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AN EXAMINATION OF THE OPTICAL PROPERTIES OF INDEX GRADIENTS CREATED BY FICK'S LAW DIFFUSION (Preprint)

Peter L. Marasco

Multispectral Sensing & Detection Division

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AIR FORCE RESEARCH LABORATORY
SENSORS DIRECTORATE
WRIGHT-PATTERSON AIR FORCE BASE, OH 45433-7320
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14. ABSTRACT

In the last few years, interest in research and development into new ways of creating gradient index optics has increased dramatically. Several new techniques were developed as part of the DARPA-sponsored Manufacturable Gradient Index Optics (M-GRIN) Program. One approach examined in this program was to employ diffusion, governed by Fick's Law, to generate both axial and radial index gradients. However, Fick's Law diffusion tends to yield index gradients that are mathematically uncommon in optical engineering and lens design. The impact of these new gradients on lens aberrations and image quality are not well understood. This paper will examine index gradients that can be described by (makeable by) solving Fick's diffusion laws for both infrared and visible light materials systems.

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An examination of the optical properties of index gradients created by Fick's Law diffusion

Peter L Marasco

Air Force Research laboratory
Wright Patterson AFB, OH, United States

ABSTRACT

In the last few years, interest in research and development into new ways of creating gradient index optics has increased dramatically. Several new techniques were developed as part of the DARPA-sponsored Manufacturable Gradient Index Optics (M-GRIN) Program. One approach examined in this program was to employ diffusion, governed by Fick's Law, to generate both axial and radial index gradients. However, Fick's Law diffusion tends to yield index gradients that are mathematically uncommon in optical engineering and lens design. The impact of these new gradients on lens aberrations and image quality are not well understood. This paper will examine index gradients that can be described by (makeable by) solving Fick's diffusion laws for both infrared and visible light materials systems.

Key Words: Index of refraction, GRIN optics, Modulation transfer function, Optical performance

1. BACKGROUND

In optical engineering, much of the magic that enables image formation is due to refraction at the boundary between optical media. For several reasons, including ease of manufacturing and mathematically simplicity, optical material interface surfaces tend to be described by some form of conic section. Common conic sections can be described by the equations noted in Table 1. [1] They are also illustrated in Figure 1.

Table 1.: Equations describing conic sections.

Name	Equation	Details
Circle	$x^2 + y^2 = \rho^2$	ρ = radius of the circle
Parabola	$(x-h)^2 = 4p(y-k)$	h, k = offsets p = direction
Ellipse	$\frac{(x-h)^2}{b^2} + \frac{(y-k)^2}{a^2} = 1$	a, b, = axis magnitudes
Hyperbola	$\frac{(y-k)^2}{a^2} - \frac{(x-h)^2}{b^2} = 1$	

In the vast majority of optics, the index of refraction is assumed to be constant, with respect to wavelength, and homogenous throughout the element. One significant exception to this rule, is Gradient Index (GRIN) optics. In GRIN optics, the refractive index is intentionally changed in some mathematically describable way to impart an additional design degree of freedom to the designer. Three common GRIN profiles are the axial gradient, the

Address Correspondence to: Peter L. Marasco, Email: Peter.Marasco@us.af.mil

spherical gradient, and the radial gradient. The first two index gradients can be considered variations of each other and have been shown to be useful in aberration correction, including chromatic aberration correction. [2,3,4] The third index gradient, radial can be used to impart optical power to an otherwise unpowered structure, such as in the example of the Wood lens.[6] All have been used with varying degrees of success in optical design

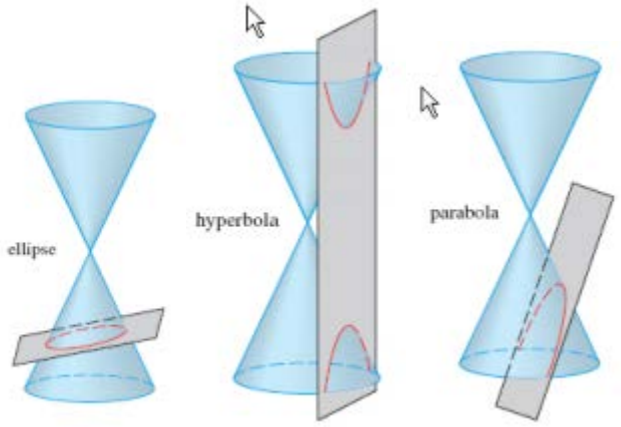


Figure 1. Illustration of common conic sections.[1]

