Computational Exploration of Anti-Reflective Nanostructures

Ganesh Petterson[1], Catherine Jahncke[1], Wataru Nakagawa[2], Jordan Baker[2]
[1]Department of Physics, St. Lawrence University, 23 Romoda Dr., Canton, NY 13617
[2]Electrical and Computer Engineering Dept, Montana State University, PO Box 173780, Bozeman, MT 59717-3780

Anti-Reflective Coatings:

- The conventional way to reduce reflection from a surface, anti-reflective coatings operate on the principle of interference
- Light is reflected from the front and rear surface of a coating, and destructively interferes with itself (Figure 1)
- For single layer coatings, this is very wavelength-specific (Figure 2)

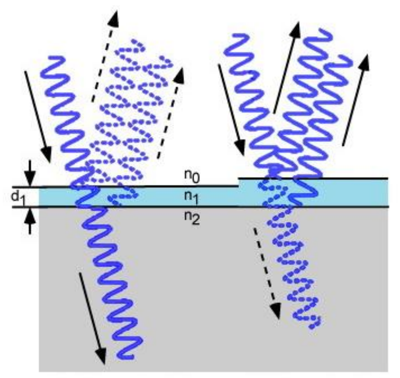

Figure 1: Constructive and destructive interference from a thin-film anti-reflective coating

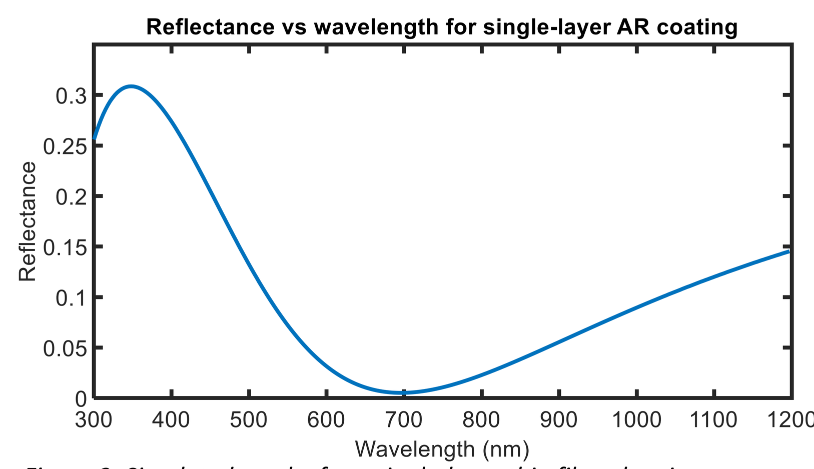

Figure 2: Simulated results for a single-layer thin film, showing a maximum reduction of reflectance for a wavelength of 700nm

Anti-Reflective Nanostructures

- Nanostructures create a refractive index gradient, reducing reflection between infinitesimal "layers"

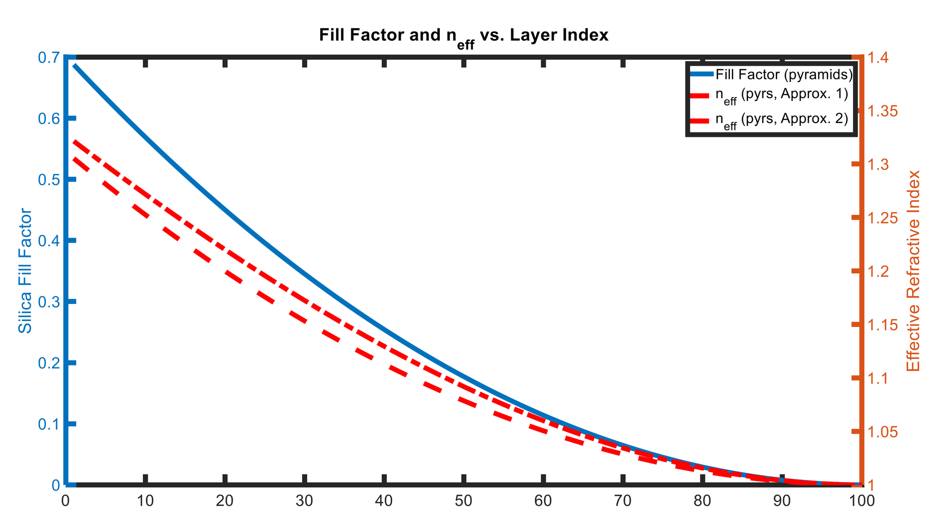

Figure 3: The "fill factor" of a pyramidal structure, representing the percentage of each layer filled by the substrate material, along with two approximations for the effective refractive index

- These structures are discretely simulated, with more layers yielding better results (Figure 4)

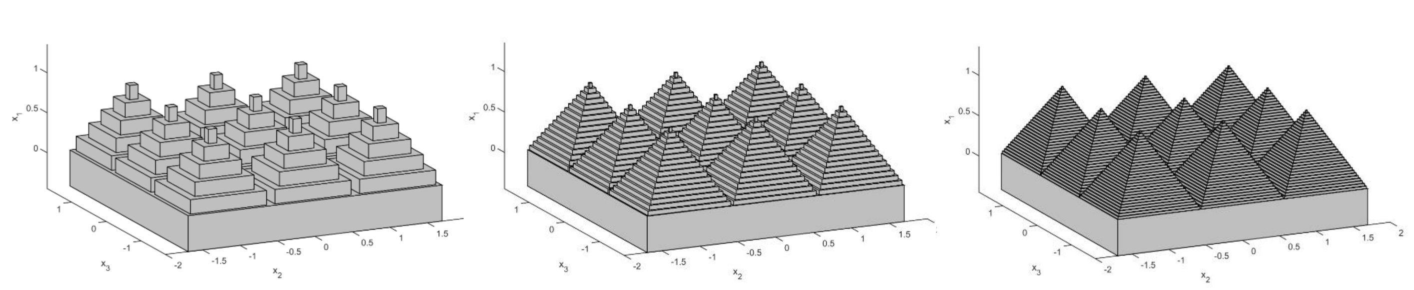

Figure 4: Pyramidal structures modeled using a varying number of layers; note the increasing accuracy with more layers

