Intuitive understanding of the connection between Pancharatnam–Berry optical beam deflectors and polarization volume holograms

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ABSTRACT

An approximate beam propagation method is proposed as an intuitive simulation of the optics of Pancharatnam–Berry phase (PPD) and polarization volume hologram (PVH) devices. Using this method, the connection between, and polarization properties of, these two types of devices are made clear.

Keywords: Pancharatnam–Berry phase, polarization volume hologram, rigorous coupled wave approach, ρ parameter.

1. INTRODUCTION

Polarization volume gratings (PVH) and Pancharatnam–Berry phase devices (PPD) have broad applications in optical systems. PPD devices, proposed in [1] and [2], have been used in optical beam steering devices [3] for applications including LIDAR, laser communication, etc., and metamaterial[4-7]. Polarization volume gratings (PVH), the physics and optics are well studied [8][9]. It can be used as an input and output coupler in a VR system. For example, a pancake optics design using a PVH has been proposed as one of the potential solutions for a lightweight headset in a virtual reality (VR) system [10].

1.1 The liquid crystal directors in PPD

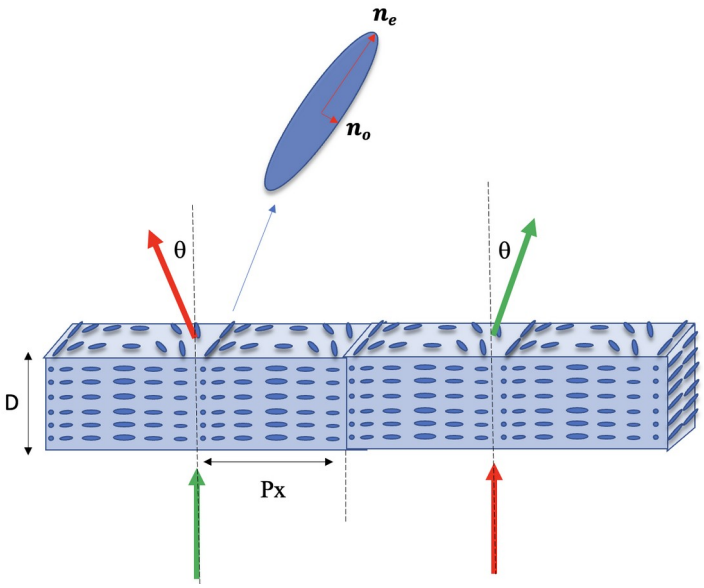

Figure 1. Liquid crystal director picture for PPD. In this picture, the blue bars are directors, which is the average direction of the long molecular axes in the liquid crystal. The birefringence Δn is the refractive index along the long ne, minus the refractive index along the short axis no(which is, Δn=ne-no). In PPD, the liquid crystal director is in the plane of the layer and spirals about the layer normal with a pitch Px. Left-hand circular light (green) is deflected to one direction with high efficiency. Right-hand circular light (red) is deflected to the opposite direction. λ is the vacuum wavelength of the incident light. The deflection efficiency is a function of thickness. While D= λ/(2Δn), its deflection efficiency is the highest.

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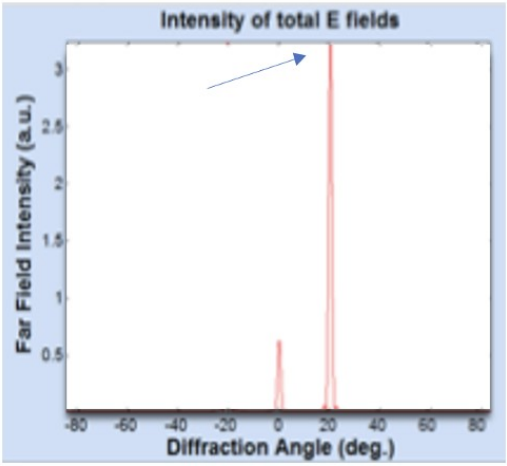

Figure 2. An example of FDTD far-field intensity result is shown when incident wavelength λ=0.633 microns, incident angle =0°, and Px=1.85 microns.

1.2 The device works as a deflector or reflector, depending on the pitch length.

Besides thickness, the deflection efficiency is a function of Px for a given wavelength.

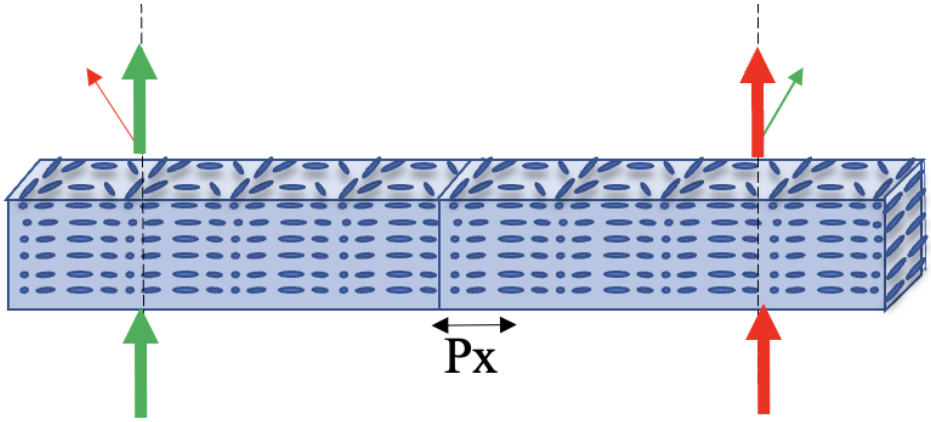

Figure 3. Liquid crystal director picture for PPD similar to, while Px is relatively small compared with the PPD in Figure 1. Later, for simplicity, we will call the structure in Figure 1 long-pitch PPD and the structure in Figure 3 short-pitch PPD.

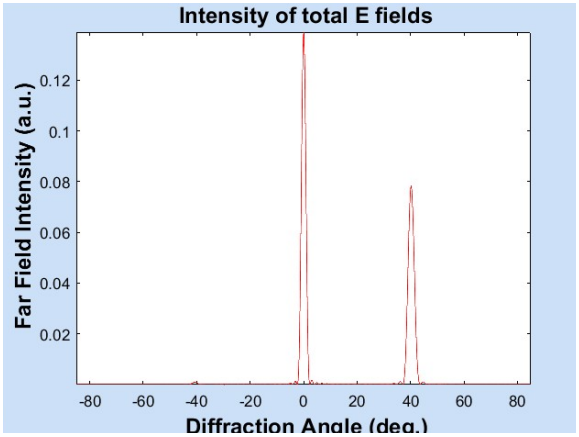

Figure 4. If λ=0.633 microns, incident angle =0°, FDTD shows short-pitch PPD with Px =0.98 microns yield a low efficiency 40° deflector.