One classic technique for creating index gradients in glass is diffusion. Two chemically similar glasses are brought together and heated for a period of time. During the process, something is transferred between the two materials (ions, atoms, molecules, etc.), creating the desired index gradient. This process can be described by Fick's Second Law which describes how concentration changes with time. Fick's Second Law can be written in one dimension as[5]:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \tag{1}$$

In the above equation, u is concentration, t is time, x is a linear dimension, and D is the diffusion coefficient, in units of area per unit time, such as m^2/s. To expand this partial differential equation to multiple physical dimensions, the equation is more commonly written:

$$\frac{\partial u}{\partial t} = D\nabla^2 u \tag{2}$$

Where ∇^2 is the Laplacian Operator. At first glance it is difficult to determine if the solution the Equation 1 will yield a solution approximating a conic section (Table 1) under any circumstances. To address this issue, the author turned to a numeric solution.

2. MODELING

The following development reflects the approach and nomenclature used in *Boundary Value Problems, Third Edition*. [5] To solve the partial differential equation, expressions for the various partial derivatives noted in Equation 1 should be derived. It can be shown that:

$$\frac{\partial u}{\partial x}(x_i, t_m) \rightarrow \frac{u_{i+1}(m) - u_{i-1}(m)}{2\Delta x} \tag{3}$$

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_m) \rightarrow \frac{u_{i+1}(m) - 2u_i(m) + u_{i-1}(m)}{(\Delta x)^2} \tag{4}$$

In these expressions, $u_i(m)$ is the concentration at time, t_m, in position x_i, $u_{i-1}(m)$ is the concentration at time t_m in position x_{i-1}, $u_{i+1}(m)$ is the concentration at time t_m in position x_{i+1}, and Δx is the change in position from x_i to x_{i+1}

It can also be shown that for the partial derivative of u with respect to time can be described as:

$$\frac{\partial u}{\partial t}(x_i, t_m) \rightarrow \frac{u_i(m+1)-u_i(m)}{\Delta t} \tag{5}$$

Here, $u_i(m+1)$ is the concentration at position x_i at time t_{m+1}, and Δt is the change in time between t_m and t_{m+1}. Now, by applying Equations 4 and 5 to Equation 1, we find:

$$\frac{u_{i+1}(m)-2u_i(m)+u_{i-1}(m)}{(\Delta x)^2} = \frac{u_i(m+1)-u_i(m)}{\Delta t} \tag{6}$$

It should be noted that this approach assumes $D = 1$ to simplify the math. Therefore:

$$u_i(m+1) = ru_{i-1}(m) + (1-2r)u_i(m) + ru_{i+1}(m) \tag{7}$$

Where:

$$r = \frac{\Delta t}{(\Delta x)^2} \tag{8}$$

It is Equation 7 that will be used to calculate the concentration at the next time step, based on the concentrations at the current time step at three locations relative to each other. One should note that in addition to $D = 1$, the position coordinate was normalized to simplify calculations ($0 < x < 1$). Also, time is always assumed to be positive ($0 < t$). This assumption is appropriate for this portion of the paper. However it does prevent this approach from being used to reverse the diffusion process.

It should also be noted that this numerical approach can become unstable, yielding answers that wildly oscillate between positive and negative infinity. Such results are not meaningful. To avoid meaningless results, two conditions must be satisfied in Equation 7. First, no coefficient of $u(m)$ may be negative. Secondly, the sum of the coefficients of the $u(m)$ terms must be less than 1. Therefore:

$$r + (1-2r) + r \leq 1 \tag{9}$$

Or, r must be less than or equal to ½. For the following analysis, r was arbitrarily set to ¼. The impact of adjusting this parameter was not thoroughly examined.

