Application of variational calculus for optimization of optic gradient coatings

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Abstract. The design optimization for n-graded optic coatings based on variational calculus is discussed. In order to exemplify the approach, the Lagrange problem for minimizing refraction is stated and solved. The refraction law is generalized for alteration of the continuous refraction index. To solve problems of reflection minimization, an integro-differential equation of retarding potentials is proposed to use as a condition to the nonholonomic Lagrange problem.

1. Introduction
Features of multilayered gradient optic coatings (with a smooth law of variation in the refractive index inside every layer – “n-graded”) are investigated in [1–7] to produce the effective coatings for photonics such as mirrors, rugate filters and, more generally, optic metamaterials. However, such coatings are conventionally fabricated as piecewise multilayer coatings with the constant refractive index inside every layer [8]. Moreover, an optimality of these piecewise structures is proved using the optimal control theory (OCT) [9]. Nevertheless, the piecewise coatings show excellent optic characteristics only in the narrow ranges of wavelengths and incident angles. Besides, the sharp stepwise variation of refraction index badly influences the mechanical and thermal ware-resistance and laser toughness [6]. A calculation algorithm for structures of any-smoothness degree also based on OCT is proposed in [10]. The solution by this algorithm still implies the use of the piecewise law for the respective order derivative of the refractive index. Whereas there exists quite a lot of problems, in which solutions may be an infinitely differentiable function, for example, Fourier series. It is applied both to reflection minimization problems mentioned in [7] and to those associated with the ray deflection from obstacles. In such problems it is convenient to use a classic calculus of variation – Lagrange problem with nonholonomic constraints [11] providing smooth solutions.

Various types of smooth laws of variation in the refractive index (monotonic, alternating and hybrid), intended to solve the listed reflection problems (figure 1), as well as technologies for deposition of coatings with the (calculated) preset properties are discussed in [7]. As for the monotonic variation laws, it is noted that J. S. Rayleigh, analyzing the light transmission through the atmosphere, showed that the n-graded layers possess antireflection properties in a wide wavelength range.

However, the main problem for optimizing antireflection properties is a definition for the refraction index itself: On the one hand, it is strictly defined “in the given point” as a ratio of speeds of light in this point and in the vacuum. On the other hand, one frequently uses the relative refractive index – the ratio of light speeds in areas adjacent to this point. These two definitions coincide only at the medium-vacuum interface where \( n_1=1 \rightarrow n_2/m_1=n_2 \). If the speed of light or the refractive index is continuous “in
the given point”, no reflection or refraction takes place. In the general case we can speak only about index change in this point \( dn(\vec{x}) \) with the argument increment \( d\vec{r} \): \( dn(\vec{x}) = (\vec{n}, d\vec{r}) \). Thus, first of all it is necessary to generalize these two laws – of refraction and reflection – in case of smooth change in the light speed.

Various methods for calculation of the refractive index as a function of the coating depth have been developed to minimize reflection. However, they all involve replacing the continuous distribution with the piecewise one. B. G. Bovard, the author of [2] admits: “This might sound disadvantageous but one should remember that the computation of the optical properties of any variable index thin film requires that the layer be approximated by thin homogeneous layers”. As for refraction, Fermat’s principle describes the deflection of a ray even with the continuous law. The question arises: is it possible to evolve the refraction and reflection laws for the continuous \( n(z) \) based on this fundamental principle and thus solve different optimization problems using variational calculus methods? It should be noted at once that the Fermat principle does not contain any assumptions about the light nature and, consequently, its quantitative characteristics, the wavelength in particular. Therefore, a spatial scale is not defined and must be introduced in the problem “forcibly”.

2. Statement of Lagrange Problem
The variational problem of refraction minimization can be set in the following way: Figure of Merit (FOM)

\[
FOM = \int_0^5 (y_1'(x) - \varepsilon)^2 dx \to \text{min} ,
\]

where \( y_1'(x) \) is a tangent of ray trajectory \( y(x) \) in the XY plane (the light motion is plane), \( \varepsilon \) is an angle of incidence (between the normal and incident ray), meaning the refraction minimization at the given refractive index at the interfaces. If instead of (1) one uses \( \int_0^5 (y(x) - f(x))^2 dx \to \text{min} \) with the known function \( f(x) \) and perhaps undefined \( L \), as FOM, then it is the problem of the ray deflection from the obstacle of the given shape. From the calculation viewpoint, these problems do not differ significantly but the last one has more important applications.