- Structures can be formed in different shapes, with varying effectiveness (Figure 5)

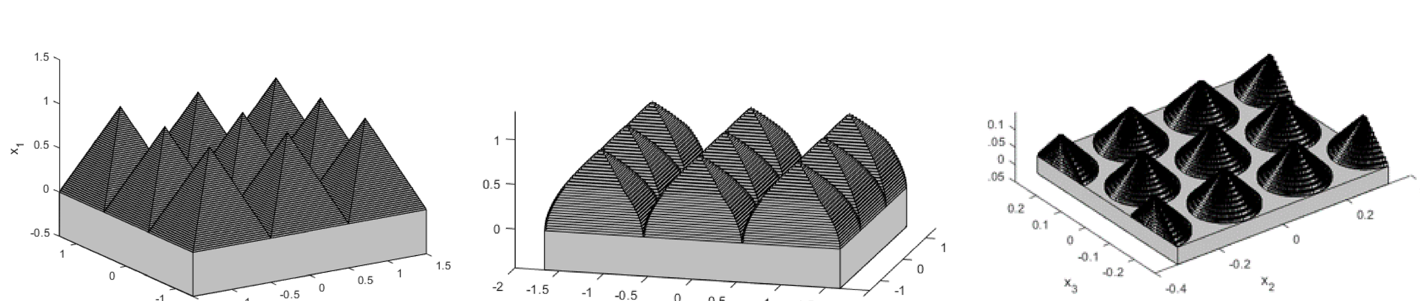

Figure 5: Different possible AR shapes. The aspect ratio, width, and pitch of structures can be changed to yield different results

Evaluation of Structures

- Structure parameters can be "swept" over a range of values to determine an optimum
- In general, the overall structure shape is kept constant while the incident field and structural parameters are changed
- Simulations yield a multidimensional matrix of reflectances

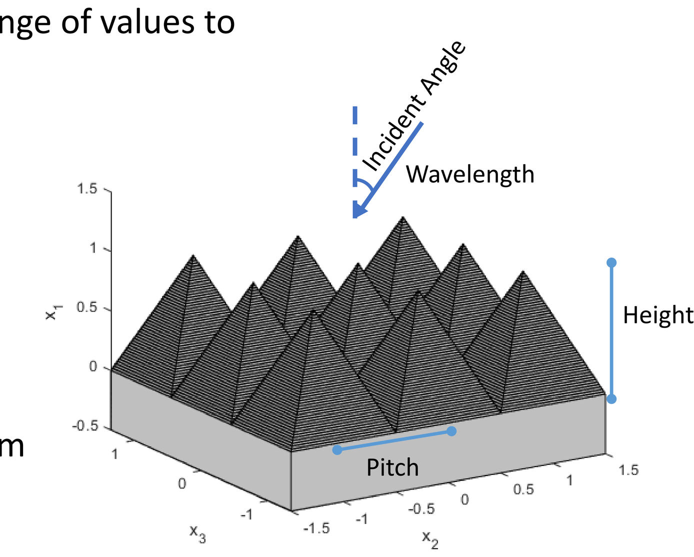

Figure 6: The parameters that are generally varied in the simulations

Structural Optimization

- A merit function is used to quantify the optimum structure and field parameters
- A Gaussian blur is used to find "stable" minima.

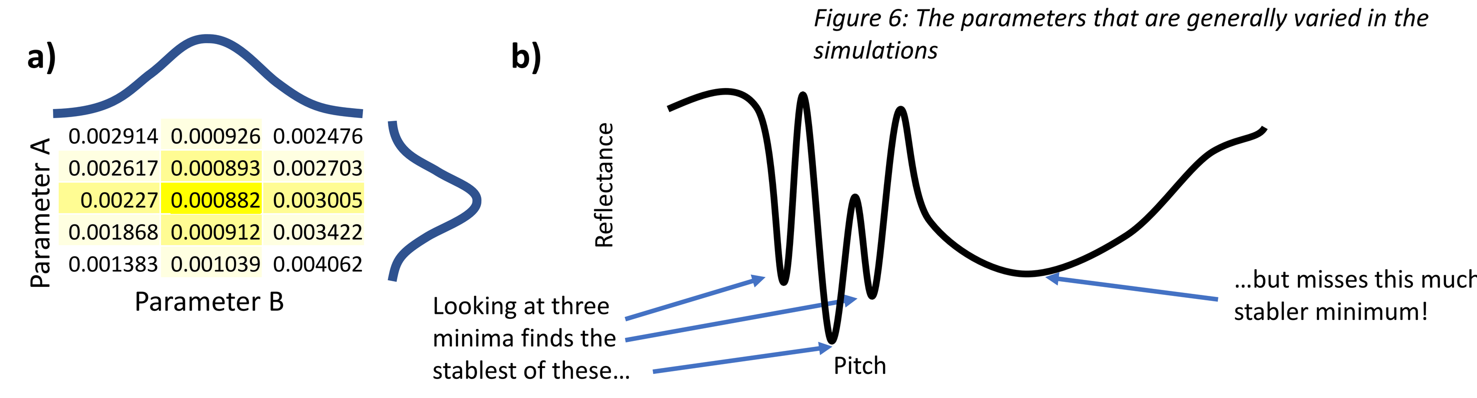

Figure 7: a) An example of the Gaussian blurring process on a two-dimensional matrix
b) A two-dimensional representation of the difference between finding absolute minima and stable minima

- The width of the Gaussian blurring function is controlled by a user-specified standard deviation for each parameter; this allows for different parameters to be prioritized

Findings

- Using the Gaussian blurring merit function, we can optimize each structure to find the configuration with minimal angular sensitivity over the simulated range
- Fused silica around 1550nm was used for all simulations to keep the material consistent
- Reflectance was plotted as a function of several parameters, in order to get a sense of overall behavior