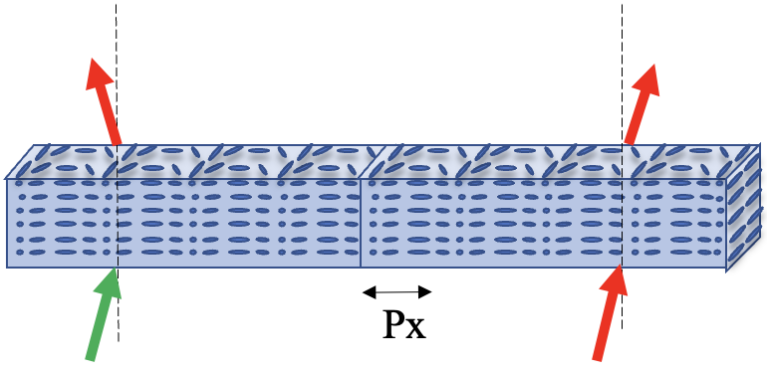

Figure 5. Short Pitch PPD, with 20° incident light, has high efficiency for LCP, while it has no effect on the RCP.

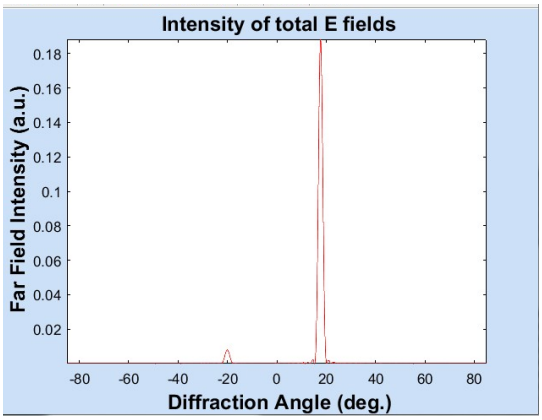

Figure 6. (b) If λ=0.633 microns, incident angle =20°, FDTD shows PPD with Px =0.98 microns yield a low efficiency 40° deflector.

We can see a PPD can behave either like a deflector or a reflector depending on the value of Px. The long-pitch PPD is a high efficiency beam deflector for normal incident light. The short-pitch PPD does not work well as a beam deflector. However, if short-pitch PPD is illuminated with 20° off-axis light, it behaves as a high efficiency polarization dependent Bragg reflector or Polarization Volume Hologram (PVH).

A device made of isotropic material behaves either like a reflector or a deflector, depending on the value of Px, is well studied. For isotropic materials, Gaylord and Moharam [11] considered a similar question in exploring the connection between Raman–Nath and Bragg type devices. They used an approximate coupled wave analysis to provide an intuitive derivation of the "ρ" parameter, which is used for distinguishing the Raman–Nath grating and Bragg grating effects [12].

To relate the PPD to isotropic gratings, the long-pitch PPD is a polarization-dependent Pancharatnam Phase Deflector (PPD) that is similar to a Rahman Nath deflector. Short-pitch PPD behaves as a polarization-dependent Bragg Reflector. However, the birefringence study on explaining the difference and connection between PPD and PVH is not yet proposed.

This difference in optical responses can be quantitatively modeled using numerical calculations, including rigorous coupled wave approach (RCWA) and the finite difference time domain (FDTD) method(as we have seen in Figure 2 and 4). However, these computational approaches are not transparent, like a black box. The output light information is given without explaining how the light interacts with the two very similar structures but gives very different outputs.

In this paper, the approach of Gaylord is extended to birefringent materials using a beam propagation method to clearly show the analytical connection between the optical properties of PPD and PVH devices.

2. APPROXIMATE COUPLED-WAVE APPROACH FOR BIREFRINGENCE MATERIAL

2.1 Overview of the calculation

In this work, the approach of Gaylord and Moharam for isotropic material [11] is extended to birefringence materials using a modified version of the dielectric tensor derivation of Sasaki [13].

The starting point is the Helmholtz equation.

$$\nabla^2 E + k^2 \varepsilon E = 0 \tag{1}$$

To show the evolution of the amplitude and polarization states of light as it propagates in a periodic birefringent structure, light is considered to be decomposed into plane waves with defined directions corresponding to the allowed diffraction orders under the Floquet condition. Further, the periodic birefringent layer is considered to be discretized into layers that are perpendicular to the plane of the film (grating k vector in the plane of film). The grating is considered to consist of N layers, each with a very small thickness d. (d=D/N)

Two assumptions are used to simplify the calculation:

1. The k vector direction of the s and p modes for each layer is assumed to be at the same angle.
2. Boundary effects are ignored.

Equations are here derived to find the amplitude and polarization state of each Floquet order in a particular layer, given the amplitude and polarization state of each of the orders in the layer before it.

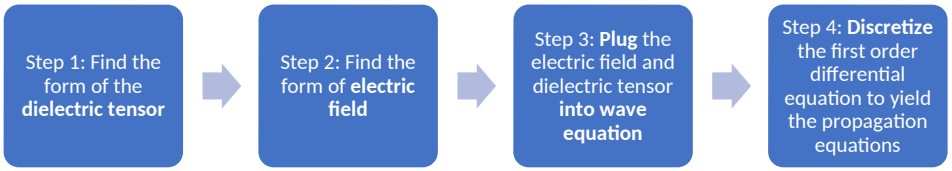

Figure 7. Calculation steps in this work.

2.2 Detailed calculation steps

2.2.1 Step1: Find the form of the dielectric tensor.

In this paper, Px is defined as positive if, along the +x direction, the director is rotated such that the right-hand rule the thumb points to the +z direction. Px is defined as negative if, along the +x direction, the director is rotated such that the right-hand rule the thumb points to the -z direction.

Similarly, the Pz is positive if, along the +z direction, the director is rotated such that the right-hand rule the thumb points to the +z direction. The Pz is negative if, along the +z direction, the director is rotated such that the right-hand rule the thumb points to the -z direction.

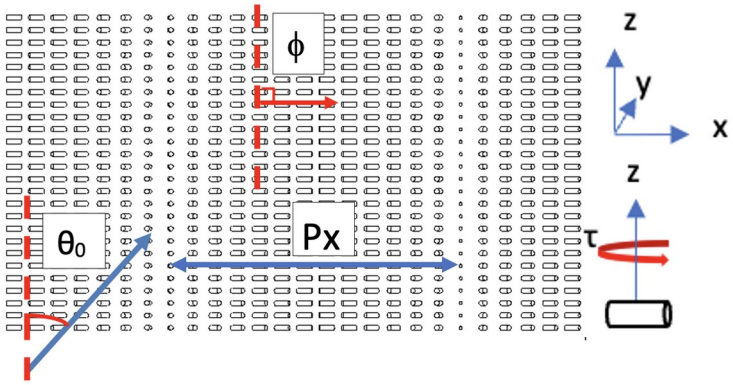

Figure 8. 2-dimensional PPD picture. The grating vector is the red arrow. The grating vector angle Φ makes =+90 ° with the +z axis. According to our definition, Px and the incident angle are positive. The angle τ describes the director rotation about the z-axis due to Px. θ_0 *is* the incident angle in the grating. When the incident angle has projections on the +x and +z axis, the incident angle is positive(In Figure 8, θ_0 is positive).

