TERAHERTZ DOMAIN RAPID PROTOTYPED GRADIENT INDEX OPTICS

By

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A Thesis Submitted to The Honors College

In Partial Fulfillment of the Bachelors degree
With Honors in

Optical Sciences and Engineering

THE UNIVERSITY OF ARIZONA

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Degree title (eg BA, BS, BSE, BSB, BFA): BS	
Honors area (eg Molecular and Cellular Biology, English, Studio Art): Optical Sciences and Engineering	
Date thesis submitted to Honors College: Wed May 4, 2011	
Title of Honors thesis: Terahertz domain Rapid Prototyped Gradient Index Optics	
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Group Project Responsibilities

May 4, 2011

1 Members

1.1 Brian Klug

As an Optical Sciences & Engineering major with an emphasis on Electrical Engineering (Optoelectronics track), responsibilities included contribution to the overall design from an antenna theory perspective in conjunction with classical optics perspective. Logistical aspects of contribution included working on engineering notebook upkeep, meeting minutes, scheduling and planning capstone project with the gantt chart, and selection as well as ordering of model polymer for the rapid prototyping machine.

Engineering contributions ranged from concept of the dithered slab model with full 3-space variation to final coding of the modified Floyd-Steinberg and ordered/Bayer dithering scheme used to realize a gradient index profile using model and support polymer. In addition, aided Alex and Duncan with remaining 'swiss cheese' model discretization by analyzing possible average index quantized levels from different size $n \times n$ grid arrangements. Further, aided in elimination of non-viable designs. Review of deliverables including final poster alongside William Duncan.

1.2 Alex Miles

Designed and coded the index profile numerical solver using differential calculus. This system derived the ideal index profile for focusing incident THz radiation to a point. Iterative derivation process created entirely from the ground up for this project which will result in the best possible behavior. Tested and verified proper behavior using Luneburg Lens.

This ideal profile then needed to be discretized, which was Brian Klug and William Duncan's responsibility, shared with Alex. In addition worked on output data formatting for further processing and leading to printing. Continued working on deliverables such as final report and poster.

1.3 William Duncan

Team leader responsible for communicating with project sponsor and mentor. Liason between everyone from the student side to ordering to other logistical communications. Organized and coordinated meetings and presentations, kept track of deadlines and deliverables. As an optical sciences student, contributed to design and analysis of dithering workflow for the lens. Initially contributed to first attempts at discretization workflow with Matlab later superceded by other methods.

Significant contribution to final printing procedure and data structure required to print the realized structure. Worked with graduate students in sponsors lab to print the final designs and provide feedback for further tweaking of the swiss cheese discretized design. Contributed majority of effort toward design and fabrication of poster.

1.4 Colton Holmes

Alongside Wanglei Han, responsible for EE analysis and testing of both designs in ANSYS HFSS. Tested and analyzed three basic designs and contributed toward the iterative process that led to our eventual two designs chosen - both the final swiss cheese and dithered system. Contributed to overall deliverables and final report.

1.5 Wanglei Han

Alongside Colton Holmes, responsible for EE analysis and testing of both designs in ANSYS HFSS. Tested and analyzed three basic designs and contributed toward the iterative process that led to our eventual two designs chosen - both the final swiss cheese and dithered system. Contributed to overall deliverables and final report.

Terahertz GRIN Rapid prototyping Engineering 498A/B - Final Report

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***Abstract*—The 'terahertz range' is a colloquial term used to describe radiation that lies between the far infrared (FIR) and microwave region in the electromagnetic spectrum, it is far less energetic than visible light. The applications of terahertz radiation are myriad: including security, military radar, product inspection, and telecommunications. These require manipulation of the radiation beyond simple transmission and detection, namely refraction: focusing, defocusing, and collimation. These operations all require waveguides and lenses.**

The current state of the art for fabricating lenses that operate in the terahertz frequency range is an expensive and time consuming processes involving high purity semiconductors, ultra precise designs, and months of lead time. Our project focused on demonstrating that an inexpensive and quick process could be implemented that reduced the investment required to produce such a lens by more than three orders of magnitude. This process consists of fabricating a novel gradient of index (GRIN) using a polymer-jetting rapid-prototyping machine with a computationally-generated design.