Up to this point, the equations have been described in terms of concentration that diffuses with time. Chemically, this is appropriate. However, from this point forward, it is assumed that the diffusion of some chemical constituent (element, molecule, ion, etc.) will yield a corresponding change in material refractive index. The change is assumed to be linear in nature (one to one). Therefore, u will be replaced with n, the common notation for refractive index.

3. ANALYSIS

Two different materials combinations were examined for this paper: a two-material and a three-material system were examined. One should keep in mind that the "materials" considered here are fictitious, described only be a refractive index at a single wavelength. Examining more realistic materials in a more realistic context was differed to future work. First the two-material system was chosen as it is a common approach to producing GRIN optics. Two glasses are brought together, heated and diffused to form a single GRIN optic with the index profile resulting from Fick's Second Law. A three-material system was considered because relatively new concepts in diffused

GRIN optics no longer are restricted to two materials. One should note that three materials were chosen arbitrarily as a starting point for this effort. The state of the art does not limit us to three. Future analyses will consider more than three.

The radial index profile for a GRIN optic is often reported in literature as an even order polynomial in radial position; in this paper, *x*. For example: [6,7]

$$N(x) = N_{00}\left(1 - \frac{N_{01}}{2}x^2 - \frac{N_{01}}{4}x^4 - \cdots\right) \tag{10}$$

If Equation 10 is used to describe a positive power element, *N(x)* is the gradient index profile, N_{00} is the maximum refractive index for the material system, and N_{01} is change in refractive index imparted by the material system, often referred to as Δn. Since even order polynomials seem to be the foundation of the radial GRIN refractive index profile, it seems most appropriate to analyze the profiles resulting from computational diffusion in terms of polynomials to determine how close to ideal they can be. One should note, this is a significant departure from the conic sections, noted earlier, that seem to be more common in optical engineering.

3.1 The two-material system

For the first examination of a computationally diffused index gradients, a two material system was chosen to have high index (n_{high}) of 2.0 and a low index (n_{low}) of 1.4 for a Δn of 0.6. One should keep in mind that this represents a material system with an unusually large Δn, larger than what is commonly available. *Δn's* of less than 0.1 are common. However, the numbers were chosen to amplify any subtle issues that might have been masked with a smaller Δn. The results of the computational diffusion appear in Figure 2. In this figure we see the starting index profile, indicated by the red line, step function, and the final diffused profile, the blue curve. A classic, x^2 GRIN profile (yellow line) is also plotted.