Let

$$\tau = \pi\left(\frac{x}{p_x} + \frac{z}{p_z}\right)$$

For the structure in Figure 8, the Px is positive, and Pz is infinite, gives,

$$\tau = \pi\left(\frac{x}{p_x}\right)$$

For the given structure that Px is positive, the grating vector is along the +x direction. According to the Floquet condition, the grating vector of the lth order can be written as,

$$\vec{k}_l = \vec{k}_0 - l\,\vec{k}_{grating}$$

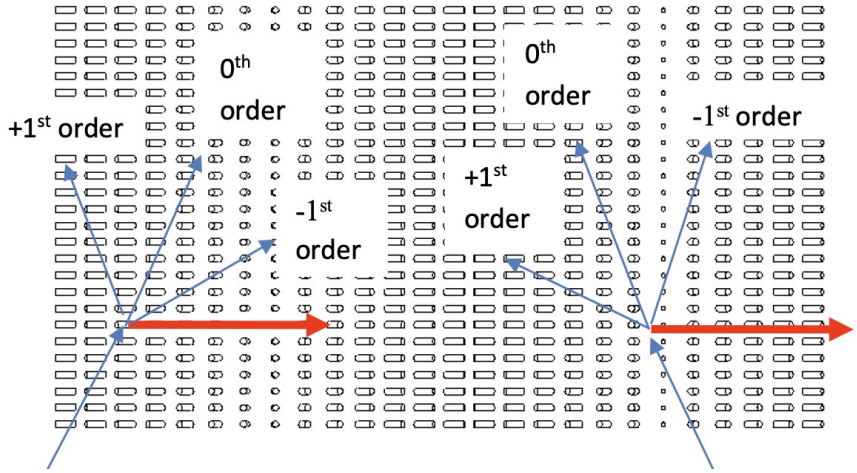

Figure 9. The three diffraction order is shown in the figure for positive(left) and negative(right) incident angles.

At Bragg condition, the incident, deflect, and grating vector forms a vector triangle[14]. Thus, the Bragg diffraction order is $+1^{st}$ when the incident angle is positive. The Bragg diffraction order is -1st when the incident angle is negative.

The Bragg diffraction order is calculated to be, from trigonometry,

$$m = \frac{2n_{ave}\Lambda}{\lambda}\cdot\cos\left(\theta_0 - \phi\right) = \frac{2\pi n_{ave}}{\lambda}\cdot 2\cos\left(\theta_0 - \phi\right)\cdot\frac{\Lambda}{2\pi} = \frac{\left|\vec{k}_{light}\right|}{\left|\vec{k}_{grating}\right|}2\cos\left(\theta_0 - \phi\right)$$

when m is the Bragg condition,

$$m = \frac{\cos\left(\theta_0 - \phi\right)}{\left|\cos\left(\theta_0 - \phi\right)\right|}$$

if $(\theta_0-\phi)$ <90°,

$$m = 1$$

otherwise,

$$m = -1$$

For the particular case of the grating vector is 90°, if light propagates to the Northeast, then θ_0 is positive, and the Bragg order corresponds to m=+1.

For a more general case of when $\phi \neq 90°$ [9],

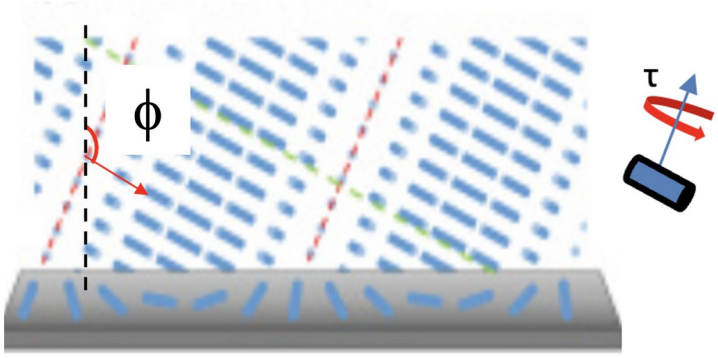

Figure 10. Slanted T-PVH director profile illustrated in [9]. The grating k vector is specified by the angle ϕ. The angle τ describes the director rotation about the Bragg plane(red dashed axis), which is perpendicular to the director rotation plane shown by the green dash line.

The director components, n_x, n_y, and n_z are,

$$n_x = \sin(\phi)\cos(\tau)$$
$$n_y = \sin(\tau)$$
$$n_z = \cos(\phi)\cos(\tau)$$

The relation between the dielectric tensor and the director orientation is,

$$\varepsilon_{ij} = n_o^{\,2}\delta_{ij} + \Delta N^2 n_i n_j$$
$$where \quad \Delta N^2 = n_e^{\,2} - n_o^{\,2}$$

As in [13], the dielectric tensor can be written in two terms. One term unrelated to the pitch is ε_a, and the other is the perturbation term $\Delta\varepsilon$.

$$\varepsilon = \varepsilon_a + \Delta\varepsilon$$

$$\varepsilon_a = \begin{bmatrix} n_o^{\,2} + \frac{\Delta N^2 \sin^2(\phi)}{2} & 0 & \frac{\Delta N^2(\sin(\phi)\cos(\phi))}{2} \\ 0 & n_o^{\,2} + \frac{\Delta N^2}{2} & 0 \\ \frac{\Delta N^2(\sin(\phi)\cos(\phi))}{2} & 0 & n_o^{\,2} + \frac{\Delta N^2 \cos^2(\phi)}{2} \end{bmatrix}$$

$$\Delta\varepsilon = \frac{\Delta N^2}{2}\begin{bmatrix} \sin^2(\phi)\cos(2\tau) & \sin(\phi)\sin(2\tau) & (\sin(\phi)\cos(\phi))\cos(2\tau) \\ \sin(\phi)\sin(2\tau) & -\cos(2\tau) & \cos(\phi)\sin(2\tau) \\ (\sin(\phi)\cos(\phi))\cos(2\tau) & \cos(\phi)\sin(2\tau) & \cos^2(\phi)\cos(2\tau) \end{bmatrix}$$

Using Euler's equation, rewriting the sine and cosine in terms of exponentials, $\Delta\varepsilon$ can be written as :

$$\Delta\varepsilon = \frac{\Delta N^2}{4} M_+ \exp(i2\tau) + \frac{\Delta N^2}{4} M_- \exp(-i2\tau)$$

Where i is the imaginary unit, and M matrices are defined as,

$$M_{+}=\begin{bmatrix} \sin^2(\phi) & -i\sin(\phi) & (\sin(\phi)\cos(\phi)) \\ -i\sin(\phi) & -1 & -i\cos(\phi) \\ (\sin(\phi)\cos(\phi)) & -i\cos(\phi) & \cos^2(\phi) \end{bmatrix}$$

$$M_{-}=\begin{bmatrix} \sin^2(\phi) & i\sin(\phi) & (\sin(\phi)\cos(\phi)) \\ i\sin(\phi) & -1 & i\cos(\phi) \\ (\sin(\phi)\cos(\phi)) & i\cos(\phi) & \cos^2(\phi) \end{bmatrix}$$

As stated in Sasaki's paper, as the incident light propagates in the grating structure, the presence of the dielectric perturbation gives rise to an additional dielectric polarization. It is considered that polarization radiates as the diffracted light [13].

