



Weekly Lab Meeting

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Second order tensor - Impermeability tensor

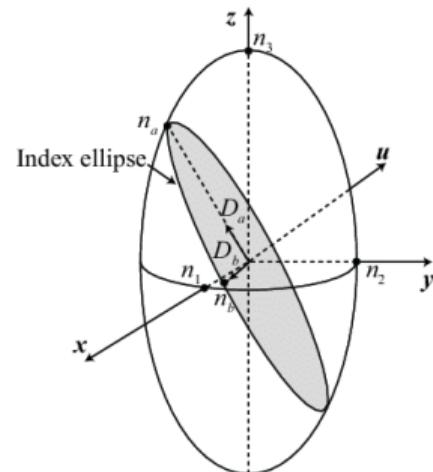
A second-order tensor η_{ij} defined as the relation of an electric field and displacement field vector:

$$\eta_{ij} E_j = D_i \quad (1)$$

Index ellipsoid has the information of impermeability tensor.

Impermeability tensor is crystallographically given by:

$$\eta = \begin{pmatrix} 1/n_1^2 & 0 & 0 \\ 0 & 1/n_2^2 & 0 \\ 0 & 0 & 1/n_3^2 \end{pmatrix} \quad (2)$$



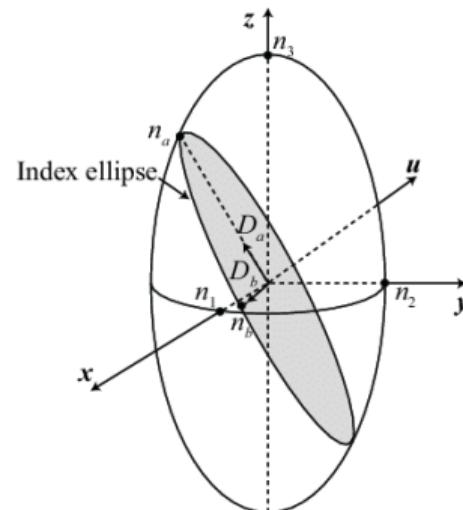
Second order tensor - Impermeability tensor

- **Transverse impermeability tensor**

The intersection of the index ellipsoid with the $\mathbf{k} \cdot \mathbf{D} = 0$ plane.

- **The information of transverse impermeability tensor**

Eigenvector of normal modes (eigenvector of transverse impermeability tensor) with their refractive index. (eigenvalues)



Pockels Perturbed Impermeability Tensor of PPKN

- **Periodically poled potassium niobate (PPKN)**

A perovskite ferroelectric crystal belonging to the orthorhombic point group mm2 at room temperature.

The crystallographic axes are labeled a , b , and c , with lattice parameters $a_0 = 5.6896 \text{ \AA}$, $b_0 = 3.9692 \text{ \AA}$, and $c_0 = 5.7256 \text{ \AA}$

For KNbO₃ at $\lambda = 1550 \text{ nm}$ and $T = 22^\circ\text{C}$, the refractive indices are $n_a = 2.1975$, $n_b = 2.2321$, and $n_c = 2.1014$, obtained from Sellmeier equations.

Assignment of dielectric and crystallographic axes : $x, y, z \equiv b, a, c (2, 1, 3)$

Quasi-phase-matched (QPM) devices in ferroelectric crystals are most commonly implemented using periodically poled 180° domains. Let [001] be $+c$ direction.

Pockels Perturbed Impermeability Tensor of PPKN

- Pockels Perturbed Impermeability

A third-order tensor r_{ijk} defined as the linear derivative of the impermeability tensor with respect to the electric field: $\Delta\eta_{ij} = r_{ijk}E_k$

$$\eta_{ij}(\mathbf{E}) = \eta_{ij}(0) + \frac{\partial\eta_{ij}}{\partial E_k} \Big|_{\mathbf{E}=0} E_k + \frac{1}{2} \frac{\partial^2\eta_{ij}}{\partial E_k \partial E_\ell} \Big|_{\mathbf{E}=0} E_k E_\ell + \dots \quad (3)$$

In our case, mm2 group is noncentrosymmetric. By using contracted notation, the Pockels term $r_{mk}E_k$ can be written explicitly as