This required several key steps. First we created a ray-tracing algorithm capable of simulating arbitrary distributions of different materials. The second was optimizing a design for ideal behavior when interacting with terahertz frequency radiation. The third and final involved descritization and realization of a the index profile into a model realizable with the prototyping machine workflow.

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I. Statement of Purpose

The purpose of this project was to produce concrete evidence - a proof of concept - that significant gradients of index of refraction could be affected by rapid-prototyped structures containing few base materials. Strictly speaking, fabrication and detailed testing of such an optic lay outside the scope of the project, but were later pursued given adequate time window.

II. Statement of Relevance

The significance of this project lies in the stark contrast it provides to current fabrication methods for optical devices operating in the terahertz frequency range. At present all optics fabricated for industrial use in the terahertz range and made by a semiconductor photolithography (CMOS manufacturing) process wherein sensitive resonating structures are patterned into silicon. This process is both time consuming as well as financially prohibitive, with a lead time from several days to several months per optic at a cost in the tens of thousands of dollars. This rapid prototyping process enables lead times on the order of hours and a material cost on the order of tens of dollars per device. In addition, the rapid-prototyping process is largely automated, meaning the highly skilled labor requisite in semiconductor processing would not be required.

The applications of terahertz radiation are myriad. The low-energy radiation reacts with few materials, namely metals and large molecules. It is this very non-reactive nature that makes it so difficult to manipulate terahertz radiation. These properties allow for military, security, inspection, medical, and telecom applications. At present terahertz radiation is utilized in some airport scanners as a safer alternative to x-ray back scatter, as terahertz radiation is low enough energy that ionization, and subsequent DNA damage, cannot occur regardless of the intensity and duration of exposure. The advent of low-cost terahertz optics would open the way for new applications that were previously barred by the prohibitive cost of fabrication.

III. Methodology

Our project was highly self-guided with some oversight from the sponsoring professors who gave insight as to which design avenues would be easier, the properties of the rapid prototyping machine and selected polymers, and the process which their graduate students were using to interface with the machine.

A. Coordinate System and Assumptions

Here, we will use the common coordinate system that has been readily adopted in the optics community. We use a Capetian coordinate system such that light or EM radiation travels along the z-axis in the positive direction. We place our optic into the coordinate system in the $x-y$ plane. While other coordinate systems provide a greater flexibility in dealing with rotationally symmetric systems (the designs presented here are no doubt square but can be called semi-rotationally symmetric at least with respect to their index profile) we will stick with a Cartesian coordinate system for greatest simplicity. Figure 1 shows a typical Cartesian coordinate system used in optics.

B. Designing the Index Profile

Traditional optics affect focusing by presenting a curved surface and a different refractive index, n. This approach is not used for terahertz radiation for two reasons: curved surfaces are difficult to fabricate given the nature of the prototyping process, and the wavelengths (much longer than the visible) involved render reasonable curvatures ineffective. A gradient of index (GRIN) was instead the goal of the project, as the features created by the rapid prototyping machine are sufficiently smaller than the wavelength such to require effective medium theory to model. In short, this theory dictates that the material properties that the wave reacts to (the refractive index n, and the dielectric constant ε) are volume-averaged over one wavelength. This means that several materials of different indices can create a spectrum of effective indices by combining blocks of them on the micron scale.

Before we could tell how much of each polymer to place where, we needed to know what sort of index profile would best create a focusing optic for the wavelengths we were interested in. We considered commercial ray tracing software available to us through the College of Optical Sciences, namely **ZEMAX** and **CODE V**, but both proved unable to simulate arbitrary distributions of index as well as incapable of simulating such long wavelengths effectively. In addition, we weren't satisfied with the index profile performance and set out to derive the best possible index for our frequency. As such, we undertook to write our own ray tracing algorithm.

