Numerical methods to compute optical errors due to stress birefringence

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ABSTRACT

A method to compute polarization changes and wavefront error due to mechanical stress in transmissive optical elements is presented. In general, stress produces an anisotropic and inhomogeneous optical medium where the magnitude and direction of the indices of refraction vary at every point. Jones calculus is used to incrementally evaluate the effects of stress for a grid of rays traced through a three-dimensional finite element stress field. For each ray, a system Jones matrix is computed representing the effective retarder properties of the stress path. The magnitude of birefringence, orientation, and ellipticity may then be derived for a grid of rays over the optical aperture. In addition, the stress-induced index changes generate wavefront error. Thus wavefront maps may be computed across the optical aperture. This method to compute the optical errors due to mechanical stress has been implemented in the optomechanical analysis software package *SigFit*. Birefringence and orientation data as computed by *SigFit* for arbitrary three-dimensional stress states may be output as CODE V® stress birefringence interferogram files to evaluate the effects of stress on optical performance.

Keywords: mechanical stress, crystalline materials, uniaxial, finite element analysis, optical design, polarization, wavefront error, CODE V, *SigFit*

1. INTRODUCTION

Mechanical stress modifies the optical properties of transmissive materials by changing the indices of refraction. For a general three-dimensional non-uniform state of stress, optical properties may become anisotropic and inhomogeneous. This results in wavefront error and polarization changes in an optical system. Optical elements may be subject to mechanical stress due to environmental effects during standard operation. Uniform temperature changes and thermal gradients cause stress due to CTE mismatches and non-uniform expansion and contraction. Gravity and dynamic loads also impart stress to an optical system. Stress birefringence is an issue for many types of optical systems including systems for optical lithography, data storage, high-energy lasers, LCD projectors, and telecommunications. For these types of optical systems, modeling techniques help enable design trades and evaluate optical performance as a function of glass type and mounting methods.

2. NATURAL BIREFRINGENCE

In general, two plane polarized waves travel along paths with different indices of refraction through an anisotropic material; this property is referred to as birefringence. The refractive indices of a given medium are defined by the direction of the wave normal and the second-order tensor known as the dielectric impermeability tensor, B_{ij}:

$$B_{ij} = \begin{bmatrix} B_{11} & B_{12} & B_{13} \\ B_{12} & B_{22} & B_{23} \\ B_{13} & B_{23} & B_{33} \end{bmatrix} . \tag{2.1}$$

The dielectric impermeability tensor may be expressed in the following form:

$$\sum_{ij} B_{ij} x_i x_j = 1 \quad \rightarrow \quad B_{11}x_1^2 + B_{22}x_2^2 + B_{33}x_3^2 + 2B_{12}x_1x_2 + 2B_{23}x_2x_3 + 2B_{13}x_1x_3 = 1, \tag{2.2}$$

which is the general equation for a second-degree surface or quadric where B_{ij} represents the coefficients of the surface. The quadric representation of the dielectric impermeability tensor completely describes the optical properties of a material and is known as the index ellipsoid (also known as the ellipsoid of wave normals, or optical indicatrix) as shown in Figure 1.

The ellipsoid defines all orientations of the second order tensor including the principal axes, which reduces the mathematical representation of the quadric surface to the following:

$$B_{11}x_1^2 + B_{22}x_2^2 + B_{33}x_3^2 = 1, \tag{2.3}$$

where x_1, x_2, and x_3 are the principal axes of the ellipsoid. Geometrically, the index ellipsoid defines the refractive indices of the optical material by its semi-axes. Mathematically, the refractive indices of a material are computed as the square root of the reciprocal of the dielectric impermeability along any principal axis. The index ellipsoid expressed along principal axes using the refraction indices as the coefficients yields:

$$\frac{x_1^2}{n_1^2} + \frac{x_2^2}{n_2^2} + \frac{x_3^2}{n_3^2} = 1 \text{ where } n_1 = \sqrt{\frac{1}{B_{11}}};\ n_2 = \sqrt{\frac{1}{B_{22}}};\ n_3 = \sqrt{\frac{1}{B_{33}}}. \tag{2.4}$$