From the perturbation term, two waves will be radiated for a given input 0th order wave.

The angle τ can be written in terms of components of the grating vector,

$$\tau=\pi\left(\frac{x}{p_x}+\frac{z}{p_z}\right)=\frac{\left(\frac{2\pi x}{p_x}+\frac{2\pi z}{p_z}\right)}{2}=\frac{\left(k_x^{\,grating}\cdot x+k_z^{\,grating}\cdot z\right)}{2}$$

Plug τ into the perturbation term Δε gives,

$$\Delta\varepsilon=\frac{\Delta N^2}{4}M_{+}\exp(i2\tau)+\frac{\Delta N^2}{4}M_{-}\exp(-i2\tau)$$

$$=\frac{\Delta N^2}{4}M_{+}\exp\left(i\left(k_x^{\,grating}\cdot x+k_z^{\,grating}\cdot z\right)\right)+\frac{\Delta N^2}{4}M_{-}\exp\left(-i\left(k_x^{\,grating}\cdot x+k_z^{\,grating}\cdot z\right)\right)$$

The final form of the dielectric tensor is,

$$\varepsilon=\varepsilon_a+\Delta\varepsilon=\varepsilon_a+\frac{\Delta N^2}{4}M_{+}\exp\left(i\left(k_x^{\,grating}\cdot x+k_z^{\,grating}\cdot z\right)\right)+\frac{\Delta N^2}{4}M_{-}\exp\left(-i\left(k_x^{\,grating}\cdot x+k_z^{\,grating}\cdot z\right)\right) \quad (2)$$

2.2.2 Find the form of the electric field

The electric field, in general, where the Jones vector describing the polarization state is expressed in a frame where the z-axis is parallel to the k vector direction is:

$$\vec{E}_l=\begin{bmatrix} E_{sl} \\ E_{pl} \\ 0 \end{bmatrix}_k=\begin{bmatrix} J_{sl} \\ J_{pl} \\ 0 \end{bmatrix}_k\exp\left(i\left(-\vec{k}_l\cdot\vec{r}\right)\right)$$

where $\vec{k}_l$ is the wave vector for the lth order.

By Floquet theorem,

$$\vec{k}_l=\vec{k}_0-l\,\vec{k}_{grating}$$

$$= \begin{pmatrix} \frac{2\pi n_{ave}}{\lambda}\sin(\theta_{in}) \\ 0 \\ \frac{2\pi n_{ave}}{\lambda}\cos(\theta_{in}) \end{pmatrix} - l\vec{k}_{grating}$$

where $\vec{k}_0$ is the incident wave vector, $\vec{k}_{grating}$–grating is the grating vector.

$$\vec{k}_{grating} = \begin{pmatrix} \left|\vec{k}_{grating}\right| \cdot \sin(\phi) \\ 0 \\ \left|\vec{k}_{grating}\right| \cdot \cos(\phi) \end{pmatrix}$$

Where above, the approximation that the direction of the k vector for the s and p modes is the same is used.

To write in the lab frame, we need to use the rotation matrix,

$$R(\theta_l) = \begin{pmatrix} \cos(\theta_l) & 0 & -\sin(\theta_l) \\ 0 & 1 & 0 \\ \sin(\theta_l) & 0 & \cos(\theta_l) \end{pmatrix}$$

$$\begin{pmatrix} J_{inx} \\ J_{iny} \\ J_{iny} \end{pmatrix} = R(\theta_l) \begin{pmatrix} J_{ins} \\ J_{inp} \\ 0 \end{pmatrix}$$

So, the electric field in the lab frame is,

$$\vec{E}_l = \begin{bmatrix} E_{xl} \\ E_{yl} \\ E_{zl} \end{bmatrix}_{lab} = \begin{bmatrix} J_{xl} \\ J_{yl} \\ J_{zl} \end{bmatrix}_{lab} \exp\left(i\left(-\vec{k}_l \cdot \vec{r}\right)\right)$$

$$= R(\theta_l) \begin{bmatrix} J_{sl} \\ J_{pl} \\ 0 \end{bmatrix}_k \exp\left(i\left\{-\left\{\left|\vec{k}_0\right|\sin(\theta_{in}) - l\left|\vec{k}_{grating}\right|\sin(\phi)\right\}x - \left\{\left|\vec{k}_0\right|\cos(\theta_{in}) - l\left|\vec{k}_{grating}\right|\cos(\phi)\right\}z\right\}\right)$$

$$= S_l * \exp\left(i\left\{-\left\{\left|\vec{k}_0\right|\sin(\theta_{in}) - l\left|\vec{k}_{grating}\right|\sin(\phi)\right\}x - \left\{\left|\vec{k}_0\right|\cos(\theta_{in}) - l\left|\vec{k}_{grating}\right|\cos(\phi)\right\}z\right\}\right)$$

where S_l is a vector in the lab frame,

$$S_l = R(\theta_l) \begin{bmatrix} J_{sl} \\ J_{pl} \\ 0 \end{bmatrix}_k$$

The total electric field is then, for all existing orders of l,

$$\vec{E}_{tot} = \sum_l S_l \exp\left(-i\left\{\left\{\left|\vec{k}_0\right|\sin(\theta_{\text{in}}) - l\left|\vec{k}_{grating}\right|\sin(\phi)\right\}x + \left\{\left|\vec{k}_0\right|\cos(\theta_{\text{in}}) - l\left|\vec{k}_{grating}\right|\cos(\phi)\right\}z\right\}\right) \tag{3}$$

2.2.3 Plug the electric field and dielectric tensor into the wave equation.

Plug the form of the dielectric tensor (2) and the form of the electric field in grating (3) in the wave equation (1),

The Laplacian term becomes,

$$\sum_l \frac{\partial^2 S_l}{\partial z^2}\exp\left(-i\left\{\left(k_x{}^{l=0} - l\cdot k_x{}^{grating}\right)x + \left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)z\right\}\right)$$

$$+\sum_l 2\left(-i\left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)\right)\frac{\partial S_l}{\partial z}\exp\left(-i\left\{\left(k_x{}^{l=0} - l\cdot k_x{}^{grating}\right)x + \left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)z\right\}\right)$$

$$-\sum_l S_l\left(\left(k_x{}^{l=0} - l\cdot k_x{}^{grating}\right)^2 + \left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)^2\right)\exp\left(-i\left\{\left(k_x{}^{l=0} - l\cdot k_x{}^{grating}\right)x + \left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)z\right\}\right)$$