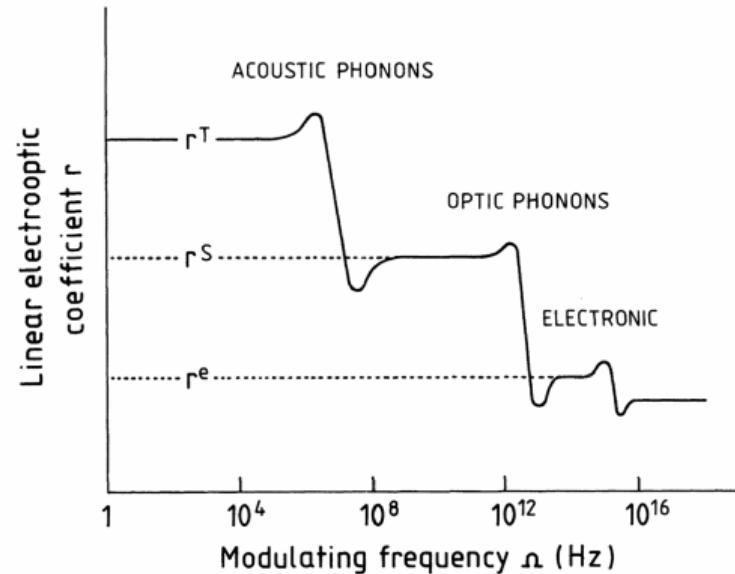
$$r_{mk}E_k = \begin{pmatrix} 0 & 0 & \pm r_{13} \\ 0 & 0 & \pm r_{23} \\ 0 & 0 & \pm r_{33} \\ 0 & \pm r_{42} & 0 \\ \pm r_{51} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix} = \begin{pmatrix} \pm r_{13}E_3 \\ \pm r_{23}E_3 \\ \pm r_{33}E_3 \\ \pm r_{42}E_2 \\ \pm r_{51}E_1 \\ 0 \end{pmatrix}. \quad (4)$$

Pockels Perturbed Impermeability Tensor of PPKN

- Pockels Perturbed Impermeability

Unclamped : T , clamped : S

Pockels Tensor	r_{mk}^T [pm/V]	r_{mk}^S [pm/V]
r_{13}	34 ± 2	20.1 ± 2
r_{23}	6 ± 1	7.1 ± 0.5
r_{33}	63.4 ± 1	34.4 ± 2
r_{51}	120 ± 10	27.8 ± 3
r_{42}	450 ± 30	360 ± 30



Pockels Perturbed Impermeability Tensor of PPKN

- Pockels Perturbed Impermeability

The index ellipsoid of the crystal in the presence of an applied field

$$\eta(\mathbf{E}) = \eta(\mathbf{0}) + \mathbf{r} \cdot \mathbf{E} = \begin{pmatrix} \frac{1}{n_1^2} \pm r_{13} E_3 & 0 & \pm r_{51} E_1 \\ 0 & \frac{1}{n_2^2} \pm r_{23} E_3 & \pm r_{42} E_2 \\ \pm r_{51} E_1 & \pm r_{42} E_2 & \frac{1}{n_3^2} \pm r_{33} E_3 \end{pmatrix}. \quad (5)$$

The magnitude of the Pockels term $r_{mk} E_k$ is typically on the order of 10^{-5} .

→ Treat as a small perturbation.

Modeling as EO Bragg Modulator

- Bragg-regime criteria

$$Q = \frac{2\pi\lambda L}{n\Lambda^2}, \quad p = \frac{\lambda^2}{n\Delta n\Lambda^2}. \quad (6)$$

Δn : the effective refractive index contrast for anisotropic medium.

For Bragg regime, $Q \gg 1$ and $p \gg 1$.