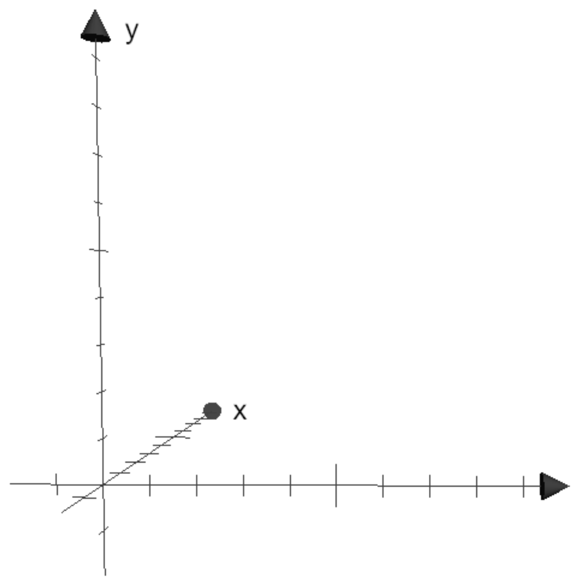


Fig. 1: Coordinate System

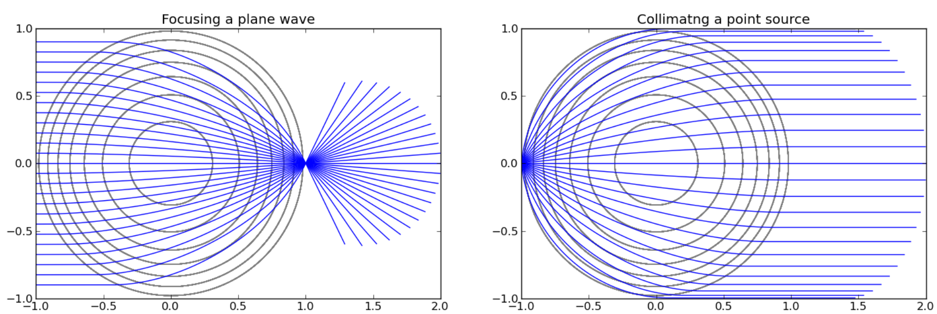


Fig. 2: Raytracing simulation of a Luneberg lens index profile for validation. Black lines are contours of equal index of refraction, blue lines are traced rays.

1) Novel Raytracing Algorithm: Our first attempts were driven by the geometric and physical optics approaches taught to the optical science members of our team during our undergraduate courses, but proved unwieldy. Consultation with Dr. Robert Erdmann in Materials Science Engineering allowed us to take on a variational calculus approach utilizing Fermat's law to derive expressions for the rays as a function of an arbitrary index field. These expressions, coupled into an differential equation solver, provided expressions for the rays for any index field.

The derivation is beyond the scope of this document, but the system of differentials being utilized as a state vector are as follows:

$$\begin{pmatrix} dx \\ dy \\ d\theta \end{pmatrix} = \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \\ \frac{1}{n(x,y)}\left[\cos(\theta)\frac{dn}{dy}(x,y) - \sin(\theta)\frac{dn}{dx}(x,y)\right] \end{pmatrix} \tag{1}$$

A proof of concept was undertaken to validate the function of the ray tracing algorithm. The test structure fed in was a Luneberg lens, a sphere with radially varying index of refraction. The index profile for this test structure can be modeled as follows, wherein r is the radial distance, R is the sphere radius, n_0 is the index of refraction of the surrounding medium, and n_1 is the highest index expected within the domain:

$$r = \sqrt{(x - x_c)^2 + (y - y_c)^2}$$

$$n(x, y) = \begin{cases} r \leq R & \sqrt{n_1 - \left(\frac{r}{R}\right)^2} \\ r > R & n_0 \end{cases}$$

The behavior of a Luneberg lens in reality is the focus collimated light entering one side onto a focused spot on the opposite side, and take light from an object in contact with one side and emit collimated light out the opposite side. The result of tracing this profile can be seen in Figure 2.