Although the variation in the refractive index with direction is defined by a second order (dielectric impermeability) tensor, the refractive index itself is not a tensor. For an isotropic optical material, $n_1 = n_2 = n_3$, there exists no birefringence, and the index ellipsoid degenerates to a sphere**.** In general, cubic crystals exhibit isotropic optical properties. For hexagonal, tetragonal, and trigonal crystals, $n_1 = n_2$? n_3, and the index ellipsoid is an ellipsoid of revolution whose principal axis is known as the optical axis. The optical axis defines the direction for which a wave traveling parallel to this axis will have no birefringence, and the material is considered uniaxial. For orthorhombic, monoclinic, and triclinic crystals, the index ellipsoid is a triaxial ellipsoid, and there exists two optical axes for which there is no birefringence. These crystals are considered biaxial. The index ellipsoids for isotropic, uniaxial, and biaxial materials are shown in Figure 2.

3. STRESS BIREFRINGENCE

The application of mechanical stress to an optical substrate modifies the optical properties of a material by modifying the dielectric impermeability tensor. Thus, a homogeneous and isotropic optical material subject to mechanical stress will become optically anisotropic. This phenomenon is known as the photoelastic effect or stress birefringence. The changes in the indices of refraction are due to the effects of stress imparting changes in the dielectric impermeability tensor that alter the size, shape, and orientation of the index ellipsoid. Changes in the dielectric impermeability tensor due to the application of mechanical stress are given by the following fourth rank tensor transformation:

$$\Delta B_{ij} = B_{ij} - B_{ij}^0 = q_{ijkl} s_{kl} \tag{3.1}$$

where q is the stress-optical coefficient matrix, and s is the stress tensor. Changes in the dielectric impermeability tensor due to the photoelastic effect may also be defined using mechanical strain as expressed below:

$$\Delta B_{ij} = p_{ijrs} e_{rs} , \tag{3.2}$$

where p is the elasto-optical coefficient, and ε is the strain tensor.

The changes in the dielectric impermeability tensor due to stress and strain are small and are considered perturbations to the index ellipsoid. Thus, a new dielectric impermeability tensor is created in the presence of a mechanical load that is no longer diagonal as defined by the principal dielectric axes. In general, changes in the dielectric impermeability tensor due to the effects of stress or strain may be superimposed on the natural birefringence for all crystal systems. The changes in the index of refraction are, therefore, expressed as additive terms of the coefficients of the index ellipsoid equation as shown below:

$$B_{11}x_1^2 + B_{22}x_2^2 + B_{33}x_3^2 = 1 \rightarrow B_{11}x_1^2 + B_{22}x_2^2 + B_{33}x_3^2 + 2B_{12}x_1x_2 + 2B_{23}x_2x_3 + 2B_{13}x_1x_3 = 1 . \tag{3.3}$$

Due to symmetry, the 3x3 matrices representing the stress and the dielectric impermeability tensors may be expressed using contracted indexes or the Voigt notation. The dielectric impermeability and stress tensors become 6×1 vectors as shown below:

$$B = [B_1 \quad B_2 \quad B_3 \quad B_4 \quad B_5 \quad B_6]^T \quad \text{and} \quad s = [s_1 \quad s_2 \quad s_3 \quad s_4 \quad s_5 \quad s_6]^T . \tag{3.4}$$