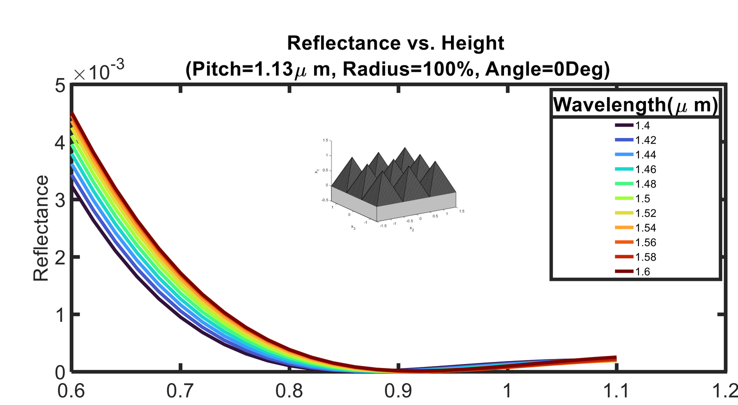

Figure 8: Reflectance dependence on height for different wavelengths of incident beam

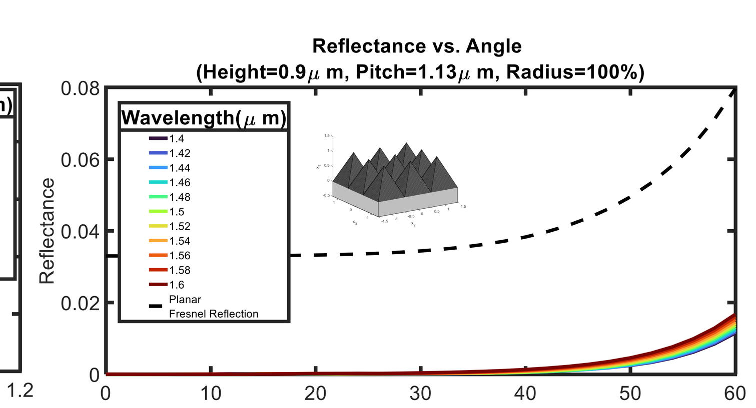

Figure 9: Reflectance dependence on angle for different wavelengths of incident beam. Note the drastic decrease as compared to an untreated surface

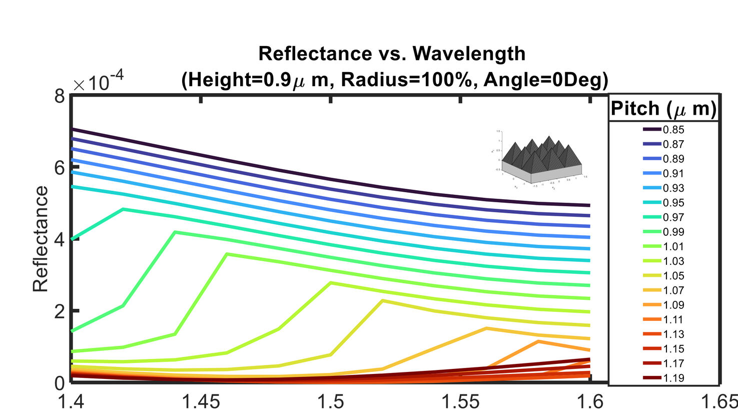

Figure 10: Reflectance dependence on wavelength, this time for different pitches; note the drastic spike in reflectance dependent on pitch

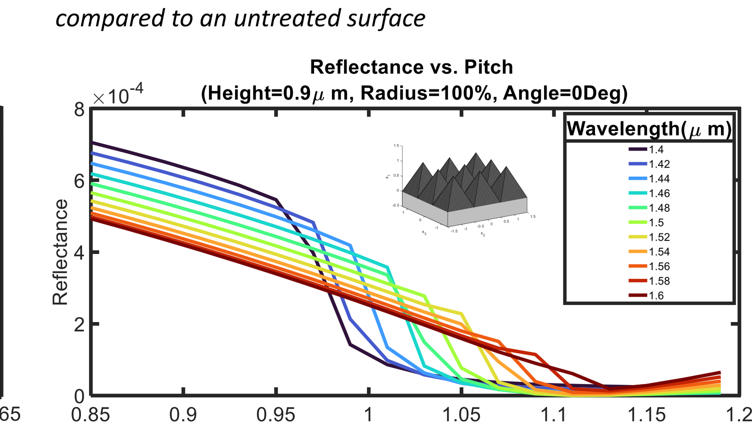

Figure 11: Reflectance dependence on pitch for different wavelengths. This is essentially the same information as Figure 10, portrayed differently.

Additional Findings

- As expected, the optimal configuration is different for different structures (Figure 12)

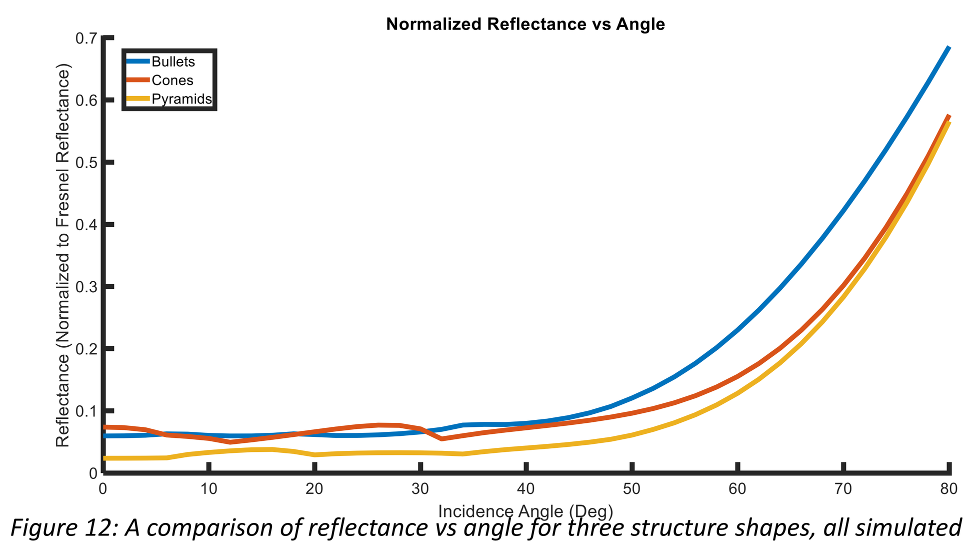

Figure 12: A comparison of reflectance vs angle for three structure shapes, all simulated with identical parameters. Note that the y-axis is normalized. Structures were simulated with a height of 0.9 μm, pitch of 1.13 μm, and 0.19 μm between bases for a 1500nm beam at normal incidence.