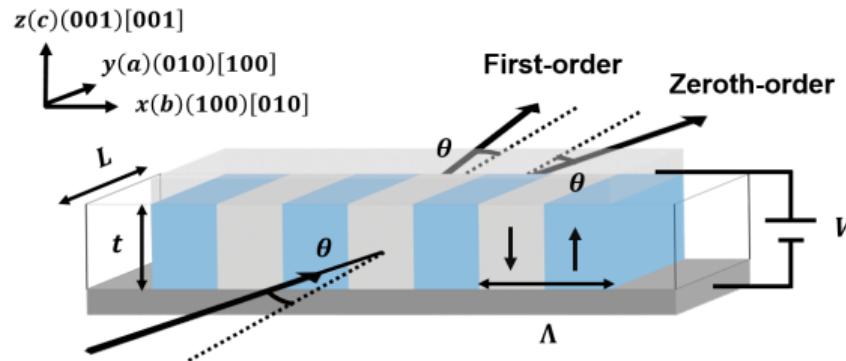
Substituting Eqs. (2) and (3) in Eq. (1) and neglecting the second derivative with respect to z , we arrive at the well-known set of coupled wave equations:

$$\frac{\partial \phi_l}{\partial \xi} = j\rho l^2(1 - B_l)\phi_l + j(\phi_{l-1} + \phi_{l+1}), \quad (4)$$

where $B_l = 2\Lambda \sin\theta_0/\lambda_0 l$, θ_0 is the external angle of incidence, $\xi = \nu(z/L)$, $\nu = \pi n_1 L / \lambda_0 \cos\theta_1$, and θ_1 is the angle of diffraction of the zero-order mode. Thus, B_l is equal to 1 for Bragg diffraction forming the l th mode, and ν is a measure of the grating strength (and appears, e.g., in the coupled mode theory of Kogelnik for Bragg diffraction³). The absorption constant α may be neglected

Modeling as EO Bragg Modulator

- Theoretical Description of EO Bragg modulator



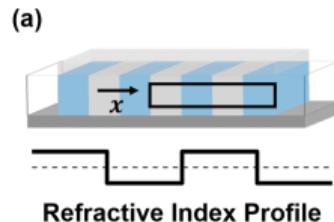
The grating vector : $\mathbf{K} = -(2\pi/\Lambda)\hat{\mathbf{x}}$

An applied field: $\mathbf{E} = (V/t)\hat{\mathbf{z}}$

The incident wavevector lies in the $x - y$ plane at an external angle θ measured from the y -axis.

Modeling as EO Bragg Modulator

- Theoretical Description of EO Bragg modulator



The square-wave grating :

$$\epsilon(x) = \epsilon^{(0)} + \sum_{\text{odd } m} \Delta\epsilon^{(m)} \cos(mKx), \quad (7)$$

The internal Bragg condition

$$\sin \theta_B = \frac{\lambda}{2n\Lambda}, \quad (8)$$

n :the refractive index of the polarization mode of 0th and 1st ordered wave.

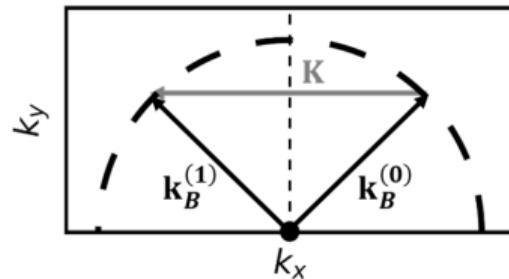
The grating is effectively treated as:

$$\epsilon(x) \approx \epsilon^{(0)} + \Delta\epsilon^{(1)} \cos(Kx), \quad (9)$$

Modeling as EO Bragg Modulator

- Theoretical Description of EO Bragg modulator

The phase matching is already satisfied by the Bragg condition,



$$\Delta \mathbf{k} = \mathbf{k}_B^{(1)} - \mathbf{k}_B^{(0)} - \mathbf{K} = 0, \quad (10)$$