2) Optimizing the Index Distribution: The optimization process was started by picking a figure of merit. We chose the axial distribution of ray crossings as our figure as we reasoned a smaller distribution indicated a tighter the bundle of rays and the more efficient the focusing effect. Later testing of the resulting fields would confirm this. The actual optimization was done by limiting our index profiles describable by the **University of Rochester** polynomial, which describes both axial (in z) and axisymmetric radial (in r) variation by a power series.

$$\begin{aligned} n(r, z) = \quad & n_{00} + n_{01}z + n_{02}z^2 + n_{03}z^3 + n_{04}z^4 \\ & +n_{10}r^2 + n_{20}r^4 + n_{30}r^6 + n_{40}r^8 \end{aligned} \qquad (2)$$

The coefficients on the various terms became the parameters for our optimization, which as done using a modification of the Levenberg-Marquardt algorithm, which converges to stable local minimum even if the initial guess is very far away.

C. Discretization

The previous step yielded a continuously defined function that returns the index of refraction at any point in space. While convenient for a simulation, this is now how it is fabricated. In order to affect the index at one given point, we fall back to the aforementioned **effective medium theory**, which holds that the material properties in a volume will act in concert as the volume-average material property. As such, we needed to find a scheme for distributing our three materials (model polymer with $n_{eff} = 1.7$, support polymer with $n_{eff} = 2.0$, and air $n_{eff} = 1.0$) in space that meshed well (no pun intended) with the capabilities of the rapid prototyping machine available. Two specific schemes were settled upon as being realistic and computationally designable (as the complexity of the profile quickly went beyond what one would want to discretize by hand).

The first such scheme was dithering. In image processing this processes takes an image possessing many intensity levels and, using a set of quantized intensity levels of our choice, rebuilds the image using only the allowed intensity levels by propagating the difference between the quantized levels and the existing level to neighboring pixels. The result is an image that resembles the original when viewed at a different scale and lacks visible quantization steps that a straight threshold or halftone dither would result in. This is the same scheme utilized by comic book printers years ago to affect gradients with only discrete points of ink, as shown in Figure 3. We implemented a modified Floyd-Steinberg dithering algorithm and used it for discretization. This algorithm is commonly used in image processing and yields good uniformity and minimal quantization error over our average sizes. We also implemented a ordered dithering algorithm, though the Swiss cheese example later on roughly approximates an ordered dither. Subjectively better smoothness was realized with the Floyd-Steinberg algorithm. Further experimentation with Bayer and other dither algorithms could potentially yield different, better results as well. This discretization algorithm was applied to each layer of the structure, in effect creating an area dither rather than a true volume dither.

The second discretization scheme is nicknamed 'Swiss cheese' since it approximates the holey structure of the cheese which it derives its namesake from. Simply put, the Swiss cheese model consists of columns of one material surrounded by another material. One structure consisting of air surrounded by model was designed, another consisting of support surrounded by model. In the Swiss cheese system, the index varies only in x and y, not z through the optic. A two-dimensional slice of material is divided up into an regular grid. Each entry in the grid is replaced with a predefined structure whose volume average is closest to the desired index.

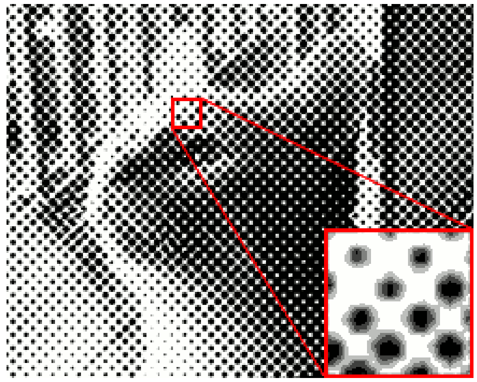


Fig. 3: An example of how a "halftone" or dithered pattern effects a gradient on different length scales

D. Electromagnetic Simulation

One avenue used to prove the focusing ability of our dithered object was simulating the structures in ANSYS HFSS. The HFSS software allowed for the structures to be built in three dimensions and simulated to observe electromagnetic plane wave behavior through and beyond our dithered structures. As discussed later, do to computer processing limitations not all of our designs were able to be simulated using HFSS. However the Lincoln Log and Swiss Cheese designs where simulated with HFSS to prove, in simulation, that terahertz plane wave focusing is possible with these structures.