- Certain structural shapes perform better across the board as compared to others

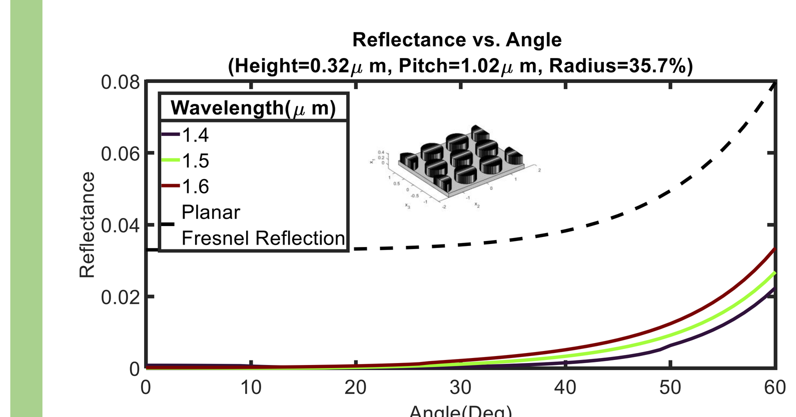

Figure 13: Reflectance dependence on height for different wavelengths of incident beam, this time for cylindrical nanostructures. Note the increased reflectance as compared to pyramidal structures

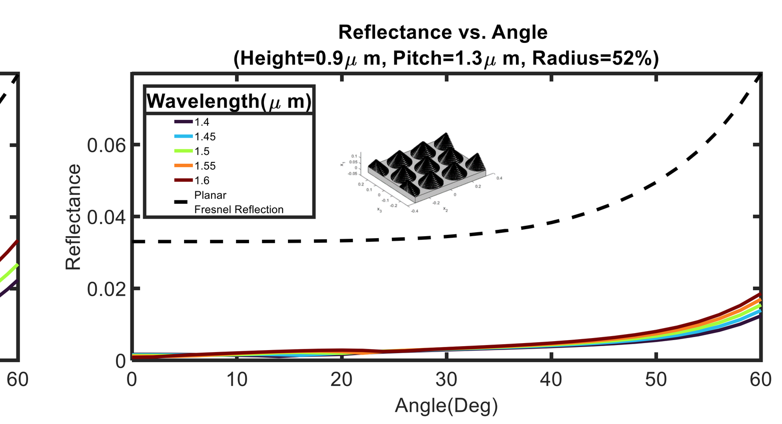

Figure 14: Reflectance dependence on height for different wavelengths of incident beam for conical nanostructures. Note the reflection reduction is relatively comparable to pyramidal results

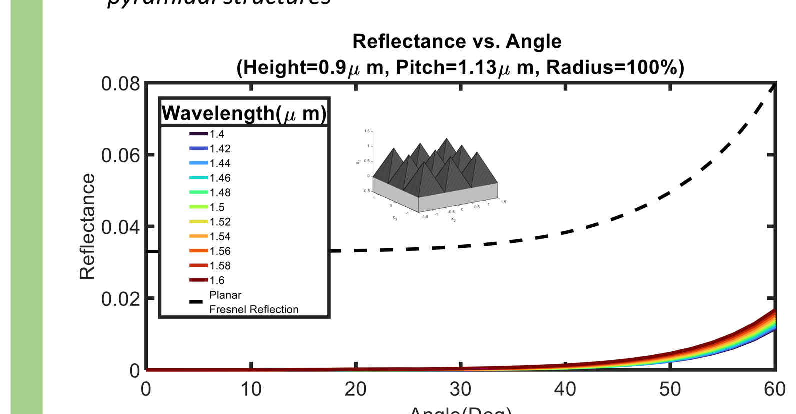

Figure 15: Reflectance dependence on angle for different wavelengths of incident beam. Note the drastic decrease as compared to an untreated surface

Conclusions

- A framework to analyze a set of simulated nanostructures and quickly determine the optimal configuration with regards to minimizing reflectance over a range of parameter values has been developed
- Pyramidal and conical nanostructures show the best performance among the structure shapes analyzed, due to the more gradual transition between air and substrate.
- Future work involves simulating over a wider range of parameter values, as well as altering structure shape.

Acknowledgements

I want to thank Dr. Catherine Jahncke of St. Lawrence University and Dr. Wataru Nakagawa and Jordan Baker of Montana State University for their immense help. I also want to thank Ken Johnson for developing GD-Calc, the simulation software largely used in this project. Finally, the faculty and students of the St. Lawrence physics department deserve acknowledgement for their constant support over the past months.

References

- PVEducation. "Anti-reflection coatings." (2022), [Online].
- E. E. Perl, W. E. McMahon, J. E. Bowers, and D. J. Friedman, "Design of antireflective nanostructures and optical coatings for next-generation multijunction photovoltaic devices," Optics Express, vol. 22, no. S5, A1243, Jul. 2014. doi: 10.1364/oe.22.0a1243.
- B. K. Mousavi, A. K. Mousavu, T. Busani, M. H. Zadeh, and S. R. J. Brueck, "Nanostructured anti-reflection coatings for enhancing transmission of light," Journal of Applied Mathematics and Physics, vol. 07, no. 12, pp. 3083–3100, 2019. doi: 10.4236/jamp.2019.712217.
- J. Cai and L. Qi, "Recent advances in antireflective surfaces based on nanostructure arrays," Materials Horizons, vol. 2, no. 1, pp. 37–53, 2015. doi: 10.1039/c4mh00140k.