The zeroth-order and first-order Bragg wavevectors

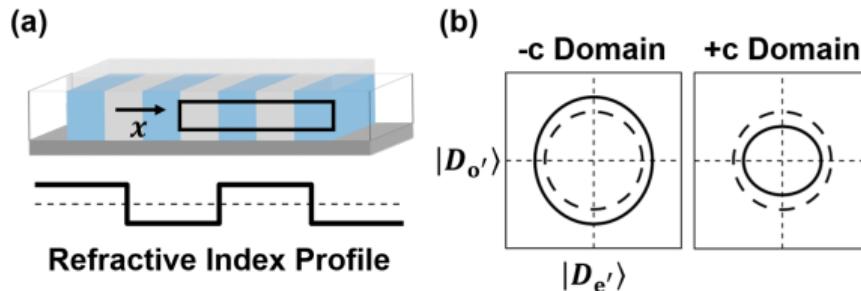
$$\mathbf{k}_B^{(0)} = k(\sin \theta_B \hat{x} + \cos \theta_B \hat{y}), \quad (11)$$

$$\mathbf{k}_B^{(1)} = k(-\sin \theta_B \hat{x} + \cos \theta_B \hat{y}), \quad (12)$$

where $k = 2n\pi/\lambda$. The polarization mode of the incident and diffracted waves are same.

Modeling as EO Bragg Modulator

- Eigenvectors of the unperturbed impermeability tensor



For Bragg-angle propagation in PPKN, the eigenvectors $|D_{o'}\rangle$ and $|D_{e'}\rangle$ of the transverse impermeability tensor are determined by the index ellipse, the intersection of the index ellipsoid with the $\mathbf{k}_B \cdot \mathbf{D} = 0$ plane.

Power splitting by superposition of two eigenvectors.

→ Decreasing the diffraction efficiency

Modeling as EO Bragg Modulator

- **Eigenvectors of the unperturbed impermeability tensor**

The eigenvectors with the condition $\mathbf{k}_B \cdot \mathbf{D} = 0$

$$|D_{o'}\rangle = \hat{x} \mp \tan \theta_{B,o'} \hat{y}, \quad (13)$$

$$|D_{e'}\rangle = \hat{z}. \quad (14)$$

The eigenpolarizations of the normal modes with $\mathbf{E} = \eta \mathbf{D}$.

$$|E_{o'}\rangle = \frac{1}{\sqrt{1 + \beta^2}} (\hat{x} \mp \beta \hat{y}), \quad (15)$$

$$|E_{e'}\rangle = \hat{z}. \quad (16)$$

where $\beta = (n_2^2/n_1^2) \tan \theta_{B,o'}$.

Modeling as EO Bragg Modulator

- **Eigenvectors of the unperturbed impermeability tensor**

Their effective refractive indices are given by

$$\frac{1}{n_{o'}^2} = \frac{\cos^2 \theta_B}{n_2^2} + \frac{\sin^2 \theta_B}{n_1^2}, \quad (17)$$

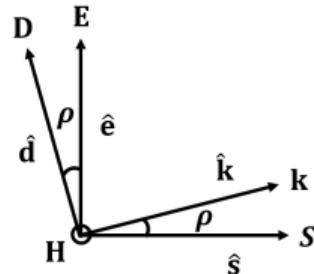
$$n_{e'} = n_3. \quad (18)$$

Small Bragg angle ($\theta_B \ll 1$)

→ zeroth-order $|E_{o'}^{(0)}\rangle$ and first-order eigenpolarization $|E_{o'}^{(1)}\rangle$ are nearly x -polarized, with their refractive index close to $n_{o'} \approx n_2$.

Modeling as EO Bragg Modulator

- Spatial Beam Walk-off of the Unperturbed Impermeability Tensor.



For a plane wave, **D**, **E**, **S**, and the wave normal **k** are coplanar.

$$\tan \rho = \frac{\hat{\mathbf{e}} \cdot \hat{\mathbf{s}}}{\hat{\mathbf{e}} \cdot \hat{\mathbf{d}}} = n^2 \left[\left(\frac{k_x}{n^{-2} - n_2^{-2}} \right)^2 + \left(\frac{k_y}{n^{-2} - n_1^{-2}} \right)^2 + \left(\frac{k_z}{n^{-2} - n_3^{-2}} \right)^2 \right]^{-1/2} \quad (19)$$

(k_x, k_y, k_z) : the components of the wavevector of the polarization modes (o' or e') along the principal axes

n_1, n_2, n_3 : refractive indices of crystallographic axes of the polarization modes.