The second term with the dielectric tensor is,

$$\left(\frac{2\pi}{\lambda}\right)^2\sum_l \varepsilon_a S_l\exp\left(-i\left(\left(k_x{}^{l=0} - l\cdot k_x{}^{grating}\right)\cdot x + \left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)\cdot z\right)\right)$$

$$+\left(\frac{2\pi}{\lambda}\right)^2\frac{\Delta N^2}{4}\sum_l M_+ S_l\exp\left(-i\left(\left(k_x{}^{l=0} - (l+1)\cdot k_x{}^{grating}\right)\cdot x + \left(k_z{}^{l=0} - (l+1)\cdot k_z{}^{grating}\right)\cdot z\right)\right)$$

$$+\left(\frac{2\pi}{\lambda}\right)^2\frac{\Delta N^2}{4}\sum_l M_- S_l\exp\left(-i\left(\left(k_x{}^{l=0} - (l-1)\cdot k_x{}^{grating}\right)\cdot x + \left(k_z{}^{l=0} - (l-1)\cdot k_z{}^{grating}\right)\cdot z\right)\right)$$

Collect the term with the same exponential; note that for the term with M+, the l-1 term is collected, and for the term with M-, the l+1 term is collected. Ignore the second derivative, rearrange the terms,

$$\exp\left(-i\left(\left(k_x{}^{l=0} - l\cdot k_x{}^{grating}\right)\cdot x + \left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)\cdot z\right)\right)*$$

$$\sum_l\left(-2\left(i\left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)\right)\frac{\partial S_l}{\partial z} - S_l\left(\left(k_x{}^{l=0} - l\cdot k_x{}^{grating}\right)^2 - \left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)^2\right) + \left(\frac{2\pi}{\lambda}\right)^2\varepsilon_a S_l + \left(\frac{2\pi}{\lambda}\right)^2\frac{\Delta N^2}{4}M_- S_{l+1} + \left(\frac{2\pi}{\lambda}\right)^2\frac{\Delta N^2}{4}M_+ S_{l-1}\right) = 0$$

For a non-trivial solution, the coefficient of the exponential need to go to 0.

Reorder terms, get,

$$-\frac{S_l\left(\left(k_x{}^{l=0} - l\cdot k_x{}^{grating}\right)^2 + \left(k_z{}^{l=0} - l\cdot k_z{}^{grating}\right)^2\right)}{2\pi^2} + \frac{2\varepsilon_a S_l}{\lambda^2} = \left\{\left(\frac{2}{\lambda^2}\right)\left(\varepsilon_a - n_{ave}{}^2\right) + \frac{2l}{\Lambda^2}(m-l)\right\}S_l$$

$$m = \frac{2n_{ave}\Lambda}{\lambda}\cdot\cos(\theta_0 - \phi)$$

So eventually, the first-order differential equation for birefringence material is,

$$-i\frac{2}{\pi}\left\{\frac{n_{ave}\cdot\cos(\theta_0)}{\lambda}-\frac{l\cdot\cos(\phi)}{\Lambda}\right\}\frac{dS_l}{dz}-+\frac{2l(m-l)}{\Lambda^2}S_l+\left(\frac{2}{\lambda^2}\right)\left(\varepsilon_a-n_{ave}{}^2\right)S_l+\frac{\Delta N^2}{2\lambda^2}M_-S_{l+1}+\frac{\Delta N^2}{2\lambda^2}M_+S_{l-1}=0 \quad (4)$$

Note this is very close to the equation in the isotropic calculation in Gaylords' paper [11]. There are two main differences:

1. There is an extra term of S_l. In isotropic material, this term drops to 0 (as $\varepsilon 0=n_{ave}{}^2$) for isotropic. This is no longer true for birefringence material.

2. The coefficient in front of S_{l-1}, S_{l+1} term is different.

2.2.4 Discretize the first order differential equation (4) to the updated equation between layers.

To numerically simulate the propagation of light, we need to discretize the continuous first-order differential equation to discrete steps through the thickness of the simulated structure.

First, we want to rewrite (4) in terms of a first-order differential of S_l.

let A equals,

$$A_l=\frac{n_{ave}\cos(\theta_0)}{\lambda}-\frac{l\cos(\phi)}{\Lambda}$$

Then we have,

$$i\frac{2A_l}{\pi}\frac{dS_l}{dz}=\frac{2l(m-l)}{\Lambda^2}S_l+\left(\frac{2}{\lambda^2}\right)\left(\varepsilon_a-n_{ave}{}^2\right)S_l+\frac{\Delta N^2 M_-S_{l+1}}{2\lambda^2}+\frac{\Delta N^2 M_+S_{l-1}}{2\lambda^2}$$

Divide by the factor in front of the derivative,

$$\frac{dS_l}{dz}=\frac{-i\pi}{2A_l}\left\{\frac{2l(m-l)}{\Lambda^2}S_l+\left(\frac{2}{\lambda^2}\right)\left(\varepsilon_a-n_{ave}{}^2\right)S_l+\frac{\Delta N^2 M_-S_{l+1}}{2\lambda^2}+\frac{\Delta N^2 M_+S_{l-1}}{2\lambda^2}\right\}$$

Now we can discretize the equation by thinking of the total thickness consisting of a very large number of layers.

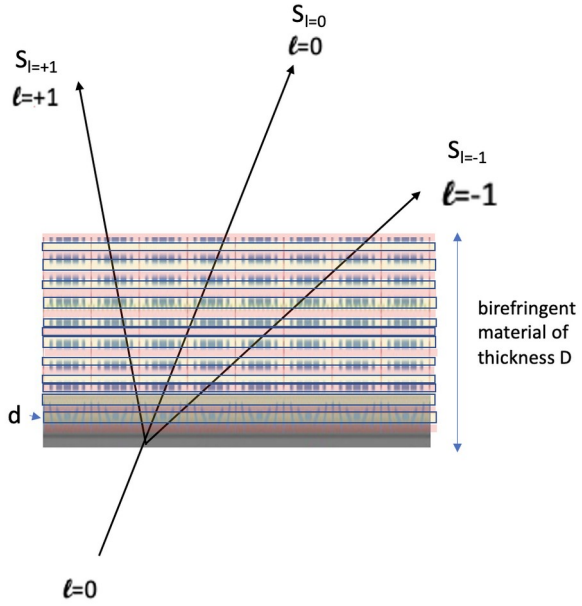

Figure 11. Discretization steps in this work

For the thickness of the grating D is one wave thickness, which is defined as,

$$\frac{\Delta n \cdot D}{\lambda} = 1$$

$$D = \frac{\lambda}{\Delta n}$$

The grating consists of N layers, each with a very small thickness d.

$$d = \frac{D}{N} = \frac{\lambda}{N \cdot \Delta n}$$

To write this equation discretely and in terms of the layer and its next layer,

$$\frac{d\, S_l(z)}{dz} = \frac{S_l^{layer+1} - S_l^{layer}}{d}$$

Finally, we obtained the equation that relates the values of the complex wave amplitude for the l_{th} diffraction order, S_l^{layer}, in one layer to those in the next layer.

$$S_l^{layer\ n+1} = -\frac{i\pi d \Delta N^2}{4 A_l \lambda^2} M_+ S_{l-1}^{layer\ n} + \left(1 - \frac{i\pi d l (m-l)}{A_l \Lambda^2} - \frac{i\pi d}{A_l \lambda^2}\left(\varepsilon_a - n_{ave}^2\right)\right) S_l^{layer\ n} - \frac{i\pi d \Delta N^2}{4 A_l \lambda^2} M_- S_{l+1}^{layer\ n}$$

$$= K_{l-1,l} M_+ S_{l-1}^{layer\ n} + K_{l,l} S_l^{layer\ n} + K_{l+1,l} M_- S_{l+1}^{layer\ n} \qquad (5)$$