To simulate the designs using HFSS the structures were built by hand using HFSSs built in three dimensional model building features. Once built individual portions of the structures were selected and given material properties, in particular the dielectric constant, similar to those of the model and support polymers. Other methods were considered but not implemented in building the structures for simulation. The first involved building the structures using the Solid Works three dimensional model building software, which allows for greater design detail, and importing the structure into HFSS using a .STEP file extension. This seemed to be illogical because our structures were able to be built with similar precision and difficulty using HFSS which excludes the process of transferring the simulated structure between different software. The second method considered was creating script files generated using MATLAB in order for the structures to be built automatically. This method would have been useful in order to build the dithered solid block design in HFSS because of the complexity of the structure. However because of foreseen computational limitations discussed later the dithered solid block was not attempted to be simulated using HFSS. Thus work in generating the script files were not undertaken.

Do to high radial symmetry and no z-directional variation in profile index it was possible to build only a quarter of the structures in HFSS to cut down computation while still able to obtain sufficient results. A radiation boundary was built around the structure and extended out to an appropriate distance where a focal point may fall inside, in general about five times the depth of the structure. An incident plane wave within the colloquial terahertz region of frequency was selected to travel normal to the surface of the selected entry plane of the structure. Also planes with unassigned material settings, so they will not interfere with the plane wave behavior, were placed at stepped z-varying distances in order to observe electromagnetic intensity activity as the plane wave travels through and beyond the structure. The simulations were then analyzed by the HFSS software which took between 20 minutes to multiple hours depending on the complexity.

Focusing effects were observed in HFSS simulation of the Swiss Cheese dithered design as seen in Figure 4. As a reminder only a quarter of the entire structure was built to decrease computation. The dimensions of the model are (2.5 cm x 2.5 cm x 1 cm) in (x y z). The original design called for a depth in z of 2 cm although when simulated an out of memory error occurred on the computer so the structure depth was cut in half so computation was possible. The incident plane wave tested on the structure was set at 100 GHz which translates to a 3 mm wavelength. By cutting

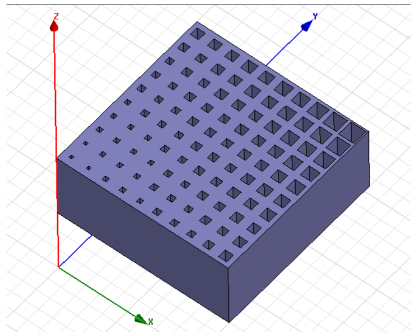


Fig. 4: HFSS Model of the Swiss cheese discretization scheme

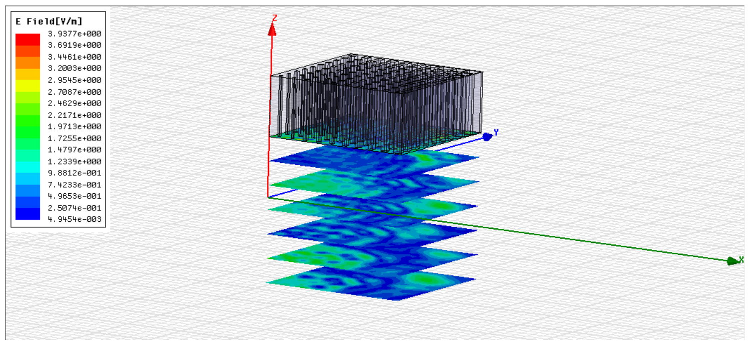


Fig. 5: HFSS Results near the focal plane

the depth of the structure in half the incident wave was still able to pass the distance of just over three wavelengths through the material. It is untested as to whether having a thicker depth would provide better or worse focusing effects. Although it would decrease the intensity of the plane wave do to absorption and reflection effects by the structure. From this simulation the results show the best focusing desired at 2 mm and 8 mm from the exiting surface of the Swiss Cheese structure. The multiple peaks of interference suggest a more collimated result than a defined focal point which is a result of having a lack of z varying index. However it does prove that focusing is possible with the use of varying polymer materials at sub-wavelength increments do to effective medium theory. As proof Figure 6 is a visual representation of the intensity of the plane wave focused at where the center of the structure would be if the whole structure was simulated.