Modeling as EO Bragg Modulator

- **Spatial Beam Walk-off of the Unperturbed Impermeability Tensor.**

Under the Bragg condition, $\mathbf{k}_B = k (\pm \sin \theta_B \hat{x} + \cos \theta_B \hat{y})$

$$\tan \rho_{o'} = n_{o'}^2 \left[\left(\frac{\sin \theta_{B,o'}}{n_{o'}^{-2} - n_2^{-2}} \right)^2 + \left(\frac{\cos \theta_{B,o'}}{n_{o'}^{-2} - n_1^{-2}} \right)^2 \right]^{-1/2}. \quad (20)$$

In our case, where the propagation vector lies in the x - y plane, the e' -polarized mode exhibits no beam walk-off, since $\hat{\mathbf{e}} \cdot \hat{\mathbf{d}} = 0$.

Analytic Expression

- Coupled Wave Theory for Anisotropic Thick Hologram Theory

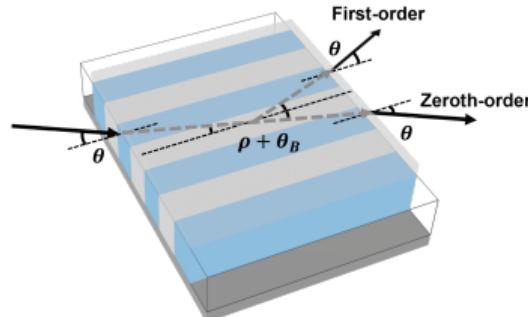
A further simplification is obtained in the case of perfect Bragg matching ($\Delta \vec{k}_r = \vec{0}$, $\xi^2 = 0$). In this case Eq. (39) becomes

$$\eta(d) = \sin^2 \left(\frac{\pi A_r d}{2\lambda(n_s n_p g_s g_p \cos \theta_s \cos \theta_p)^{1/2}} \right) e^{-2\alpha d}, \quad (41)$$

where λ is the vacuum wavelength. The argument of the sin function is of the form $(\pi \Delta n d / \lambda \cos \theta)$ in analogy with Ref. [1], with $\Delta n = A_r / [2(n_s n_p g_s g_p)^{1/2}]$ and $\cos \theta = (\cos \theta_s \cos \theta_p)^{1/2}$. In nonabsorbing materials the maximum

Analytic Expression

- Coupled Wave Theory for Anisotropic Thick Hologram Theory



The First-order diffraction efficiency at $y = L$ under the perfect phase matching,

$$\eta_d(L) = \sin^2 \left(\frac{\pi \Delta n L}{\lambda \cos(\theta_B - \rho)} \right), \quad (21)$$

The effective index contrast Δn for an anisotropic medium

$$\Delta n = \frac{\langle E^{(1)} | \Delta \epsilon^{(1)} | E^{(0)} \rangle}{2n \cos \rho}. \quad (22)$$

Here, $\theta_i = \theta_B = -\theta_d$ in the Bragg configuration.

Analytic Expression

- **Coupled Wave Theory for Anisotropic Thick Hologram Theory**

the dielectric contrast $\Delta\epsilon$ to the first Fourier component $\Delta\epsilon^{(1)}$ of the square-wave grating

$$\Delta\epsilon^{(1)} \approx -\frac{2}{\pi}\epsilon(\mathbf{0})\Delta\eta\epsilon(\mathbf{0}) \quad (23)$$

where unperturbed dielectric tensor $\epsilon(\mathbf{0}) = (\eta(\mathbf{0}))^{-1}$.

Analytic Expression

- **180°-domain PPKN**

The contrast of the impermeability tensor

$$\Delta\eta = \begin{pmatrix} 2r_{13}E & 0 & 0 \\ 0 & 2r_{23}E & 0 \\ 0 & 0 & 2r_{33}E \end{pmatrix} \quad (24)$$

The first-order Fourier component of the dielectric tensor modulation

$$\Delta\epsilon^{(1)} = -\frac{2}{\pi} \begin{pmatrix} 2n_1^4 r_{13}E & 0 & 0 \\ 0 & 2n_2^4 r_{23}E & 0 \\ 0 & 0 & 2n_3^4 r_{33}E \end{pmatrix} \quad (25)$$