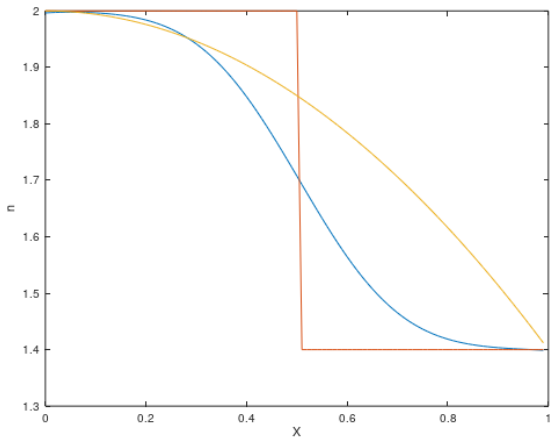


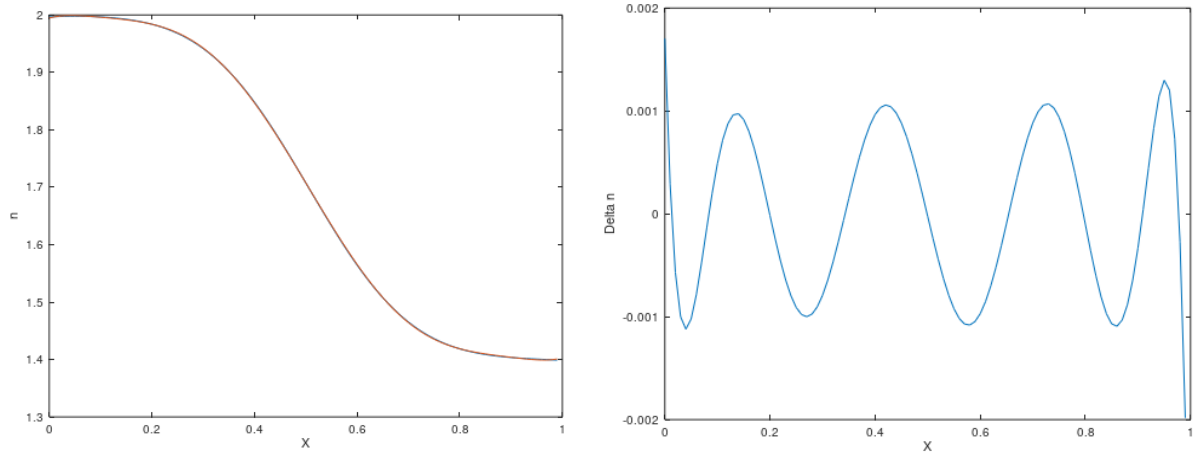
Figure 2. The two-material system. Refractive index profile before diffusion (red line) and after diffusion (blue line) plotted as a function of position against the x^2 radial profile assumed for a radial GRIN optic (yellow line).

It is clear to see from Figure 2 that there is a significant difference between the diffused and the x^2 profiles. Therefore, higher order polynomial statistical curve fits were applied to model the diffused gradient. A fourth order fit was employed first and reported here. For the two-material system, statistical fitting yielded:

$$0.42110x^4 + 2.04541x^3 - 3.81543x^2 + 0.82805x + 1.96537 \tag{11}$$

A correlation coefficient (R^2) was calculated to be 0.9959 to assess "goodness" of fit. From Equation 11, one can see surprisingly large coefficients for the odd order terms in the polynomial. This was unexpected. To explore the

goodness of the fit in greater detail, the diffused curve and its statistical fit were plotted together. In addition, the difference between fit and diffused curve was calculated. Both are plotted in Figure 3 A and B respectively. While the fit seems to follow the diffused curve quite closely, one can see that there are still significant refractive index differences between the two, on the order of +/- 0.001.

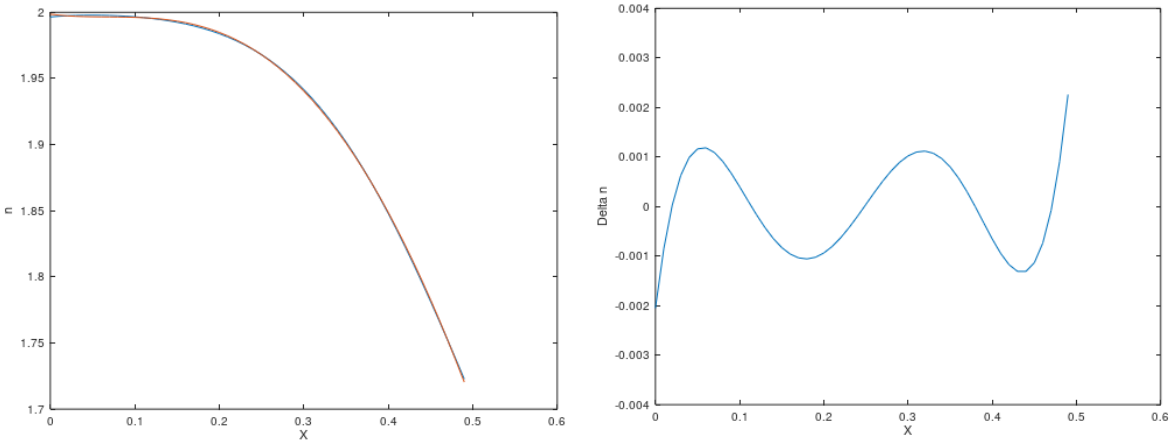


A B

Figure 3. (A) Index profile for the diffused two-material system (blue line) plotted with a statistical curve fit (red line) as a function of position. (B) The difference in refractive index between the diffused profile and the statistical fit plotted as a function of position.