We forcibly introduce the spatial scale as shown in figure 1: 1 \( \mu m = 5 \) arbitrary units (au). The initial value of refraction index at the external coating interface is equal to 1.6. The final one at the 1 \( \mu m \) depth is 2.4.

The additional condition is the Euler equation of the Fermat principle [8]

\[
\frac{d}{dx} \left( \frac{n(x)y_1'(x)}{(1+y_1'^2(x))} \right) = 0
\]

To reduce the problem to the canonic form, denote \( y',(x)=y_1(x) \), \( n(x)=y_2(x) \) and the Lagrange
undetermined multiplier $\mu(x) = y_3(x)$.

The equation (1) may be rewritten as

$$y'_1 (x) \cdot y_2 (x) + y_3 (x) \cdot \left(1 + y_2^2 (x)\right) \cdot y'_2 (x) = 0$$  \hspace{1cm} (3)

Thus, the auxiliary Lagrangian has the following view:

$$L(x) = (y_1 (x) - \varepsilon)^2 + y_3 (x) \left[y'_1 (x) \cdot y_2 (x) + y_1 (x) \cdot \left(1 + y_2^2 (x)\right) \cdot y'_2 (x)\right]$$  \hspace{1cm} (4)

So, the whole system of Euler equations is (to shorten equation, we omit the argument, (x)):

$$\begin{align*}
\left\{ \begin{array}{c}
y'_3 = y_2^{-1} \left[2 (y_1 - \varepsilon) + 3 y_1 y_3 y'_2 \right], y_3 (0) = y_{30}, \\
y'_2 = - \frac{3 y'_3 y_1}{1+y_2^2}, \\
y'_1 = - \frac{y'_3 y_1}{y_1 (1+y_2^2)}, \\
y_1 (0) = \varepsilon, \\
y_2 (0) = 1.6
\end{array} \right. $$  \hspace{1cm} (5)

The initial condition $y_{30}$ can be found from the condition $y_2 (5) = 2.4$. Note that the 3rd equation of the system (4) is nothing but the refraction law with continuous variation of refractive index. In fact, the sine of the angle between the refracted ray and the normal is calculated from the equality:

$$\sqrt{\frac{n_1}{n_3}} \cdot \sqrt{\frac{n_2}{n_3}} = 1 + \frac{\varepsilon^2}{n_3}.$$  \hspace{1cm} (6)

Hence, the refraction law in the general case is just the same as in the case of the sharp interface with the natural substitution of the “angle of refraction” with the “angle increment” or “sine increment”.

This 3rd equation (5) or refraction law in its continuous form allows us to have the explicit relation between $y_1$ and $y_2$ or the ray trajectory tangent and the refraction index:

$$\ln \left(\frac{n(x)}{n(x) + n(x) dx}\right) = 1 - \frac{n(x)}{n(x)} dx \Rightarrow \frac{y'_1}{y_1 \sqrt{1+y_2^2}} = - \frac{y'_2}{y_2} = - \left(\ln (n(x))^'\right) = \frac{(\sin(\varepsilon))^'}{y_2 \sin(\varepsilon)} = (\ln(\sin(\varepsilon)))'. $$  \hspace{1cm} (7)

Hence, we have solution in the form of an implicit function (figure 2):
\[ \int_{1.6}^{y} \frac{2y^3(1-\varepsilon(A^2y^2-1))}{3B(A^2y^2-1)(y^2-A^2y^2-1)} \, dy = x, \]  
but it may be calculated only if \( \varepsilon \) in (10) is more than \( \varepsilon_0 \) – the real initial angle due to singularity. It is because the optimal solution tends to stepwise function being equal to 1.6 in the range \( x \in [0,5] \) and becoming equal to 2.4 in final point 5. Just as commonsense and OCT predict! For instance, if \( \varepsilon=1 \) the solution (9) in MathCad15 results in \( C=160.528 \). The Lagrange multiplier turns out to be practically constant varying from 83.9 to 84.6 in the integration interval \([0,5] \) at \( \varepsilon=0.05 \) rad.

3. Results and discussion

The solutions compared with different approximations are shown in figure 2 (\( \varepsilon=1 \)) and 3 (\( \varepsilon=0.0505 \)). Uppermost, note the decrease in the tangent with an increase of refractive index (from 0.05 to 0.033): the denser optic medium acts like a focusing lens.