Analytic Expression

- o' -polarized wave of 180° -domain PPKN

Diffraction efficiency

$$\begin{aligned}\eta_d(L) &= \sin^2 \left[\frac{2}{1 + \beta^2} \frac{L (n_2^4 r_{23} - \beta^2 n_1^4 r_{13}) V}{\lambda t n_{o'} \cos(\theta_B - \rho_{o'}) \cos \rho_{o'}} \right] \\ &\approx \sin^2 \left[\frac{2 L n_2^3 r_{23} V}{\lambda t \cos(\theta_B - \rho_{o'}) \cos \rho_{o'}} \right].\end{aligned}\tag{26}$$

Half-wave voltage V_π

$$\begin{aligned}V_\pi &= \frac{(1 + \beta^2)\pi n_{o'} \lambda t \cos(\theta_B - \rho_{o'}) \cos \rho_{o'}}{4 L n_2^4 r_{23}} \\ &\approx \frac{\pi \lambda t \cos(\theta_B - \rho_{o'}) \cos \rho_{o'}}{4 L n_2^3 r_{23}}.\end{aligned}\tag{27}$$

Analytic Expression

- **e'-polarized wave of 180°-domain PPKN**

Diffraction efficiency

$$\eta_d(L) = \sin^2 \left[\frac{2L n_3^3 r_{33} V}{\lambda t \cos \theta_B} \right]. \quad (28)$$

Half-wave voltage V_π

$$V_\pi = \frac{\pi \lambda t \cos \theta_B}{4L n_3^3 r_{33}}. \quad (29)$$

Benchmarking Results with RCWT

- Setting physical device parameter

Table 2: Reported fabrication parameters of bulk 180°-domain PPKN devices, reformulated for the EO Bragg modulator considered in this work. In this convention, the crystal thickness t is along the c axis, whereas the interaction length L is defined along the a axis.

Thickness t (mm)	Length L (mm)	Poling period Λ (μm)	Reference
0.925	3	32.5	Kim & Yoon, Appl. Phys. Lett. 81 , 3332 (2002) [24]
1.0	10	35.5	Hirohashi <i>et al.</i> , Jpn. J. Appl. Phys. 43 , 559 (2004)[25]
1.0	8	14.4	Yu <i>et al.</i> , Appl. Phys. Lett. 85 , 5839 (2004) [26]
1.0	10	30	Meyn <i>et al.</i> , Opt. Lett. 24 , 1154 (1999) [27]

This thickness is consistent with domain measurements on a 0.6 mm-thick c -cut KNbO₃ plate, we adopt 0.5 mm in our simulations.

A crystal length $L = 1$ cm, a crystal thickness $t = 500 \mu\text{m}$, and a poling period $\Lambda = 14.4 \mu\text{m}$ at an operating wavelength of $\lambda = 1550 \text{ nm}$.

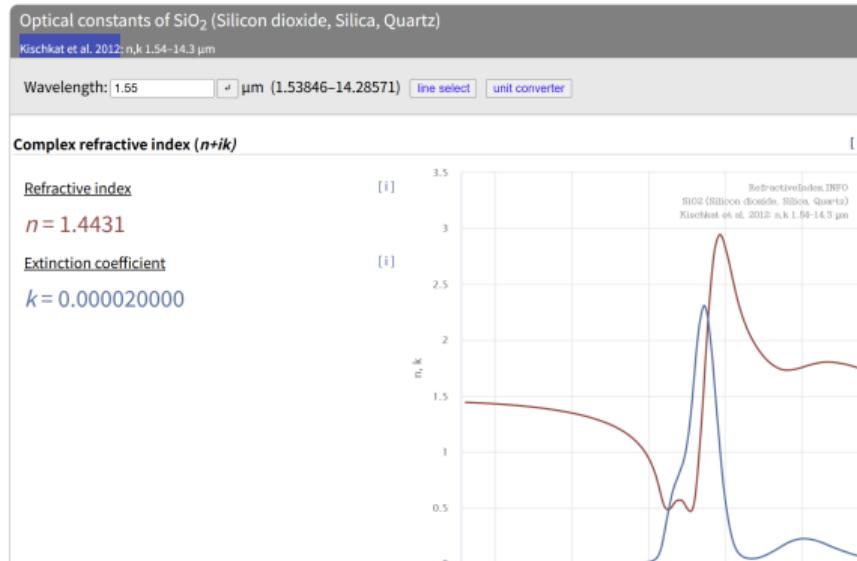
Benchmarking Results with RCWT

- Anti-reflection coating (single layer AR coating)

For so small Bragg angle, the incident wave is close to normal.