It is possible that issues arise when attempting to fit to the entire diffused profile. The inflection the curve experiences as x exceeds 0.7 may be problematic. It is also possible that part of the profile could be discarded during manufacturing and yield a more parabolic and desirable GRIN profile. To examine this, a statistical fit was performed on the data falling between $0 < x < 0.5$. This zone was chosen to avoid an anticipated inflection point in the index profile that could become significant when $x > 0.5$. This statistical fitting yielded:

$$3.801902x^4 - 6.257491x^3 + 1.159575x^2 - 0.080675x + 1.998546 \quad (12)$$



A B

Figure 4. (A) Index profile for the diffused two-material system (blue line) plotted with a statistical curve fit (red line) as a function of position (half profile). (B) The difference in refractive index between the diffused profile and the statistical fit plotted as a function of position.

R^2 was calculated to be 0.99988. This is better than the fit for the full $0 < x < 1$ profile. However, the odd order terms still seem significant, especially x^3. To further examine the restricted profile, the diffused curve and its statistical fit were plotted together along with the difference between the two and displayed in Figure *4*. Unfortunately, the differences are still on the order of +/- 0.001 or larger. So while limiting the range of x reduced the number of zero crossings, improving R^2, the magnitude of the differences increased, making the gradient less desirable from an optical engineering standpoint.

3.2. Three-material system

To examine a more complex system, enabled by advances in material science and the desire to make larger clear aperture GRIN optics, a three material system was considered. This system was chosen to have an n_{high} of 2.2, a middle refractive index (n_{mid}) of 2.0, and an n_{low} of 1.4 yielding an Δn of 0.8. The results of the computational diffusion appear in Figure 5. In this figure we see the starting index profile, indicated by the red line, a combination of step functions, and the final diffused profile, the blue curve. Again, a classic, x^2 GRIN profile (yellow line) is also plotted. It should be noted that the magnitudes of n_{high} and n_{mid} and the widths of these two bands were chosen to yield a diffused profile closer to the x^2 classic profile then could be achieved in the two-material system. This improvement is noticeable in Figure 5.

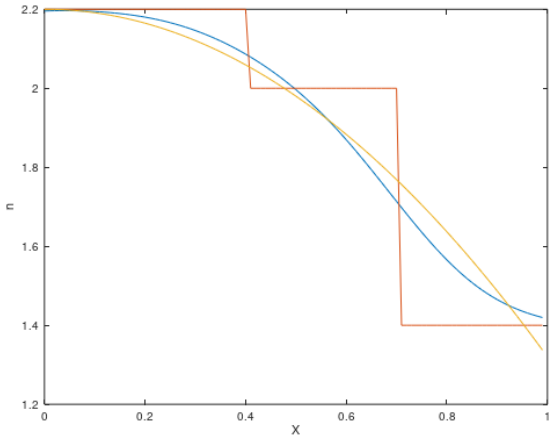
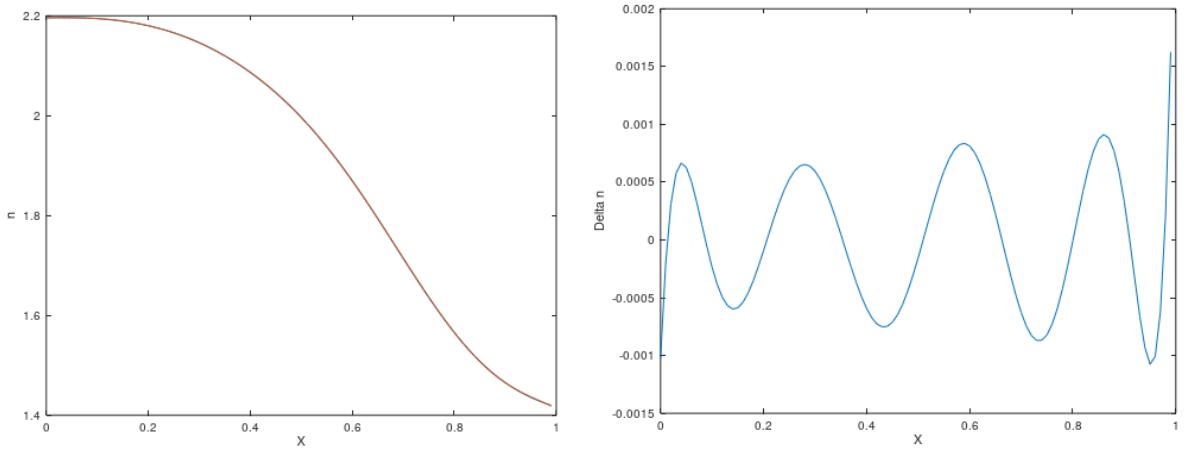


Figure 5. The three-material system. Refractive index profile before diffusion (red line) and after diffusion (blue line) plotted as a function of position against the x^2 radial profile assumed for a radial GRIN optic (yellow line).