E. Interfacing with the EDEN 350V Rapid Prototyping machine

Interfacing with Objet EDEN 350V is through a MATLAB Graphical User Interface (GUI). The GUI was written by members of the two sponsors' research groups. To port our results and output to the printer via the provided MATLAB GUI a number of steps were taken. First, a binary image of our desired spatial distribution of polymers was created from our matrix or functional form. The creation of these images translated a matrix of 1's and 0's, representing the spatial distribution of polymer and air respectively, into a binary image (black and white) with the same spatial distribution of black and white pixels as 1's and 0's. Porting out two designs into MATLAB each needed individual consideration due to the fact that the Swiss Cheese model was non-varying along the z-axis and was essentially many of the same layers stacked while the dithered model included 50 different layers that were used to affect an index variation both radially and along the z-axis. Further, due to memory limitations on the machine running the MATLAB that interfaced with the Objet EDEN 350V, one image layer often had to be broken down into many sub-layers.

Resolution of the Objet EDEN 350V is given as 42μm in x, 84μm in y, and 15μm in z. This caused the need for stretching our image by a factor of two in x direction thus giving us a final output from the printer that was square. Further, to create the desired aspect ratio for the optic (4:1) many of the same image had to be printed to create one "layer" in our design.

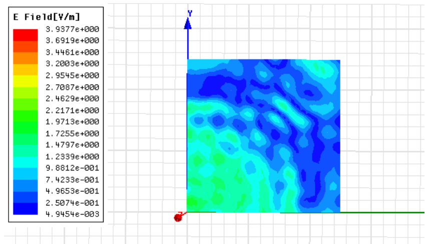


Fig. 6: HFSS Results near the focal plane

Our image for each layer had a resolution of 2000×1000 pixels producing an optic measuring 8.4cm along each edge of the face. To create the desired aspect ratio each image file or "layer" was ported to MATLAB and thus the Objet EDEN 350V printer a total of 28 times, giving each layer a thickness of $15\mu\text{m} \times 28 = 420\mu\text{m}$ in z. Finally each optic, dithered and Swiss cheese, we given a total of 50 "layers" for a final thickness of 2.1cm.

F. Failed Design Avenues

Initially, a structure dubbed "Lincoln Log" was considered but scrapped to to the required complexity in discretization. The idea here was to use a stacked of crossed variable size rectangular rods. An example of the Lincoln Log structure is shown below in Figure 7a.

This design was eventually scrapped due to the complexity required for discretization. Eventually this design was evolved into the Swiss Cheese model such that it had a index profile that didn't vary along the z, or propagation, axis. The simplification from Lincoln Log design to the Swiss Cheese model allowed for discretization of one layer that would be essentially extruded to the full 2.1cm thick model through layering of 1400 of the same layer while discretization of the Lincoln Log structure required the spatial averaging of index values along a complicated structure with a further boundary condition that every Lincoln Log must be continuous between discretization steps.

IV. Literature Review

The literature review was very brief, as even in-depth searches showed that the two sponsoring professors had a hand in every inroad into this technological territory. Dr. Gehm and Dr. Xin have published papers on creating volumetric optics in the GHz and THz regions, creation of bandgap structures by the same technology, and prototyping crystalline waveguide structures in ordered polymers. These papers were used to determine a large amount of the information we used to proceed regarding the nature of the polymers being used, as well as the nature of the interaction. Some of their projects focused on the micro-resonator effect that the structures could have on the incident wave, while others utilized the periodicity of the fabricated structure to impose a specific band-structure to influence the electronic properties of the bulk material.