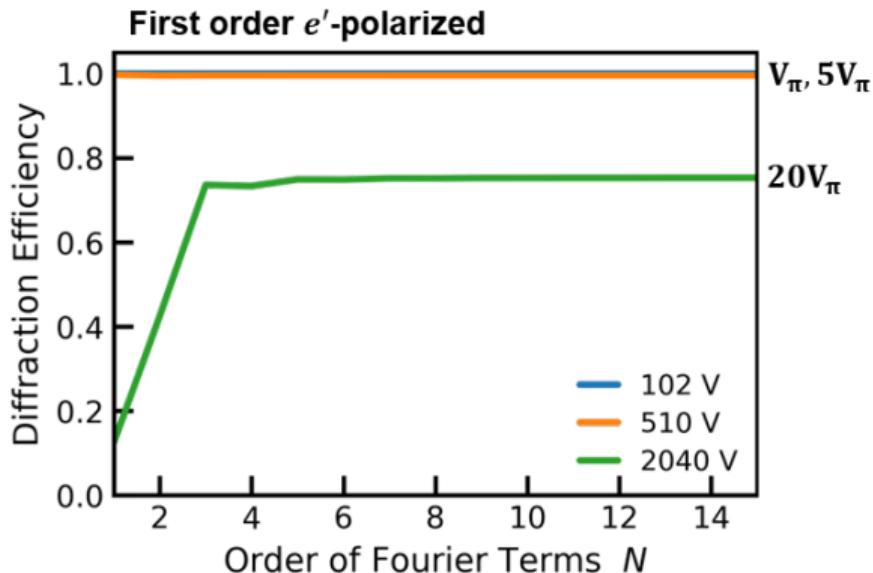
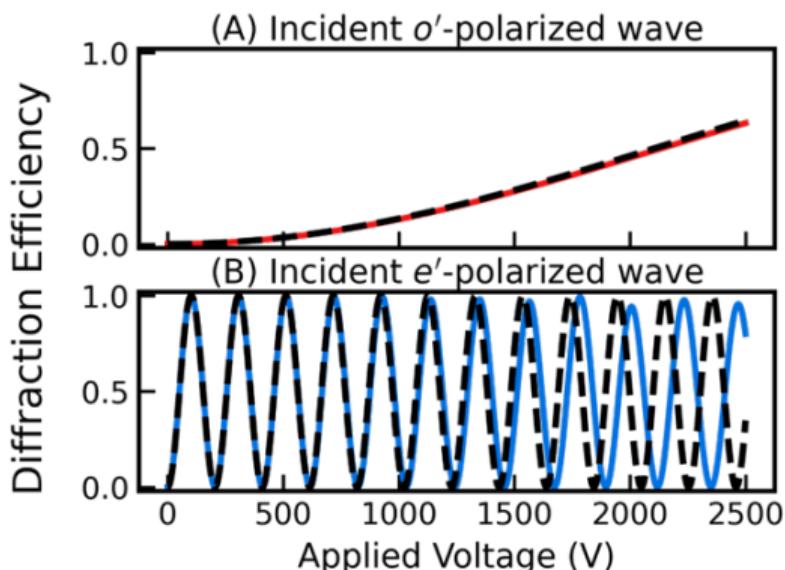
The thickness $t_f = \lambda/(4n_f)$, where $n_f \approx \sqrt{n_{\text{air}} n_j}$ for $j = o', e'$.

This design value is close to that of SiO_2 with $n_f = 1.4431$, yielding a film thickness of $t_f \approx 268$ nm at $\lambda = 1550$ nm.



Good Convergence

$L = 1 \text{ cm}$, $t = 500 \mu\text{m}$, $\Lambda = 14.4 \mu\text{m}$ and $\lambda = 1550 \text{ nm}$



As the applied voltage increases (the refractive index contrast increases), the period (\sin^2) of the diffraction efficiency becomes longer and higher-order Fourier components redistribute the diffraction efficiency.