This results in the following relationship between the applied stress and the dielectric impermeability:

$$\Delta B_m = q_{mn} s_m . \tag{3.5}$$

The photoelastic effect is a function of the crystalline structure of the material. A different stress-optical coefficient matrix represents each crystal class. For example, under a uniform state of stress, isotropic materials become uniaxial. Conversely, various classes of cubic crystals that nominally exhibit isotropic properties may become biaxial. Consider the effect that stress has on the cubic crystal calcium fluoride under a uniaxial stress acting along the [100] axis. Nominally, the material is isotropic (this excludes the intrinsic birefringence of the material at ultraviolet wavelengths) and the index ellipsoid is expressed as:

$$B_0x_1^2 + B_0x_2^2 + B_0x_3^2 = 1 . \tag{3.6}$$

The change in the dielectric impermeability tensor is expressed by the following:

$$\begin{Bmatrix} \Delta B_1 \\ \Delta B_2 \\ \Delta B_3 \\ \Delta B_4 \\ \Delta B_5 \\ \Delta B_6 \end{Bmatrix} = \begin{Bmatrix} B_1 - B_0 \\ B_2 - B_0 \\ B_3 - B_0 \\ B_4 \\ B_5 \\ B_6 \end{Bmatrix} = \begin{bmatrix} q_{11} & q_{12} & q_{12} & 0 & 0 & 0 \\ q_{12} & q_{11} & q_{12} & 0 & 0 & 0 \\ q_{12} & q_{12} & q_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & q_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & q_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & q_{44} \end{bmatrix} \begin{Bmatrix} s_1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} = \begin{Bmatrix} q_{11}s_1 \\ q_{12}s_1 \\ q_{12}s_1 \\ 0 \\ 0 \\ 0 \end{Bmatrix} . \tag{3.7}$$

This yields the updated index ellipsoid, expressed as:

$$B_1x_1^2 + B_2x_2^2 + B_3x_3^2 = 1 . \tag{3.8}$$

The index ellipsoid changed shape, but the principal axes stayed the same. Thus, the indices of refraction may be computed as:

$$n_1 = \sqrt{\frac{1}{B_1}};\; n_2 = \sqrt{\frac{1}{B_2}};\; n_3 = \sqrt{\frac{1}{B_3}}\,. \tag{3.9}$$

The changes in the indices of refraction, Δn, may be computed by differentiating ΔB and assuming that the changes in index are comparatively small, which yields the following:

$$\Delta n = -\frac{1}{2} n_0^3 \Delta B \;\rightarrow\; \Delta n_1 = -\frac{1}{2} n_0^3 q_{11} s_1,\;\; \Delta n_2 = -\frac{1}{2} n_0^3 q_{12} s_1,\;\; \Delta n_3 = -\frac{1}{2} n_0^3 q_{12} s_1\,. \tag{3.10}$$

Since $\Delta n_2 = \Delta n_3$ the impact of the stress is to create a uniaxial crystal.

In general, the changes in the optical properties of the material are reflected in the updated dielectric impermeability tensor by using the appropriate stress-optical coefficient matrix. Typically, the stress-optical coefficient matrix is defined along the axes of a crystal. Coordinate transformations are required to orient the matrix in another direction. For a given wave normal traversing the optical medium, the principal indices of refraction in the plane defined by the wave normal may be geometrically constructed using the index ellipsoid representation. This is shown for an arbitrary ray passing through a point in Figure 3. Geometrically, the indices of refraction are computed as the semi-axes of the ellipse, which is normal to the ray direction and centered at the origin of the index ellipsoid.

4. MODELING STRESS BIREFRINGENCE

A technique is described in this section to account for the change in the optical properties for a ray traced through a three-dimensionally spatially varying stress field of an optical element. The effect of the stress distribution is analogous to a spatially varying optical retarder. Hence, a Jones matrix whose retarder properties are derived - namely the magnitude of birefringence, orientation, and ellipticity, may be used to represent the effect of the stress distribution. This is repeated for a grid of rays through the optical element.