$K_{l+1,l}$, $K_{l,l}$, and $K_{l-1,l}$ is the coupling coefficient that relates the complex amplitude of the $(l+1)^{th}$, l^{th}, $(l-1)^{th}$ diffraction order in layer n to the lth diffraction order next layer (layer n+1).

$$K_{l-1,l} = -\frac{i\pi d \Delta N^2}{4 A_l \lambda^2} M_+ \qquad K_{l,l} = 1 - \frac{i\pi d l (m-l)}{A_l \Lambda^2} - \frac{i\pi d}{A_l \lambda^2}\left(\varepsilon_a - n_{ave}^2\right) \qquad K_{l+1,l} = -\frac{i\pi d \Delta N^2}{4 A_l \lambda^2} M_-$$

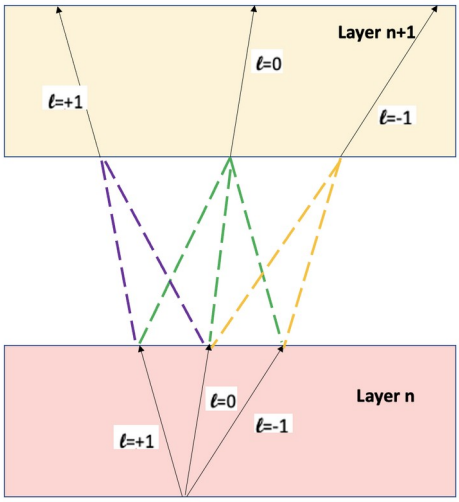

Figure 12. The diffraction order in layer n+1 can be defined by the diffraction orders in layer n and coupling constants K.

These equations can be used to find the output amplitude and polarization state of light exiting a film of many layers. It turns out that this simple method provides quite accurate results compared with RCWA, at least for the case where the grating k vector is in the plane of the layers(ϕ = 90°). More details can be found in the supplemental material in [15].

Given the verification of this method to predict the amplitude and phase of light exiting a film of a periodic birefringent media, we can use the simple form of these equations to analyze the evolution of light going through the film as a function of the parameters they contain.

3. APPROXIMATIONS FOR Φ=90° PPD/PVH WITH THREE DIFFRACTION ORDERS

In $K_{l,l}$, there is a term with $\left(\varepsilon_a - n_{ave}^{\,2}\right)$. If ϕ=90°, for the 'unslanted' director configuration of Figure 8,

$$\varepsilon_a - n_{ave}^{\,2} = \begin{bmatrix} \frac{n_e^{\,2}+n_o^{\,2}}{2} - n_{ave}^{\,2} & 0 & 0 \\ 0 & \frac{n_e^{\,2}+n_o^{\,2}}{2} - n_{ave}^{\,2} & 0 \\ 0 & 0 & n_o^{\,2} - n_{ave}^{\,2} \end{bmatrix}$$

If the average index is taken as**,**

$$n_{ave} = \sqrt{\frac{\left(n_e^{\,2}+n_o^{\,2}\right)}{2}}$$

the expression is further simplified to,

$$\varepsilon_a - n_{ave}^{\,2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\Delta N^2}{2} \end{bmatrix}$$

When light is nearly normally incident (electric field has a small component along the z-direction), and birefringence is low, the effect of this term is very close to 0.

Note when grating vector angle $\phi = 90°$, M+ and M- are also simplified to,

$$M_{+}=\begin{bmatrix}1 & -i & 0\\ -i & -1 & 0\\ 0 & 0 & 0\end{bmatrix}$$

$$M_{-}=\begin{bmatrix}1 & i & 0\\ i & -1 & 0\\ 0 & 0 & 0\end{bmatrix}$$

And A_l is also simplified to,

$$A_l=\frac{n_{ave}\cos(\theta_0)}{\lambda}-\frac{l\cos(\phi)}{\Lambda}=\frac{n_{ave}\cos(0°)}{\lambda}-\frac{l\cos(90°)}{\Lambda}=\frac{n_{ave}}{\lambda}$$

The coupling coefficients then are simplified to,

$$K_{l-1,l}=-\frac{i\pi d\Delta N^2}{4n_{ave}\lambda}M_{+} \qquad K_{l,l}=1-\frac{i\pi dl(m-l)\lambda}{n_{ave}\Lambda^2} \qquad K_{l+1,l}=-\frac{i\pi d\Delta N^2}{4n_{ave}\lambda}M_{-}$$

Write (5) for -1st,0th,and 1st diffraction order, we have,

$$\begin{aligned}S_{-1\,order}^{layer\,n+1}&=K_{-1,-1}S_{-1\,order}^{layer\,n}+K_{0,-1}S_{0\,order}^{layer\,n}\\ S_{0\,order}^{layer\,n+1}&=K_{-1,0}S_{-1\,order}^{layer\,n}+K_{0,0}S_{0\,order}^{layer\,n}+K_{+1,0}S_{+1\,order}^{layer\,n}\\ S_{+1\,order}^{layer\,n+1}&=K_{0,+1}S_{0\,order}^{layer\,n}+K_{+1,+1}S_{+1\,order}^{layer\,n}\end{aligned} \tag{6}$$

K is the coupling coefficient that relates the complex amplitude in layer n+1 to layer n for different diffraction orders.

$$K_{-1,-1}=1+\frac{2i\pi d\lambda}{n_{ave}\Lambda^2} \qquad K_{0,-1}=-\frac{i\pi d\Delta N^2}{4n_{ave}\lambda}M_{-}$$

$$K_{-1,0}=-\frac{i\pi d\Delta N^2}{4n_{ave}\lambda}M_{+} \qquad K_{0,0}=1 \qquad K_{+1,0}=-\frac{i\pi d\Delta N^2}{4n_{ave}\lambda}M_{-}$$

$$K_{0,+1}=-\frac{i\pi d\Delta N^2}{4n_{ave}\lambda}M_{+} \qquad K_{+1,+1}=1$$

For simplification, let C and E to be real numbers of,

$$C=\frac{\pi d\Delta N^2}{4n_{ave}\lambda}$$

$$E=\frac{2\pi d\lambda}{n_{ave}\Lambda^2}$$

Coupling coefficient becomes,

$$K_{-1,-1}=1+iE \qquad K_{0,-1}=-iCM_{-}$$

$$K_{-1,0} = -iC\,M_{+} \qquad K_{0,0} = 1 \qquad K_{+1,0} = -iC\,M_{-}$$

$$K_{0,+1} = -iC\,M_{+} \qquad K_{+1,+1} = 1$$

We have two important observations for the coupling coefficient:

1. There are no $K_{-1,+1,}$ or $K_{+1,-1}$, meaning energy only transfers between adjacent orders.

2.What special to the -1st order is, while both $K_{0,0}$ and $K_{+1,+1}$ is 1, $K_{-1,-1}$ have two terms of different phases. Later we can see how this leads to the difference between PPD and PVH.