Numerical results

external incidence angle in air : 3.085°

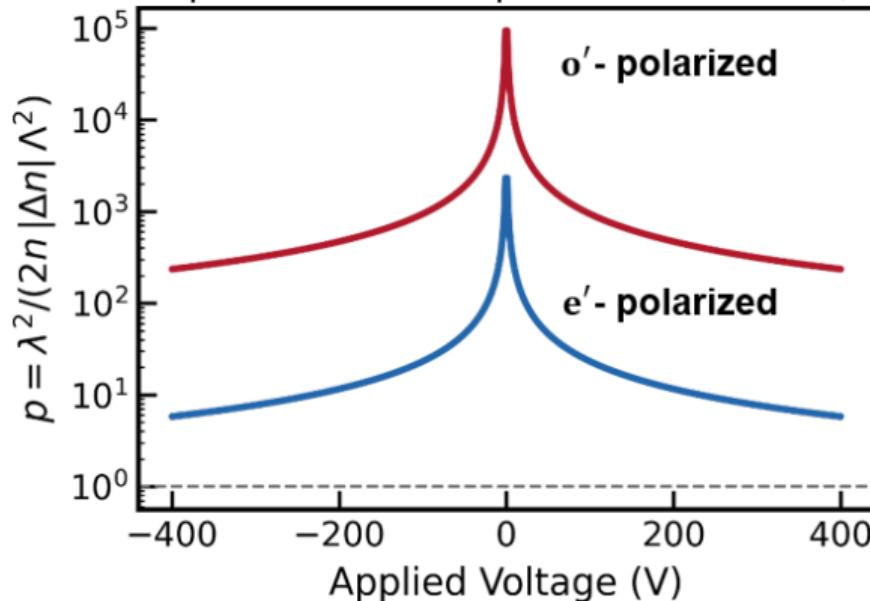
internal incidence angles of 1.468° and 1.382° for the o' - and e' -polarized waves, respectively.

The beam walk-off angle of the o' -polarized wave, $\rho_{o'} = 0.0439^\circ$

The e' -polarized wave exhibits no beam walk-off.

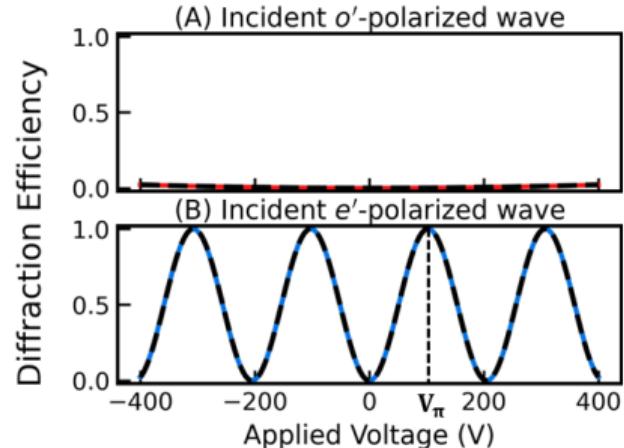
Bragg or not?

$Q = 210.4$ and $Q = 223.5$ for o' -polarized and e' -polarized incidence, respectively.



These results indicate that the applied voltage controls the contrast of effective refractive index and that p decreases as the voltage increases.

RCWT vs anisotropic Thick hologram theory



r_{33} of e' -polarized wave

→ In unclamped KNbO₃, r_{33} is approximately twice that of congruent LiNbO₃ (Li/Nb = 0.937), while their principal refractive indices are comparable ($n_3 \approx 2.10$ for KNbO₃ and $n_e \approx 2.14$ for LiNbO₃).

The half-wave voltage V_π of the EO PPLN Bragg modulator can be expected to be roughly half that of a comparable PPLN device.

Conclusion

- (1) The half-wave voltage V_π of the EO modulator in KNbO₃ can be expected to be roughly half that of a comparable PPLN device.
- (2) When the Bragg angle or beam walk-off cannot be neglected, the full anisotropic expressions derived in this work must be used.
 - The analytic expressions derived in this work can be directly applied to many other periodically poled ferroelectric crystals, our analysis naturally extends beyond PPKN devices.