![Figure 2 and 3](image-url)

Comparing this “optimal” FOM=\( K_5=5.108 \cdot 10^4 \) with the calculated from the relation (6) \( y_1(x) \) for sinusoidal \( n_1(x)=1.6+0.8 \cdot \text{Sin}((\pi/10) \cdot x) \), linear \( n_2(x)=1.6+(2.4/5) \cdot x \) and “cubic-sine” \( n_3(x)=1.6+0.8 \cdot \text{Sin}((\pi/10) \cdot x) \) approximations one makes sure in the absence of real optimality of the calculated one. The “sinusoidal FOM” \( K_5=7.822 \cdot 10^4 \) and the “linear” \( K_5=5.619 \cdot 10^4 \) are larger than the “optimal” one. But “cubic-sine” approximation \( K_5=4.979 \cdot 10^4 \) is less. Reducing the initial value \( \varepsilon_0 \) consequently to minimal possible values we see the decrease of the “optimal” FOM: 0.06 - 4.045 \cdot 10^{-4} that is already less than \( K_4=0.055 - 3.583 \cdot 10^{-4} ; 0.052 - 2.965 \cdot 10^{-4} \) that is already less than 7th power sinusoidal approximation (fig. 3); 0.0501 – 1.838 \cdot 10^{-5}. The tendency is obvious.

However, the final angle values are equal for any \( \varepsilon_0 \): \( \theta_2(4) = \Theta_1(5) = \Theta_2(5) = \Theta_3(5) = 0.033 = 0.05 = (1.6/2.4)! \) It means that the refraction law (Snell’s law) holds globally. In other words, the beam trajectory tangent is the potential function of the refractive index that is depends only upon its values in separated points according to the Snell’s law. At the same time the generalized refraction law (6) holds locally. We could say that this fact is the consequence of the space scale absence in the Fermat principle marked above. These “5 arbitrary units” may be 0.5 nm as well 1 μm or 1 m so that the interface or boundary between two adjacent areas is quite “a conditional idea from the light beam viewpoint”.

But what about reflection? It is well known that \( \lambda/4 \) coating is the really antireflection one. And the space scale is obviously denoted by the \( \lambda \) value. Whereas the \( n \)-graded coating shown in fig. 1 [6] is declared to be “antireflecting” in a rather wide \( \lambda \) range. The form of the optimal solution (the stepwise function in the limit \( \varepsilon \rightarrow \varepsilon_0 \)) obtained above is far from similar to this one. It means that this “optimal
solution” is not so optimal from the reflection point of view. In other words, these are quite different problems, though related through the Fermat principle but only in terms of statement on equality of angles of incidence and reflection. However, intensities of this reflected ray and of the refracted one remain uncertain. To calculate them, one has to use a light model, e.g. the wave model that means exploiting the Fresnel formulas. Still, they are based on the plane wave approximation that significantly limits their application. In order to overcome this limitation, we should apply the Huygens principle that is to use the integro-differential equation with retarded potentials as nonholonomic condition of the Lagrange problem [8, chapter 2], but it is the subject of the other much more complex research.

![Figure 3](image.png)

**Figure 3.** (ε=0.052) Refraction index vs coating thickness: y – the optimal one (black), n1(ξ) – the sinusoidal approximation (blue), n2(ξ) – the linear approximation (green), n3(ξ) – the “7th power-sine” approximation (red) (a) Light beam tangents vs coating thickness: θ(y) – the optimal one (black), Θ1(ξ) – the sinusoidal approximation (blue), Θ2(ξ) – the linear approximation (green), Θ3(ξ) – the “7th power -sine” approximation (red) (b).

4. Conclusions

Actual algorithms for optimizing the n-graded coatings based on calculation of characteristic matrices are complex and self-contradictory as applied to variation of the continuous refractive index. The OCT application cannot give infinitely smooth solutions either. In order to overcome these contradictions, the classic variational calculus, i.e. the Lagrange problem without nonholonomic constraints is investigated. The Euler equations of the Fermat principle are utilized as these constraints in the case of refraction or deflection from a given trajectory minimization. The simplest example described above proves the absence of strict smooth optimal solutions and tendency to stepwise functions. However, this example generalizes the refraction law in case of continuous change in the speed of light. This generalized refraction law holds locally, whereas the Snell’s law holds globally due to the lack of the space scale in the Fermat principle.

As for optimization of antireflection properties, the use of this principle is insufficient due to the lack of ray quantitative characteristics. In this case the integro-differential equation of retarded potentials must be introduced as an auxiliary condition.

References

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