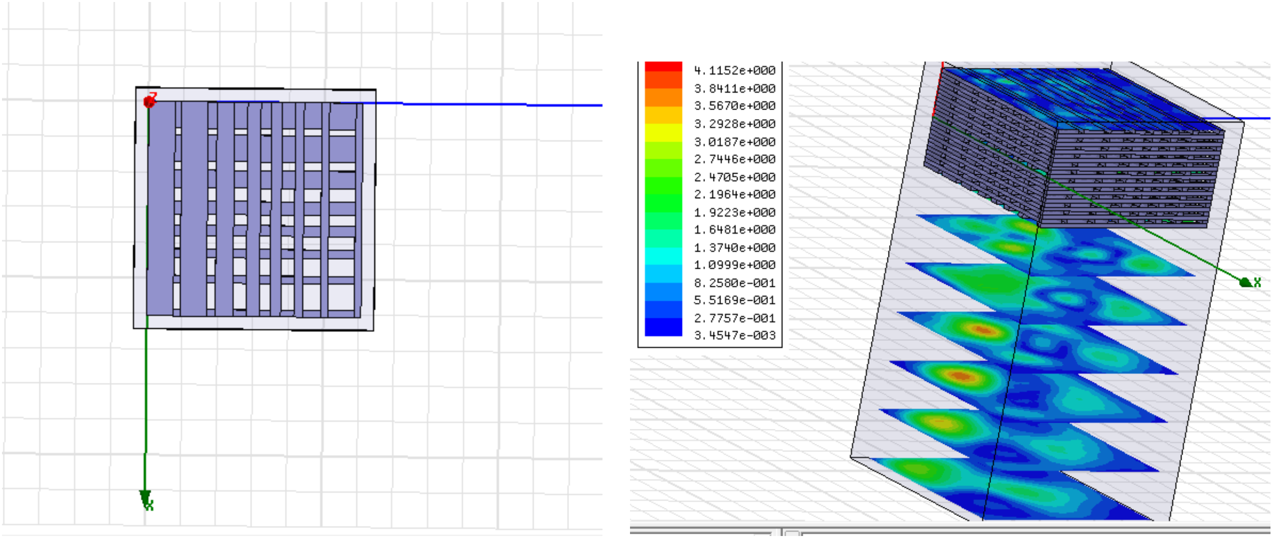
V. Results and Issues

Simulations of several test structures were run using ANSYS HFSS. This software is able to solve Maxwell's equations in three dimensional volumes using any combination of boundary conditions specified, translating to any use-specific geometry and material properties. We encountered several issues in running these simulations, which will be detailed.

A. Simulation Issues

The first hurdle in simulation lay in the long computation time required. This was exacerbated by our requirement for complex geometries, and furthermore by the long focal lengths being affected by the GRIN optic. As a longer focal length is simulated, a larger volume of simulation is required to actually observe the electric field amplitude (the square of which would be proportional to our observed spot intensity) at the focal spot. This was addressed, in part, by running the simulations on a powerful computing cluster run by Dr. Xin. A second step was taken to reduce the simulation time: we simulated only one quadrant of our optic, knowing that the profile is highly rotationally symmetric. This causes the simulations to show radiation converging to one corner of the simulated region, being the center of the optic.

The second issue encountered lies with the complexity of each model. The Swiss cheese model presented the least issues of the pursued designs, as it required only one bulk structure with rectangular regions of air removed from it. In this way the fifty fabricated layers could be represented by a bare minimum of boundary conditions upon Maxwell's equations.



(a) 1/4 of Lincoln Log optic in HFSS

(b) Plane wave showing focusing characteristics to upper left corner

Fig. 7: Lincoln Log Structure used in HFSS Simulation

The other model designed, the dithered distribution, ended up requiring far too many conditions. This arises from the fact that each cube of material would require six boundary conditions to separate it from the neighboring material, and a longitudinal variation means that each of the fifty layers would be distinct from the next. In sum-total, this would require 600 million boundary conditions to be specified (50 layers $\times$ 1000 px $\times$ 2000 px $\times$ 6 sides). Comparing this to the swiss cheese model, which possessed roughly 100 column-shaped holes and therefore roughly 600 boundary conditions, the computational load is unrealistically large.

VI. Analysis and Conclusions

Our work has shown that rapid prototyping can be an effective way to produce optical devices in the low terahertz and high gigahertz region. Physical testing, in additional to stringent simulation, would be the final step to pursue this as a pathway for product production. Figures on loss, reflection, and scattering would also be of prime importance to investigate.

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