As in the two-material system, a fourth order statistical curve fit was applied to the diffused gradient, yielding:

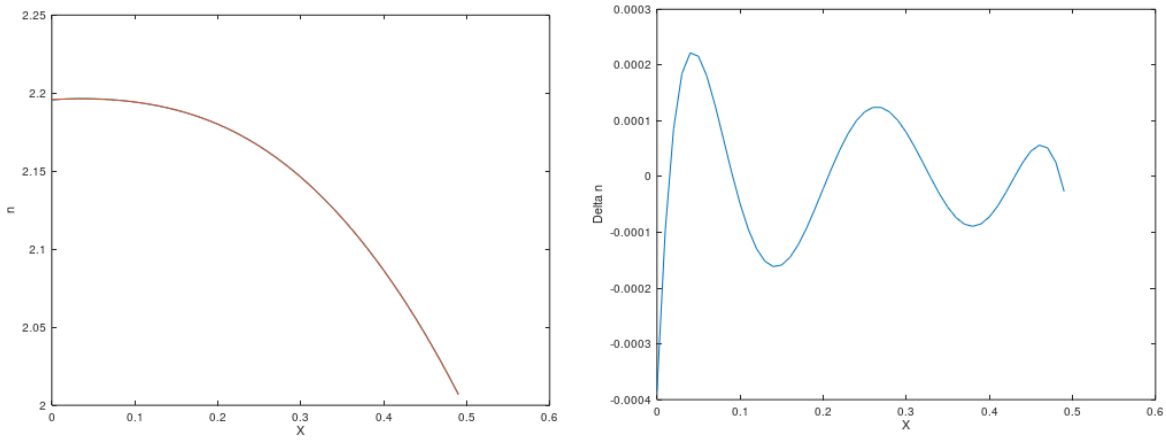
$$3.80329x^4 - 6.13173x^3 + 1.83493x^2 - 0.28397x + 2.20529 \qquad (13)$$

R^2 was calculated to be 0.9998. Again, this is a noticeable improvement over the two-material system. But again, the magnitude of the coefficients of the odd order terms were larger than anticipated, in particular the x^3 term. The diffused curve and its statistical fit were plotted together. In addition, the difference between fit and diffused curve was calculated and plotted, yielding Figure 6 A and B respectively. The fit seems to follow the diffused curve quite closely, but again, there are still significant refractive index differences between the two, on the order of +/- 0.001. But for some of the profile, $x < 0.5$, the differences are less than 0.001. This warrants a closer look.



A B

Figure 6. (A) Index profile for the diffused three-material system (blue line) plotted with a statistical curve fit (red line) as a function of position. (B) The difference in refractive index between the diffused profile and the statistical fit plotted as a function of position.



A B

Figure 7. (A) Index profile for the diffused three-material system (blue line) plotted with a statistical curve fit (red line) as a function of position (half profile). (B) The difference in refractive index between the diffused profile and the statistical fit plotted as a function of position.

To examine this, a statistical fit was performed on the data falling between $0 < x < 0.5$. Unlike the two-materila system, this zone included an anticipated inflection point in the index profile (at $x = 0.4$) that could become significant. This statistical fitting yielded:

$$0.513398x^4 - 1.500658x^3 - 0.215572x^2 + 0.019840x + 2.195946 \qquad (14)$$

R^2 was calculated to be 0.99999. This is better than the fit for the full $0 < x < 1$ profile. The inclusion of the inflection point seemed to have little impact in this case. However, the odd order terms still seem significant, especially x^3. To further examine the restricted profile, the diffused curve and its statistical fit were plotted together along with the difference between the two and displayed in Figure 7. One should note that in Figure 7 B, the differences shrink considerably, on the order of +/- 0.0002. It is believed that theses index changes are small enough to accommodate in an optical design.

