that are not reflected or transmitted out of the cell can generate collectable carriers. By measuring the reflection and transmission of a device, the $EQE$ curve can be corrected to obtain the $IQE$ curve.$^1$ The equation for calculating $IQE$ is shown below:

$$IQE = \frac{EQE}{1 - R}$$  \hspace{1cm} (6)
However, for measuring the effectiveness of these multi-layer AR coatings in reducing optical losses, \( EQE \) was the more important of the 2 measurements in characterizing the performance of these solar cells. The results of the \( EQE \) measurements are shown in Fig. 10.

![Comparison of EQE for GaAs control, Sample A, and Sample B](image)

**Fig. 10**  \( EQE \) measurements for GaAs solar cell control, sample A and sample B

As the data show, \( EQE \) values increased for both AR-coated GaAs solar cell devices, with a peak value in the 800-nm wavelength region. Sample A demonstrated the most improvement, with a slightly higher \( EQE \) value in the 600–820 nm region. This increase in \( EQE \) suggests that the actual power of the solar cell device will also increase.

### 3. Conclusion

A process for calculating the correct index of refraction of an as-deposited dielectric material for use as an AR coating was developed. Two dielectrics with reported refractive indices were individually deposited on to GaAs substrates and characterized. The corrected index of refractions for the dielectrics \( Y_2O_3 \) and \( Ta_2O_5 \) were calculated. Two multi-layer AR structures were designed and fabricated using these dielectric materials. They were deposited onto real GaAs solar cell devices and characterization of the AR coatings performed. Both multi-layer AR structure designs were found to be effective in substantially reducing the surface reflection off of the GaAs solar cells in the 600 to 900 nm wavelength spectral range. This reduction in optical loss enhanced the absorption of charge carriers into the active
region of the solar cell devices, as seen in the $EQE$ measurement results. A
difference in efficiency was seen between the 2 AR multi-layer structures as well,
with the higher indexed Ta$_2$O$_5$ next to the solar cell demonstrating a higher $EQE$
value in the wavelength spectral range of 600 to 820 nm. This result is dictated by
Snell’s Law.
4. References


5. www.britannica.com/photovoltaics


### List of Symbols, Abbreviations, and Acronyms

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>AlGaAs</td>
<td>aluminum gallium arsenide</td>
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<tr>
<td>AR</td>
<td>anti-reflective</td>
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<tr>
<td>Au</td>
<td>gold</td>
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<td>Cr</td>
<td>chromium</td>
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<td>EQE</td>
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<td>GaAs</td>
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<td>MBE</td>
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<td>QE</td>
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<td>Sn</td>
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<td>Ta$_2$O$_5$</td>
<td>tantalum pentoxide</td>
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<tr>
<td>Y$_2$O$_3$</td>
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