4. THE EFFECT OF THE INCIDENT LIGHT POLARIZATION STATE ON THE RESPONSE OF PPD AND PVH DEVICES

When the incident polarization state is LCP, and the incident angle is close to 0 °(normal incidence), calculate the complex amplitude of diffraction orders in layer 2 from layer 1, because the incident beam is 0th order only, gives,

$$S_{-1\,order}^{layer\,2} = K_{0,-1} S_{0\,order}^{layer\,1} = -iC \begin{bmatrix} 1 & i & 0 \\ i & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} = 0$$

$$S_{0\,order}^{layer\,2} = K_{0,0} S_{0\,order}^{layer\,1} = S_{0\,order}^{layer\,1} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix}$$

$$S_{+1\,order}^{layer\,2} = K_{0,+1} S_{0\,order}^{layer\,1}$$

$$= -iC\,M_{+} S_{0\,order}^{layer\,1}$$

$$= -iC \begin{bmatrix} 1 & -i & 0 \\ -i & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} = -\sqrt{2}\,iC \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix}$$

Calculate complex amplitude of diffraction orders in layer 3 from layer 2, gives,

$$S_{-1\,order}^{layer\,3} = K_{-1,-1} S_{-1\,order}^{layer\,2} + K_{0,-1} S_{0\,order}^{layer\,2} = 0 + K_{0,-1} S_{0\,order}^{layer\,1} = 0$$

$$S_{0\,order}^{layer\,3} = K_{-1,0} S_{-1\,order}^{layer\,2} + K_{0,0} S_{0\,order}^{layer\,2} + K_{+1,0} S_{+1\,order}^{layer\,2} = 0 + S_{0\,order}^{layer\,1} + iC\,M_{-} \sqrt{2}\,iC \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} - \sqrt{2} C^2 \begin{bmatrix} 1 & i & 0 \\ i & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix} = \left(\frac{1}{\sqrt{2}} - 2\sqrt{2} C^2 \right) \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix}$$

$$S_{+1\,order}^{layer\,3} = K_{0,+1} S_{0\,order}^{layer\,2} + K_{+1,+1} S_{+1\,order}^{layer\,2} = -iC\,M_{+} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} - \sqrt{2}\,iC \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix}$$

$$= -2\sqrt{2}\,iC \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix}$$

The calculation can go on, but we can see some very interesting conclusions in terms of polarization responses of PPD/PVH:
For LCP incidence, throughout the thickness,

1. -1st order is not activated(no energy is flowing into -1st order).
2. The 0th order is always LCP.
3. +1st order beam is always RCP.

The same calculation steps can be applied for RCP incidence, in which case the -1st order is activated instead of the +1st order.

Note when the incident angle is negative(m= -1), the same calculation can be applied to find the same incident polarization state that will activate the same diffraction order as when the incident angle is positive.

To summarize the polarization response for a PPD/PVH structure with positive Px,
1. 0th order does not change its polarization state.

2. LCP incidence can only activate the +1st order.

3. RCP incidence can only activate the -1st order.

5. THE DIFFERENCE IN POLARIZATION RESPONSE OF PPD AND PVH DEVICES

In [11], the 'ρ' parameter is derived for an isotropic material which is the ratio of the two terms for the complex amplitude S_l. In this section, the ρ parameter is proposed, applying a method similar to the isotropic material. In this section, a positive angle of incidence is assumed.

It will be shown below that, the ratio of E(for -1st order, describes the coupling to itself with different phase) and C(for -1st order, describes the coupling to 0th order) is significant in differentiating the PPD and PVH optical effects. The ratio, is,

$$ratio = \frac{E}{C} = \frac{\left(\frac{2\pi d\lambda}{n_{ave}\Lambda^2}\right)}{\left(\frac{\pi d\Delta N^2}{4 n_{ave}\lambda}\right)} = \frac{\left(\frac{2\lambda}{\Lambda^2}\right)}{\left(\frac{\Delta N^2}{4\lambda}\right)} = \frac{4\lambda^2}{\left(\frac{\Lambda^2\left(n_e{}^2 - n_o{}^2\right)}{2}\right)} = \frac{4\lambda^2}{\left(\frac{\Lambda^2\left(n_e + n_o\right)\left(n_e - n_o\right)}{2}\right)} = \frac{4\lambda^2}{\left(\Lambda^2 \cdot n_{ave}{}' \cdot \Delta n\right)}$$

where,

$$n_{ave}{}' = \frac{\left(n_e + n_o\right)}{2}$$

This ratio will be designated as the 'ρ' parameter for birefringence material,

$$\rho = \frac{4 * \lambda^2}{Px^2 * n_{ave}{}' * \Delta n}$$

The effect of the value of the 'ρ' parameter can be clearly seen by looking at the propagation of light in the birefringent periodic material through its first two layers.

As shown in section 4, assuming the incident angle is close to 0, energy does not flow to +1st order with RCP incidence. We, therefore, only need to calculate the 0 and -1st order when exiting the second layer.

Light incident on the first layer only has energy in the 0th order. With RCP incident light, calculate the complex amplitude of diffraction orders in layer 2 from layer 1, get

$$S_{-1\,order}^{layer\,2} = K_{-1,-1} S_{-1\,order}^{layer\,1} + K_{0,-1} S_{0\,order}^{layer\,1} = K_{0,-1} S_{0\,order}^{layer\,1} = -iC\,M_{-} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix} = -\sqrt{2}\,iC \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} = \sqrt{2}\,C \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} \exp\left(-i\frac{\pi}{2}\right)$$

$$S_{0\,order}^{layer\,2} = S_{0\,order}^{layer\,1} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix}$$

Calculate complex amplitude of diffraction orders in layer 3 from layer 2, gives,

$$S_{-1\,order}^{layer\,3} = K_{-1,-1} S_{-1\,order}^{layer\,2} + K_{0,-1} S_{0\,order}^{layer\,2} = -(1+iE)\sqrt{2}\,iC \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} - iC\,M_{-} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix}$$

$$= -(1+iE)\sqrt{2}\,iC \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} - iC\sqrt{2} \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} \left\{ -i\,2\sqrt{2}\,C + \sqrt{2}\,CE \right\}$$

$$= \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} \left\{ 2\sqrt{2}\,C\left(-\frac{\pi}{2}i\right) + \sqrt{2}\,CE(0\,i) \right\}$$

$$S_{0\,order}^{layer\,3} = K_{-1,0} S_{-1\,order}^{layer\,2} + K_{0,0} S_{0\,order}^{layer\,2} = iC\,M_{+}\ \sqrt{2}\,iC \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix} + S_{0\,order}^{layer\,1} = -2\sqrt{2}\,C^2 \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix} + \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix} = \left(-2\sqrt{2}\,C^2 + \frac{1}{\sqrt{2}}\right) \begin{bmatrix} 1 \\ -i \\ 0 \end{bmatrix}$$

We can see that the 0th order has a constant phase when propagating through the layers. When propagating through the layers, the -1st order picked up the boxed term, which has a phase of 0 that is -π/2 different from -1st order in the previous layer. This phase difference originates from $K_{-1,-1}$, which has two terms of different phases.