4. DISCUSSION

There is a very real possibility that the diffused gradients simply do not conform to conic sections and cannot be made to conform to them. The magnitude of the x3 terms seems to indicate that the classic, even order GRIN should be difficult to achieve by diffusion without some intervention. This may be a significant issue hampering the adoption of diffused index gradients in optical design. Polynomial fits can be used to describe index gradients. But in simpler cases, such as a two-material system, there seems to always be a small index residual on the order of 0.001 or more. It is believed that such differences are significant enough to significantly hamper a design, especially in complex, long focal length optical systems. [8] However, it may be possible to engineer your materials prior diffusion to improve performance. This treatment of the three-material system supports this possibility. Greater study of the concept should be undertaken.

Since implementing index profiles that behave like and can be described by conic sections may be more difficult than desirable, one must explore possibilities that can be pursued using some form of polynomial expression. One such concept is that of freeform optics. Traditionally, freeform surfaces are described using some kind of polynomial fit, be it in terms of x and y position coordinates, Zernike polynomials, or some other more exotic expression. Transmissive, refractive freeform optics may be an appropriate application of diffused gradients since the optics will necessarily have to be described to great precision with high-order polynomials. The design strategy, employing a large number of degrees of freedom, could work with the substrate, not against it. Perhaps it is unlikely to develop a physical instantiation of this concept. But it should be explored from a theoretical point of view.

5. CONCLUSION AND FUTURE WORK

Diffused index profiles seem to not match a typical conic section. Deviations from ideal tend to be on the order of 0.001 in refractive index, significantly hampering their applicability in an optical system. The addition of a large number of curve fit terms did not seem to help the quality of the fit considerably in most cases examined. This is possibly due to the fact that when calculated, correlation coefficients were found to be in the range of 0.9999 for fits using four terms or more. Statistically speaking, there is already a high degree of agreement between the calculated diffused index profile and the statistical curve fit. However, the agreement needs to be better to ensure the desired optical performance.

Literature indicated that such refractive index changes would negatively impact imaging performance in general. However, literature also indicated that small index changes in an axial gradient could be insignificant. If so, diffusion might be more appropriate for forming axial GRIN optics. However, for radial gradients, the impact was far more significant.

It might be possible to calculate an index profile from which to begin diffusion that will enable one to arrive at or get closer to a better behaved conic section. However, the computational techniques used in this paper assumed that time would always be positive. Starting from an ideal, diffused profile and working backwards violates this assumption. Therefore, another computational technique must be found that does not rely on a positive time assumption. Once found, it starting homogenous profiles will have to be calculated and examined for manufacturability.

The impact of these gradients in terms of lens modulation transfer function (MTF) still needs to be explored. This paper illustrates index errors or profile differences that need to be compensated for in an optical design. The impact of those issues in terms image quality parameters common in optical engineering remains incomplete. An understanding of the optical performance impact of this issues remains the subject of another paper.

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Peter L Marasco joined the Air Force Research Laboratory in 1991 as a civilian research physicist. In his 24 years with AFRL, he led or significantly contributed to research and development in many technology areas related to optical and electro-optical engineering including night vision, imaging technology in all major electro-optical bands and infrared atmospheric windows, multispectral imaging, body-mounted sensing, display technology (helmet- and head-mounted displays, microdisplays, and 3 dimensional visualization), aerospace transparency characterization, optical scattering, and visual performance testing. Dr. Marasco is currently the Technology Advisor for Electro-Optical Sensing in the Air Force Research Laboratory, Sensors Directorate, Multispectral Sensing and Detection Division. He holds degrees in optical and electro-optical engineering from the University of Rochester, the University of Arizona, and the University of Dayton. His current work focuses primarily technologies for surveillance and target recognition with an emphasis on reducing imaging system volume, weight, power consumption, and cost. In his career, he authored 38 papers, holds 4 patents, and has been a member of SPIE since 1994.