This method requires a three-dimensional representation of the stress field typical of finite element analysis output. Thus at discrete points within the optical element (we assume at finite element node points), the stress tensor, as expressed below, is known.

$$s = [s_1 \quad s_2 \quad s_3 \quad s_4 \quad s_5 \quad s_6]^T \tag{4.1}$$

The change in the dielectric impermeability tensor for each node in the finite element model is computed using equation 3.5.

$$\Delta B_m = q_{mn} s_m \qquad \rightarrow \qquad \Delta B = [\Delta B_1 \quad \Delta B_2 \quad \Delta B_3 \quad \Delta B_4 \quad \Delta B_5 \quad \Delta B_6]^T \tag{4.2}$$

A grid of rays is then 'traced' through the perturbed optical model. For a given ray direction that is 'traveling' from a front surface to the rear surface, it is the refractive indices in the plane normal to the ray direction that are desired. A coordinate transformation is then performed to orient one of the axes of ΔB tensor to be perpendicular to the ray direction. (In our case, a transformation is performed to orient the z-axis to be parallel with the ray direction). This yields the transformed ΔB tensor

$$\Delta B' = [\Delta B'_1 \quad \Delta B'_2 \quad \Delta B'_3 \quad \Delta B'_4 \quad \Delta B'_5 \quad \Delta B'_6]^T \tag{4.3}$$

Next, the principal ΔB values and the rotation angle, γ_{12}, are determined for the plane normal to the ray direction for each increment. This rotation occurs about the z'-axis, which is parallel to the ray direction. The rotation angle is computed as

$$g = \frac{1}{2} \tan^{-1} \frac{2\Delta B'_{12}}{\Delta B'_1 - \Delta B'_2} \tag{4.4}$$

This yields the following ΔB configuration (the cross-term in the x'y'-plane vanishes):

$$\Delta B'' = [\Delta B''_1 \quad \Delta B''_2 \quad \Delta B''_3 \quad 0 \quad \Delta B''_5 \quad \Delta B''_6]^T \tag{4.5}$$

The new coordinate system is defined by x" and y" which define the directions of the in-plane ΔB values, $\Delta B''_1$ and $\Delta B''_2$. (The z"-axis is parallel to both the z'-axis and the ray direction). The principal ΔB directions in the x"y" plane define the directions of the principal indices of refraction. The indices of refraction are given below

$$\Delta n_1 = -\frac{1}{2} n_0^3 \Delta B''_1 \;\;\&\;\; \Delta n_2 = -\frac{1}{2} n_0^3 \Delta B''_2 \tag{4.6}$$

For a non-uniform stress field, the magnitude of the indices of refraction, Δn_1 and Δn_2, and orientation, γ, of the index change vary at every point along the path of the ray path. This is equivalent to the ray traversing a series of uniaxial crystals or a series of crossed waveplates of varying birefringence.

Computing the integrated optical effects of a non-uniform stress distribution is performed by the use of Jones calculus. At incremental points along the ray path, Jones rotation and retarder matrices are defined. The retarder matrix is used to modify the optical phase of the two orthogonal electric field components due to the different indices of refraction in the two directions, Δn_1 and Δn_2. Computationally, the phase is added to each component by the retarder matrix given below:

$$R(d) = \begin{bmatrix} e^{i d_1} & 0 \\ 0 & e^{i d_2} \end{bmatrix} \tag{4.7}$$

where the phase change, expressed in radians, is given by

$$d_1 = \frac{2p\Delta n_1 L}{l} \tag{4.8}$$

$$d_2 = \frac{2p\Delta n_2 L}{l} \tag{4.9}$$

The above phase equations assume the ray distance, L, is in units of wavelengths.

The rotation matrix is used to rotate between the x'y'z' coordinate system and the principal coordinate system x"y"z" and is defined below.

$$R(\gamma) = \begin{bmatrix} \cos\gamma & \sin\gamma \\ -\sin\gamma & \cos\gamma \end{bmatrix} \tag{4.10}$$

A Jones matrix is computed for each incremental stress field, *i*, using the following relationship:

$$M_i = R(\gamma)_i^T R(\delta)_i R(\gamma)_i \tag{4.11}$$

For a ray traveling through a non-uniform stress state, a system level matrix, M_s, is developed by multiplying each incremental matrix, M_i. This is analogous to using Jones calculus to compute the effects of a cascade of optical elements as illustrated in Figure 4.a.

$$M_s = M_i \ldots M_2 M_1 \tag{4.12}$$

The system Jones matrix, M_s, for a given ray defines the integrated effects of the stress field on the optical properties of the material. The magnitude of birefringence, orientation, and ellipticity may be computed from the system Jones matrix. A grid of rays may then be traced to evaluate the effects of stress over the aperture as depicted in Figure 4.b.