If the 'ρ' parameter is small, the "out of phase term" is negligible, which results in the phase of the -1st order being constant as it propagates from layer to layer through the material. However, if the 'ρ' parameter is large, "the out of phase term" is not negligible. In this case, the phase of the -1st order changes when it propagates from layer to layer, and its phase changes with respect to the other orders.

In [11], the boxed term is called a "dephasing" term. [15] plots the phase and amplitude of each of the considered three orders as a function of film thickness, that clearly shows that, with an increasing 'ρ' parameter, the rapidly changing phase of the -1st order leads to the transition from PPD to PVH.

The physical explanation of this rapidly varying phase of the -1st order with respect to the zero order for the case of a large 'ρ' value can be roughly seen by considering the simplified ray trace diagrams in Figure.13.

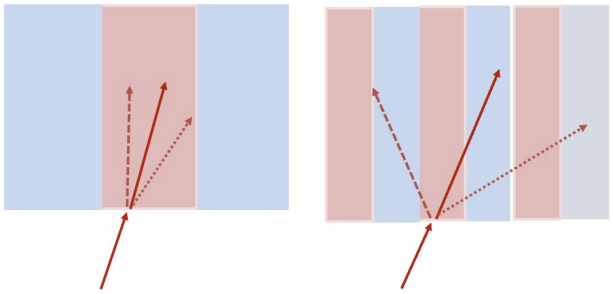

Figure 13. Figure shows an incident light beam to a periodic media and the resulting diffracted orders for PPD(left) and PVH(right).

For PPD, because the grating period is large, there is not expected to be a large phase difference for the +1st (long dashes) and -1st(dotted line)order beam. For PVH, with a much smaller grating period, the 0th order deflected beam (solid line) and the +1st order beam traverse regions of a similar index of refraction and are expected to have a similar phase variation as they propagate through the media. However, the -1st order sees a greater variation in the index of refraction, and therefore is expected to have a changing phase relationship to the 0th order beam.

Note when the incident angle is negative, m= -1, the +1st order has a dephasing term(instead of -1st order for positive incident angle). Following the same calculation in this section, the +1st order will not have a constant phase with a large 'ρ' parameter because of the dephasing effect illustrated.

6. LIMITATION OF THE WAVE PROPAGATION SIMULATION

Unlike FDTD and RCWA, the proposed beam propagation method is very transparent in showing the intensity and phase change of each diffraction order when propagating through an anisotropic media. However, the drawback is, the proposed beam propagation method is not as accurate as FDTD and RCWA because of the necessary approximations that we used to arrive at a simple expression of complex amplitudes.

The first approximation is the k vector direction of the s and p modes for each layer are assumed to be at the same angle. This limit the simulation to be less accurate for large birefringence. In future work, a more accurate beam propagation method can be worked on by studying the s and p modes separately.

The second approximation is the boundary effects are ignored. This means the reflections at the interfaces are not considered.

The third approximation is the term with $\left(\varepsilon_a - n_{ave}^{\ 2}\right) S_l^{\ layer}$ in (5) is assumed to be 0.
When the ϕ=90°, the expression simplifies to,

$$\left(\varepsilon_a - n_{ave}^{\ 2}\right) S_l^{\ layer} =$$

$$= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\frac{\Delta N^2}{2} \end{bmatrix} \begin{bmatrix} S_x \\ S_y \\ Sz \end{bmatrix}$$

$$= -\frac{\Delta N^2}{2} Sz$$

This shows the third approximation yields a simulation result that is less accurate for large birefringence, large incident angle (non-zero Sz), and when the grating vector is different from 90°.

7. CONCLUSION

In this work, the approximate coupled-wave approach is extended from isotropic to birefringent materials. Compared with the RCWA, the approximate approach has limitations but is more intuitively understandable.

Using the (6) from the beam propagation method of the solution to the wave equation, an explanation is provided for the difference between PPD and PVH gratings. First, the incident polarization state only has the possibility to excite either the $+1^{st}$ or -1st order depending on its polarization state being LCP or RCP (for an assumed +Px structure as in Figure.8). Second, for the case when the incident angle and the grating k vector have the same sign, the distinction between the optical effect of a PPD vs. a PVH is related to the changing relative phase between the non-Bragg diffraction order(In this paper, is -1st order) and the 0th order. If the 'ρ' parameter is small, the phase relation between the 0th and non-Bragg diffraction order is relatively unchanged, and the energy can flow into the non-Bragg diffraction order, making the device behaves like a PPD deflector. If the 'ρ' parameter is large, no net energy to be transferred from the 0th order to the non-Bragg diffraction order, and the device behaves like a PVH reflector.

In the case where the incident angle and the grating k vector are of the opposite sign, the distinction between the optical effect of a PPD vs. a PVH is related to the changing relative phase between the $+1^{st}$ order and the 0th order that results in no net energy to be transferred from the 0th order to the $+1^{st}$ order if the 'ρ' parameter is large. These results are summarized in Figure.14 for the case of the grating k vector and incident angle are both positive.

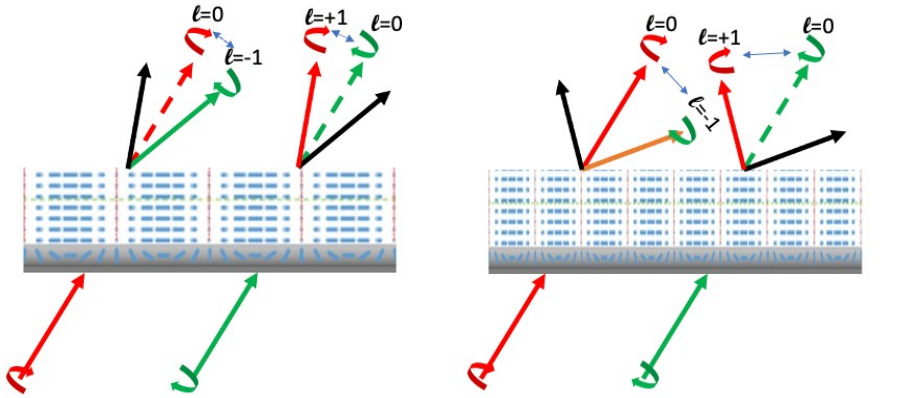

Figure 14. Explanation of the different polarization responds of PPD(a) and PVH(b). The polarization state of light represented by the green arrow is LCP, while the red arrow is RCP. The black arrows represent a diffraction order that is not allowed. In the case of optimized device thickness , no energy is transferred to the direction of the dashed vectors.

In Figure 14, as shown in section 4, energy transfer to the order indicated by the black arrow is prevented because the order is not activated by the incident polarization state. The difference between PPD and PVH devices is shown in section 5. For PVH device, the energy transfer to the -1st order is prevented because of the rapidly changing phase relationship between this order and the 0th order incident beam. The polarization explanation, as shown in section 4, and the phase explanation, as shown in section 5, combines to give us a complete answer to why there is a transition between PPD and PVH.

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