Computational Exploration of Anti-Reflective Nanostructures

Ganesh Petterson, Dr. Catherine Jahncke
Department of Physics, St. Lawrence University, 23 Romoda Dr., Canton, NY 13617

Reflection from an Interface

- Every optical material can be characterized by a *refractive index (n)*
  - The index describes how much light "bends" when entering said material.
- The refractive index and incidence angle govern the reflection from an interface through the Fresnel equations:

$$R_s = \left(\frac{n_i \cos\theta_i - n_t \cos\theta_t}{n_i \cos\theta_i + n_t \cos\theta_t}\right)^2$$

$$R_p = \left(\frac{n_t \cos\theta_i - n_i \cos\theta_t}{n_i \cos\theta_t + n_t \cos\theta_i}\right)^2$$

- R_s and R_p denote the reflectance for s and p polarizations; we average these quantities for the remainder of the poster.

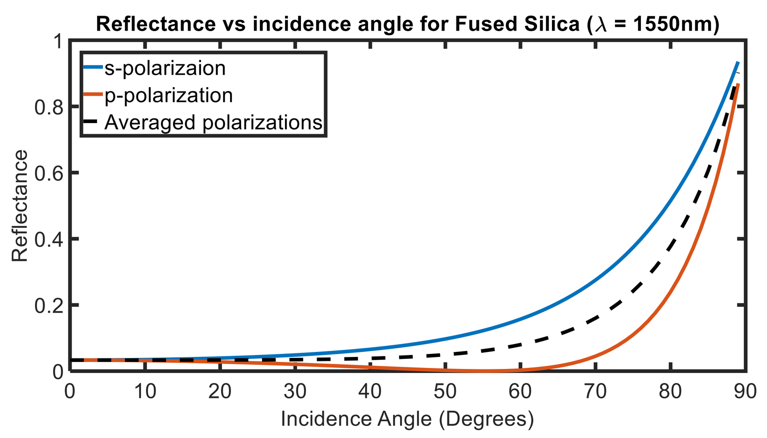

Figure 1: Reflectance as a function of incidence angle from a simple interface. Note the different values for s- and p- polarizations.

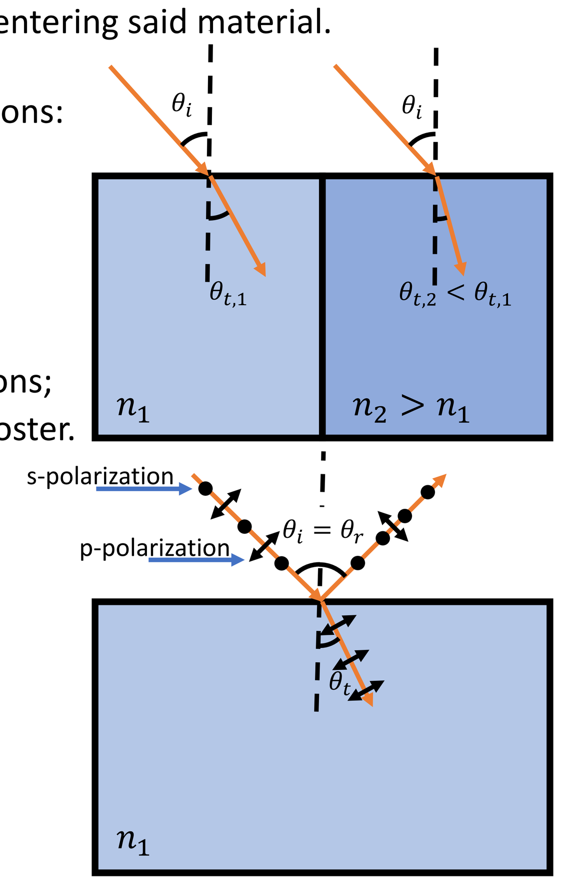

Figure 2: (Top) An image demonstrating the effect of different refractive indices.
(Bottom) The parameters and polarization behavior of reflection.

Interference of Light

- Light can be modeled as a wave, and as such, exhibits interference.
- This interference can be desired, as in the case of anti-reflective coatings, or undesired, as in the case of back-reflection in benchtop optical experiments.

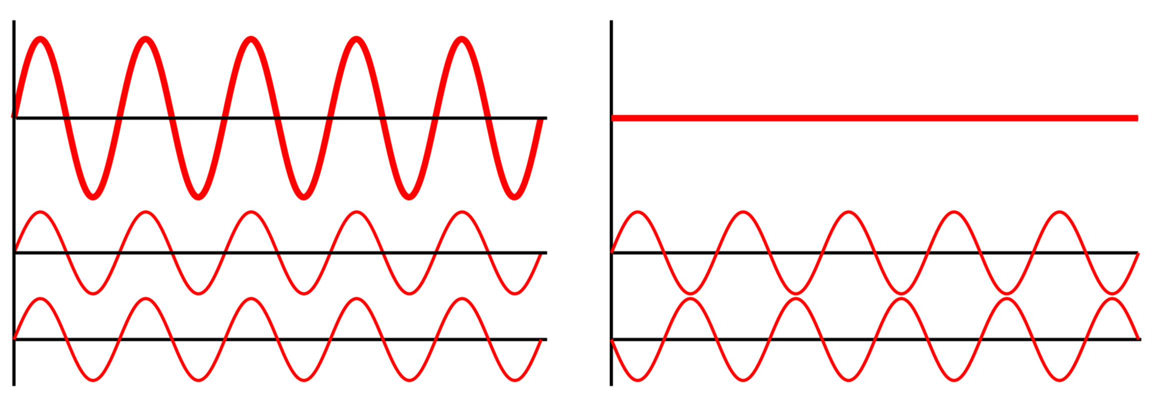

Figure 3: Constructive and destructive interference of two waves. The theory of interference is used in the design of anti-reflective optical coatings, detailed below.

Anti-Reflective Coatings:

- Light is reflected from the front and rear surface of a coating, and destructively interferes with itself (Figure 1)
- For single layer coatings, this is very wavelength-specific (Figure 2)

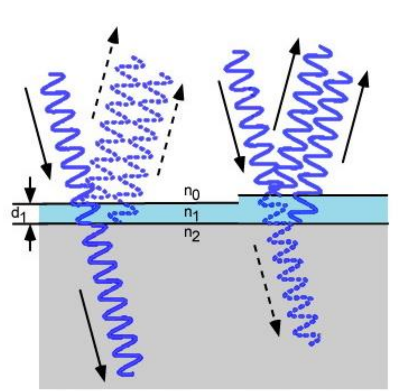

Figure 4: Constructive and destructive interference from a thin-film anti-reflective coating.