An additional effect on optical systems due to mechanical stress is wavefront error. Wavefront error is due not only to surface deformations and mis-positioning (ignored here) but also due to the gross index change caused by the stress field. This may be approximated by averaging the optical path of the two electric field components for each incremental length, L_i, and summed for a given ray path:

$$OPD_i = \left(\frac{\Delta n_1 + \Delta n_2}{2}\right)_i L_i \rightarrow \text{WFE} = \sum_{i=1}^{n} OPD_i \tag{4.13}$$

5. STRESS BIREFRINGENCE OPTICAL DESIGN SOFTWARE TOOLS

Many optical design codes, such as CODE V, offer the ability to model birefringent materials with homogeneous properties, where the birefringence is the same at every point in the material. The difference in the index between orthogonal axes (i.e. birefringence) is specified along with an orientation value. Thus an optical element with a uniform stress distribution may be represented using this approach. However, mechanical stress typically varies in three dimensions within an optical element. The optical design software program CODE V®[1] also offers an approximate technique to model the effects of a spatially varying stress field using interferogram files. Interferogram files represent perturbations in the optical properties due to stress, which are superimposed upon the nominal isotropic or anisotropic properties of the optical medium.

Stress birefringence interferogram files (magnitude and orientation) are based on a linear retarder model and require two sets of data, with each set in a different interferogram file. One data set (or interferogram file) represents the magnitude of birefringence, i.e., the difference in the refractive index between the orthogonal plane wave components expressed in nm/cm. The second interferogram file represents the crystal axis orientation. Stress birefringence interferogram files may be assigned to surfaces in the optical model using Zernike polynomials or a uniform rectangular grid. The use of stress birefringence interferogram files assumes small amounts of stress birefringence such that the ray splitting effect is negligible.

The two stress birefringence interferogram files are attached to the front surface of the optical element to be evaluated. The data represents an average value through the thickness of the lens. For a skew ray traversing the element, the magnitude and orientation is computed as the average value from the point on the interferogram file where the ray enters the front surface and the point where the ray exits the rear surface.

Greater accuracy may be obtained by using multiple surfaces to represent a single element. Stress birefringence interferogram files may then be assigned to each surface. This method may also be used in the situation where the Jones matrix is not representative of a linear retarder model in which the stress birefringence interferogram are based. In this case, the ellipticity value derived from the Jones matrix is non-zero and the more general elliptical retarder model must be used to represent the integrated effects of the stress field. In general, using multiple surfaces to represent a lens element and applying stress birefringence interferogram files to each surface approximate the elliptical retarder.

6. STRESS BIREFRINGENCE OPTOMECHANICAL SOFTWARE TOOLS

The optomechanical interface software package *SigFit*[2,3] uses finite element derived stress distributions to compute the retarder properties (birefringence, orientation, and ellipticity) for a grid of rays. A solid 3-D finite element model of the optical elements is required. The supplied stress tensor from the FEA solid elements is read directly into *SigFit*. The stresses are transformed into a common surface coordinate system using a stress transformation. The transformed stress tensors for each element are then averaged with all other elements at the common nodes to provide a single, unambiguous stress state per node throughout the solid optic. Rays are then traced through the optical element stress field. The user specifies the number of integration increments. At each integration point, the stress tensor is interpolated from the average nodal stress tensor in the optic using 3D finite element shape functions. The local interpolated stress tensor is then transformed into the ray coordinate system with the stress along the ray.

The change in the dielectric impermeability tensor is computed at each incremental point along the ray path. The magnitude and the direction of the indices of refraction are then computed along with Jones retarder and rotation matrices at each point. Then for a given ray path through the stress field, a system Jones matrix is computed and the magnitude of birefringence, orientation, and ellipticity values are derived. Wavefront error is also computed using the index changes at each increment along the ray path. SigFit outputs the birefringence, orientation, ellipticity, and wavefront maps into results files for graphical representation via contour plotting using the finite element model.