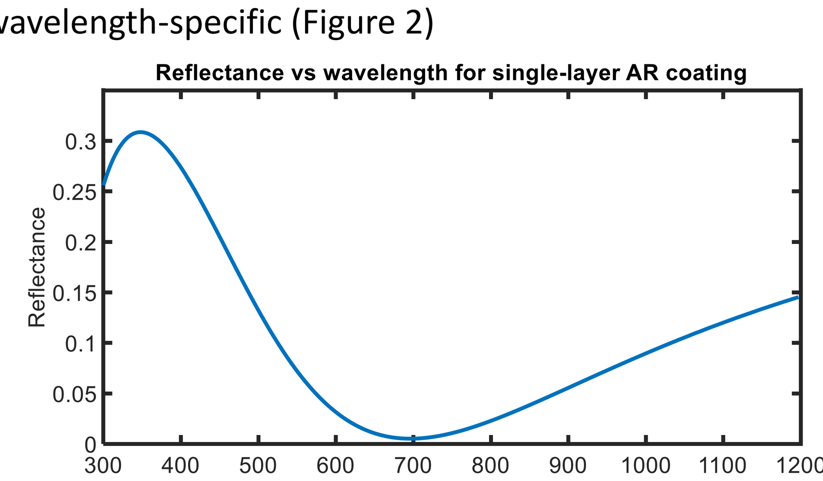

Figure 5: Simulated results for a single-layer thin film, showing a maximum reduction of reflectance for a wavelength of 700nm.

Anti-Reflective Nanostructures

- Nanostructures create a refractive index gradient, reducing reflection between infinitesimal "layers"
- The lack of reliance on interference means that they have the potential to perform better over wide angular or wavelength ranges
- We largely investigate the performance of AR nanostructures over a wide angular range

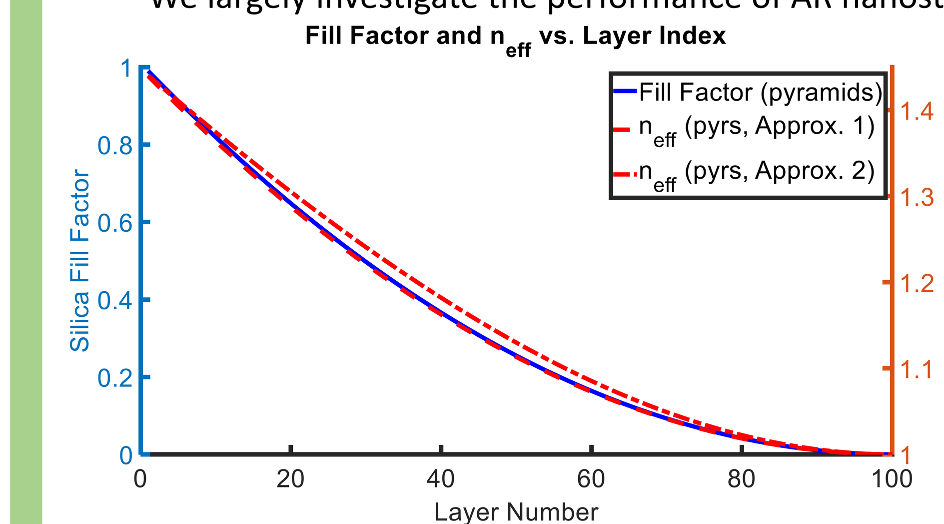

Figure 6: The "fill factor" of a pyramidal structure, representing the percentage of each layer filled by the substrate material, along with two approximations for the effective refractive index.

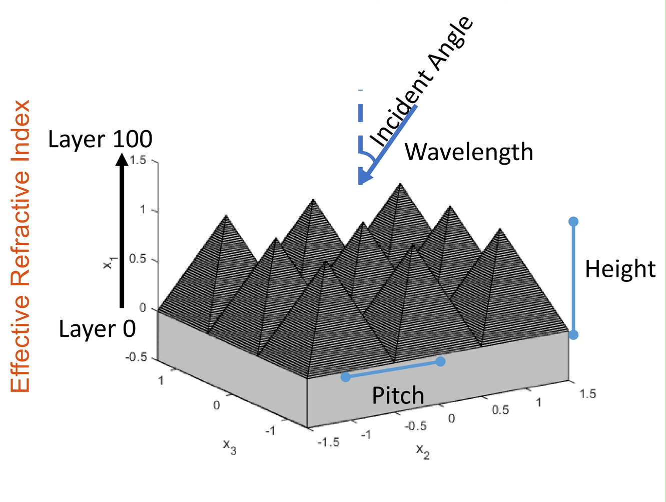

Figure 7: A diagram showing the different parameters that were varied for each shape.

- Structures can be formed in different shapes, with varying effectiveness (Figure 8)

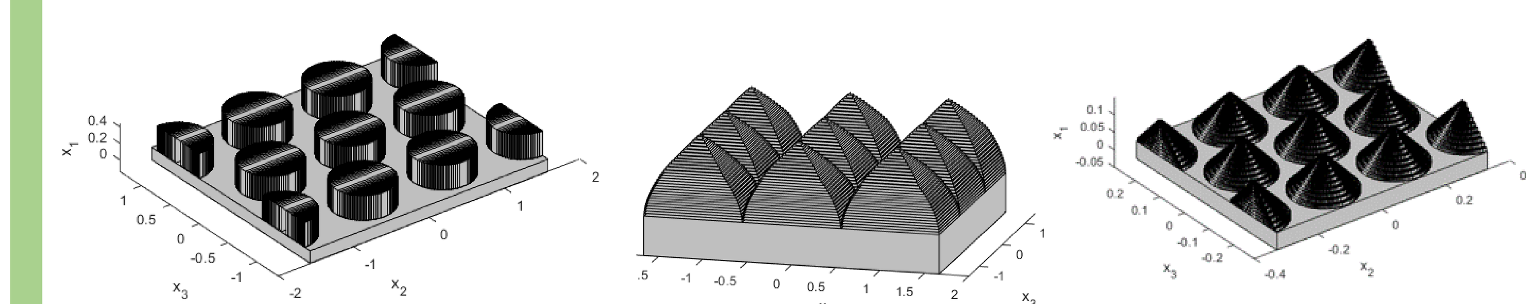

Figure 8: Different possible AR shapes. The aspect ratio, width, and pitch of structures can be changed to yield different results.