Specifying front and rear apertures define the ray paths through the stress field. Rays are passed from nodes on the front surface, defined by coordinates R_i, θ_i, and Z_i, through the optic to a corresponding rear surface point with coordinates R_o, θ_o, and Z_o, using a ray angle determined by the ratio of the radius of the front and rear apertures, A_i and A_o, respectively, as given by the following equation**.**

$$R_o = R_i \, (A_o/A_i) \qquad (6.1)$$

The birefringence, orientation, and wavefront values computed by *SigFit* for a grid of rays may be fit to Zernike polynomials or interpolated to a uniform grid. The birefringence and orientation data may then be output into CODE V stress birefringence interferogram files. Typically, to create stress birefringence interferogram files, the front and rear apertures are set equal. Skew rays are accounted internally by CODE V. The wavefront data may be output into wavefront interferogram files.

Doyle[4] discusses the use of stress birefringence interferogram files to model the effects of stress in focusing and collimating lens elements as a function of temperature for a telecommunication component. Rays traversing the focusing and collimating lens stress distribution are shown in Figure 5. Birefringence and wavefront maps computed by *SigFit* are shown for both elements (front and rear) of the doublet lens in Figure 6.

SUMMARY

Accounting for mechanical stress is critical for polarization and wavefront sensitive optical systems. In general, stress produces an anisotropic and inhomogeneous optical medium where the magnitude and direction of the indices of refraction vary at every point. Jones calculus is used to incrementally evaluate the effects of stress for a grid of rays traced through a three-dimensional finite element stress field. Birefringence, orientation, ellipticity, and wavefront maps may be computed over the optical aperture. Commercial software tools exist to evaluate the effects of mechanical stress within the optical model. The optomechanical analysis program *SigFit* creates stress birefringence and wavefront interferogram files using optical element stress data computed via finite element analysis. The optical design software program CODE V® uses interferogram files to represents the integrated effects of mechanical stress in an optical element. These tools allow design trades to be examined among glass types and mounting methods.

REFERENCES

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[2]*SigFit* written by Sigmadyne, Inc., Rochester, NY

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FIGURES

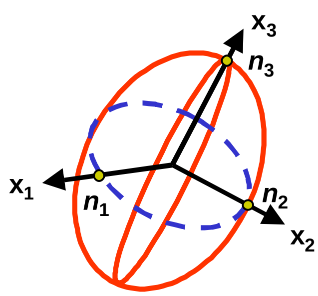
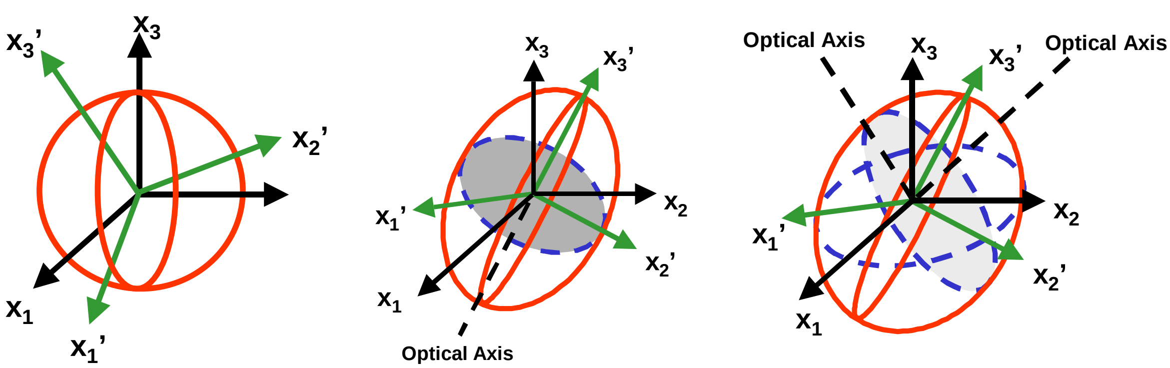