- Each shape has a different fill-factor curve, yielding different effective refractive index profiles

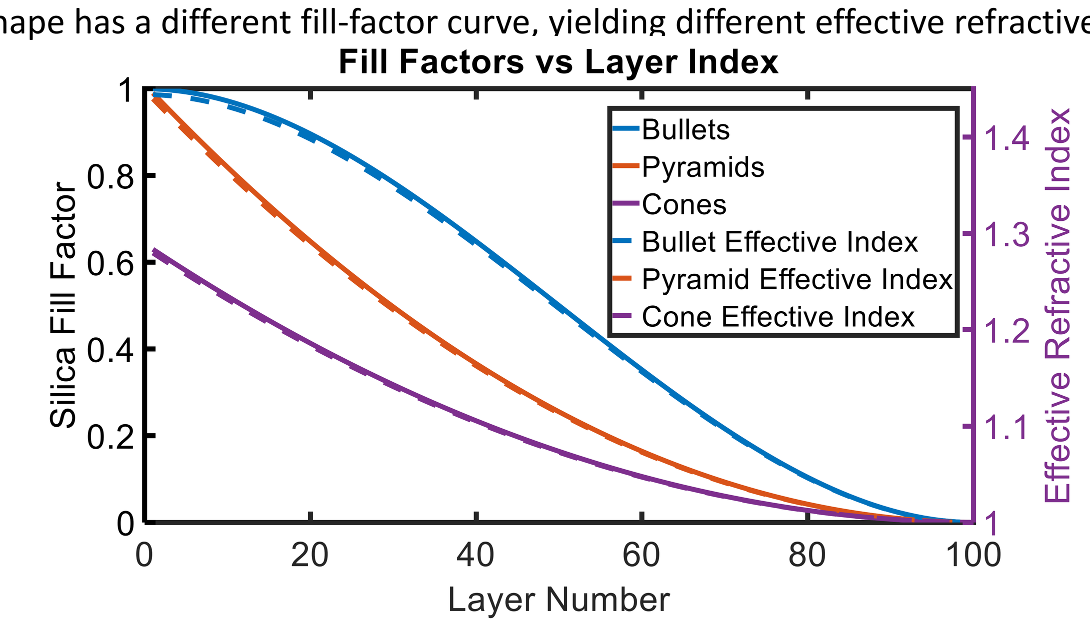

Figure 9: Fill factors and approximate effective refractive indices for three different structure shapes.

- The "smoothest" effective index transition surprisingly does not yield the best results!

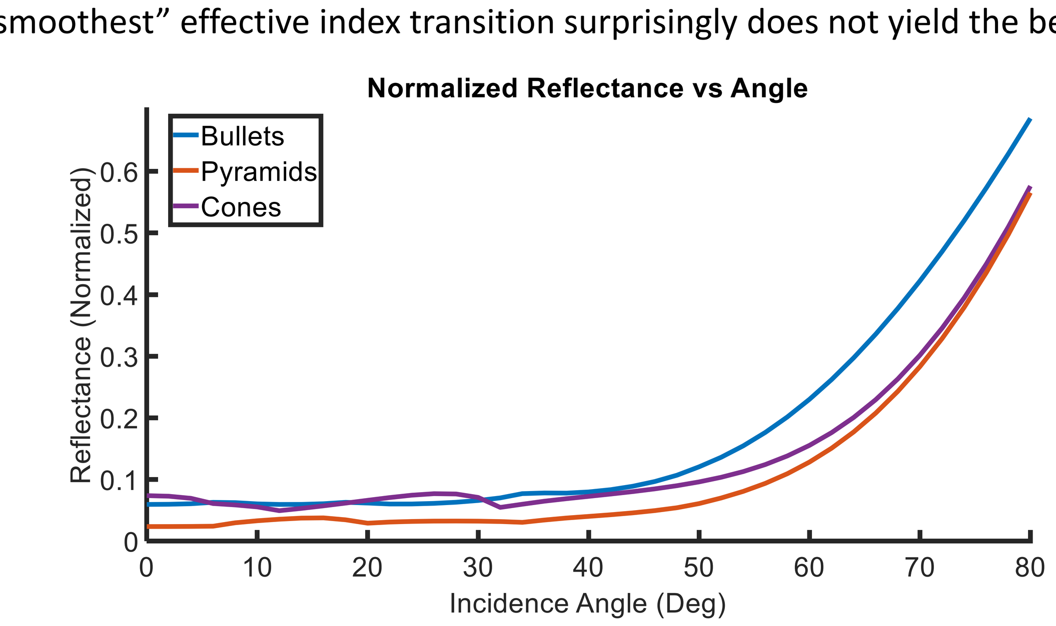

Figure 10: A comparison of reflectance vs angle for three structure shapes, all simulated with identical parameters. Note that the y-axis is normalized to the "baseline reflectance"; that is, the reflectance of a flat pane of fused silica. Structures were simulated with a height of 0.9 μm, pitch of 1.13 μm, and 0.19 μm between bases for a 1500nm beam at normal incidence.

Findings

- Results, such as those in Figure 10, were obtained through the use of the MATLAB simulation package GD-Calc
- Fused silica was used for all simulations to keep the material consistent.
- The input wavelength was around 1550nm for all simulations.
- Reflectance was plotted as a function of several parameters, in order to get a sense of overall behavior
  - The following figures demonstrate that the optimization of these structures is a multi-faceted problem. Even considering a single structure shape, reflectance varies widely based on structure pitch and height.

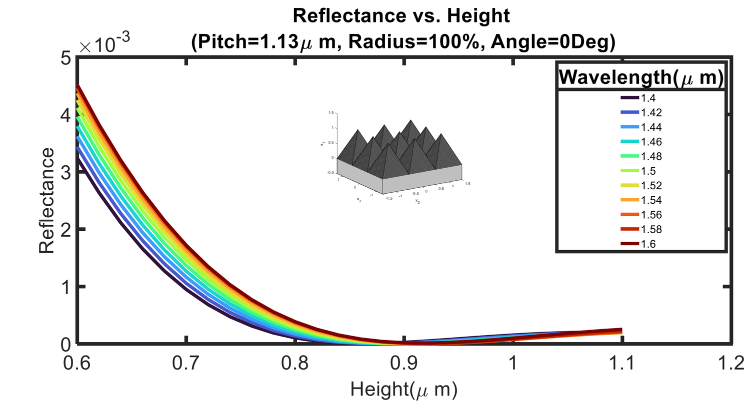

Figure 11: Reflectance dependence on height for different wavelengths of incident beam.

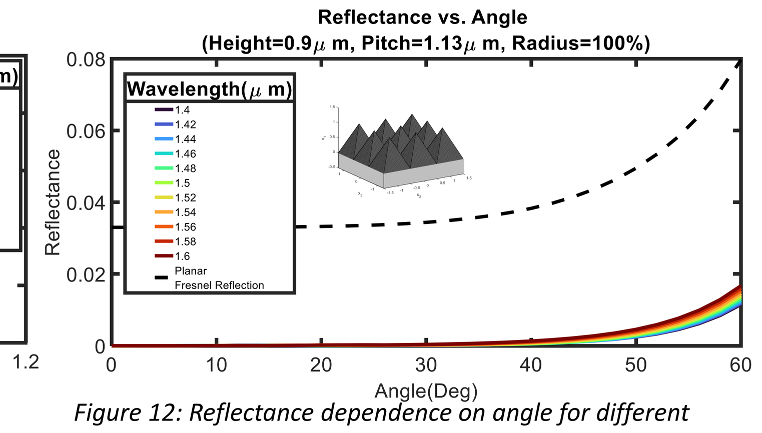

Figure 12: Reflectance dependence on angle for different wavelengths of incident beam. Note the drastic decrease as compared to an untreated surface.

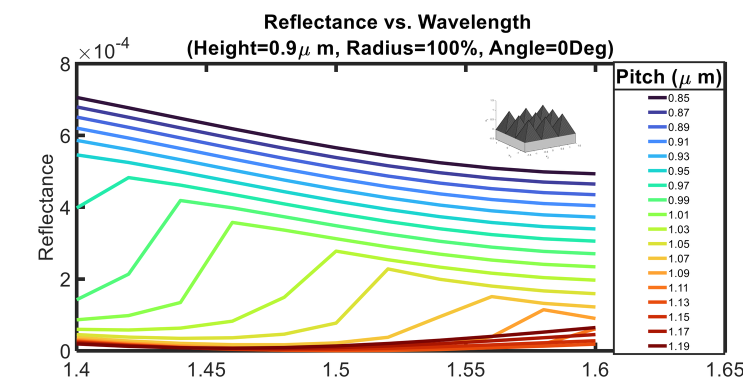

Figure 13: Reflectance dependence on wavelength, this time for different pitches; note the drastic spike in reflectance dependent on pitch.

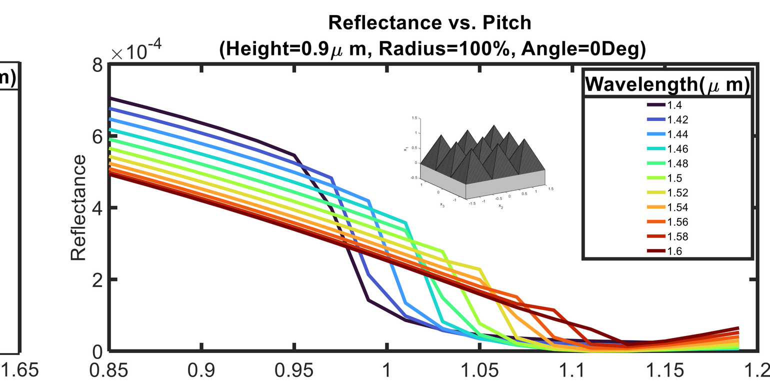

Figure 14: Reflectance dependence on pitch for different wavelengths. This is essentially the same information as Figure 10, portrayed differently.

Conclusions

- A framework to analyze a set of simulated nanostructures and quickly determine the optimal configuration with regards to minimizing reflectance over a range of parameter values has been developed
- Future work involves simulating over a wider range of parameter values, as well as altering structure shape.
- Bullet-shaped structures show promise, due to the smoother transition in effective refractive index. However, in the structure ranges simulated, they have shown to be inferior to pyramids.
- The problem of finding an "optimum solution" that minimizes reflectance for a given situation is complex and multi-faceted and requires the use of an iterative process to find an optimum for a specific situation.

Acknowgements

I want to thank Dr. Catherine Jahncke of St. Lawrence University and Dr. Wataru Nakagawa and Jordan Baker of Montana State University for their immense help. I also want to thank Ken Johnson for developing GD-Calc, the simulation software largely used in this project. Finally, the faculty and students of the St. Lawrence physics department deserve acknowledgement for their constant support over the past months.

References

- PVEducation. "Anti-reflection coatings." (2022), [Online].
- E. E. Perl, W. E. McMahon, J. E. Bowers, and D. J. Friedman, "Design of antireflective nanostructures and optical coatings for next-generation multijunction photovoltaic devices," Optics Express, vol. 22, no. S5, A1243, Jul. 2014. doi: 10.1364/oe.22.0a1243.
- B. K. Mousavi, A. K. Mousavu, T. Busani, M. H. Zadeh, and S. R. J. Brueck, "Nanostructured anti-reflection coatings for enhancing transmission of light," Journal of Applied Mathematics and Physics, vol. 07, no. 12, pp. 3083–3100, 2019. doi: 10.4236/jamp.2019.712217.
- J. Cai and L. Qi, "Recent advances in antireflective surfaces based on nanostructure arrays," Materials Horizons, vol. 2, no. 1, pp. 37–53, 2015. doi: 10.1039/c4mh00140k.