Figure 1. Index Ellipsoid: Geometric representation of the dielectric impermeability tensor; the refractive indices are defined by the semi-axes of the ellipsoid



(a) (b) (c)

Figure 2. Index Ellipsoid for a) isotropic material; b) uniaxial material; and c) biaxial material

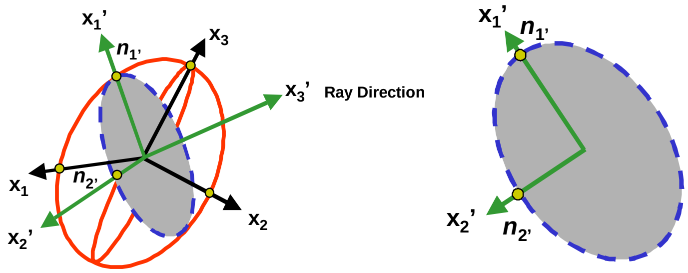
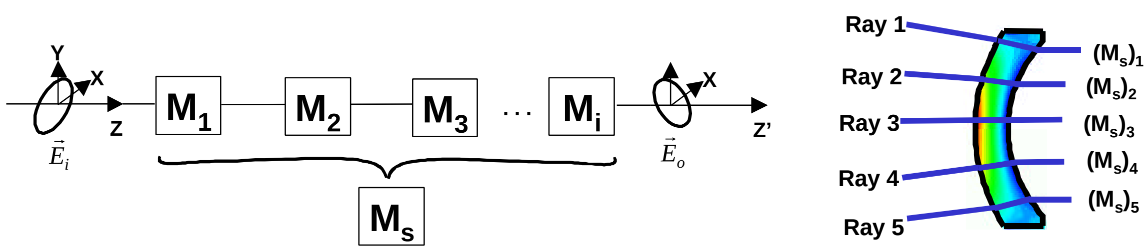


Figure 3. Indices of refraction for an arbitrary ray may be computed as the semi-axes of the ellipse that is normal to the ray direction and centered at the origin of the index ellipsoid



(a) (b)

Figure 4. a) The integrated effects of the stress field may be represented as a cascade of optical systems using Jones calculus; and b) System Jones matrix computed for a grid of rays

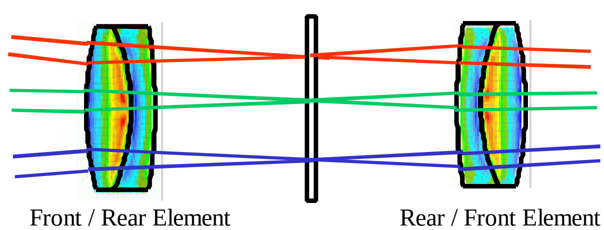
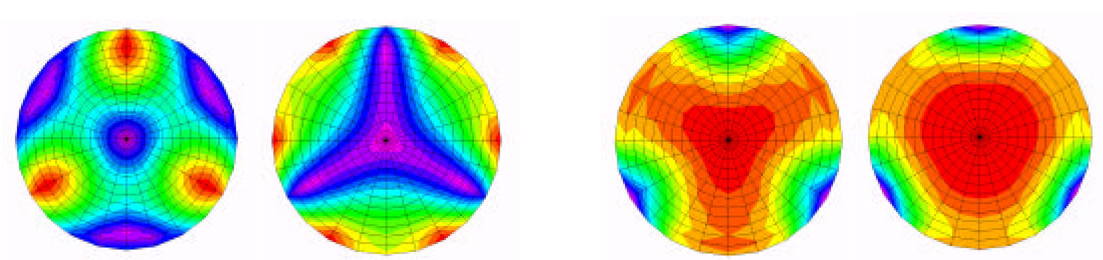


Figure 5. Doublet focusing and collimating lenses with stress distribution overlaid



(a) (b)

Figure 6. a) Front and rear birefringence maps and b) front and rear wavefront maps