Analysis of strain-induced Pockels effect in Silicon

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Outline

• Electro-optic effect in crystal
• Strain-induced Pockels effect
• The proposed model and the overlap functions
• Conclusion
Nonlinear optics

Nonlinear effect can be mathematically described by the polarization vector

\[ D_i(r, t) = \varepsilon_0 E_i(r, t) + P_i(r, t) \]

The general formula of the polarization vector is quite complicated*

\[ P_i(r, t) = \varepsilon_0 \int \chi^{(1)}_{ij}(r-r', t-t') E_j(r', t') dr' dt \]
\[ + \varepsilon_0 \int \chi^{(2)}_{ijk}(r-r_1, t-t_1, r-r_2, t-t_2) E_j(r_1, t_1) E_k(r_2, t_2) dr_1 dt_1 dr_2 dt_2 \]
\[ + \varepsilon_0 \int \chi^{(3)}_{ijkl}(r-r_1, t-t_1, r-r_2, t-t_2, r-r_3, t-t_3) E_j(r_1, t_1) E_k(r_2, t_2) E_l(r_3, t_3) dr_1 dt_1 dr_2 dt_2 dr_3 dt_3 + \ldots \]

For a local medium, in the frequency domain we have

\[ P_i(r, \omega) = \varepsilon_0 \chi^{(1)}_{ij}(r, \omega) E_j(r, \omega) \]
\[ + \varepsilon_0 \chi^{(2)}_{ijk}(r, \omega_1, r, \omega_2) E_j(r, \omega_1) E_k(r, \omega_2) \]
\[ + \varepsilon_0 \chi^{(3)}_{ijkl}(r, \omega_1, r, \omega_2, r, \omega_3) E_j(r, \omega_1) E_k(r, \omega_2) E_l(r, \omega_3) \]  
\[ \text{Linear term (refractive index)} \]
\[ \text{Quadratic term (Pockels effect, SHG)} \]
\[ \text{Cubic term (Kerr effect, FWM)} \]

*Einstein notation is used. The sum over repeated indices is always understood.
Electro-optic effect in crystal

The quadratic nonlinear susceptibility is responsible of the Pockels effect

\[ P_i^{(2)}(\omega) = \varepsilon_0 \chi_{ijk}^{(2)} E_j(0) E_k(\omega) \]

\( \chi^{(2)} \) is a 3-index tensor

- 27 components
- 18 independent components

Our goals

1. \( \chi^{(2)} \) as a function of the strain gradient tensor
2. Theory and optimization of nonlinear effects in silicon waveguides
Centrosymmetric crystal and deformations

- Inversion point
  - for every point \((x, y, z)\) in the unit cell there is an indistinguishable point \((-x, -y, -z)\).
- No native \(\chi^{(2)}\)

- Surface interface or Non uniform strain
  - Centrosymmetry is broken
  - \(\chi^{(2)}\) appears

\( \chi^{(2)} \) as a function of the strain gradient tensor

Approximation of \( \chi^{(2)} \) with its Taylor series with respect to the strain tensor and strain gradient tensor

\[
\chi_{ijk}^{(2)} (\varepsilon, \zeta) = \chi_{ijk}^{(2)} (\varepsilon = 0, \zeta = 0) + \sum_{l,m} \frac{\partial \chi_{ijkl}^{(2)}}{\partial \varepsilon_{lm}} \varepsilon_{lm} + \sum_{l,m,n} \frac{\partial \chi_{ijkl}^{(2)}}{\partial \zeta_{lmn}} \zeta_{lmn} + o \left( \max \{|\varepsilon_{lm}|, |\zeta_{lmn}|\} \right)
\]

Vanishes as a 5 index tensor and as all the Tensors with odd number of indices

\[
T_{ijk\alpha\beta\gamma} = \left. \frac{\partial \chi_{ijkl}^{(2)}}{\partial \zeta_{\alpha\beta\gamma}} \right|_{\varepsilon = 0}
\]

6-index tensor \( \Rightarrow \) Survives!

3\(^6\) = 729 components!
Symmetries

Symmetry of the strain tensor

\[ \varepsilon_{\alpha\beta} = \varepsilon_{\beta\alpha} \quad \Rightarrow \quad \zeta_{\alpha\beta\gamma} = \zeta_{\beta\alpha\gamma} \]

Symmetry of the Pockels effect

\[ \chi^{(2)}_{ijk}(\omega, 0) = \chi^{(2)}_{ikj}(0, \omega) , \]

\[ \chi^{(2)}_{ijk}(\omega, 0) = \chi^{(2)}_{ijk}(-\omega, 0) = \chi^{(2)}_{jik}(\omega, 0) , \text{ Lossless condition} \]

48 symmetry operations compatible with cubic lattice of silicon

\[
\begin{pmatrix}
\pm1 & 0 & 0 \\
0 & \pm1 & 0 \\
0 & 0 & \pm1
\end{pmatrix},
\begin{pmatrix}
\pm1 & 0 & 0 \\
0 & 0 & \pm1 \\
0 & \pm1 & 0
\end{pmatrix},
\begin{pmatrix}
0 & \pm1 & 0 \\
0 & 0 & \pm1 \\
\pm1 & 0 & 0
\end{pmatrix},
\begin{pmatrix}
0 & \pm1 & 0 \\
\pm1 & 0 & 0 \\
0 & 0 & \pm1
\end{pmatrix},
\begin{pmatrix}
\pm1 & 0 & 0 \\
0 & \pm1 & 0 \\
0 & 0 & \pm1
\end{pmatrix}.
\]

Due to symmetries, only 15 components of \( \chi^{(2)} \) are independent!
What can we measure? ...the effective susceptibility

The effective index can be experimentally measured

$$\Delta n_{\text{eff}} = \frac{\varepsilon_0 c}{N} \int_A E_i^* \chi_{ijk}^{(2)}(\omega, 0) E_j^* E_k^{dc} \, dA,$$

$$N = \frac{1}{2} \int_{A_\infty} (\mathbf{E} \times \mathbf{H}^* + \mathbf{E}^* \times \mathbf{H}) \cdot \mathbf{i}_z \, dA.$$

The effective susceptibility vector can be defined as

$$\chi_{\text{eff}}^k E_k^{dc} = n_{\text{eff}} \Delta n_{\text{eff}},$$

$$\chi_{k, \alpha\beta\gamma}(\omega, 0) = T_{ik\alpha\beta\gamma}(\omega, 0) \cdot \frac{\varepsilon_0 c}{N} \int_A E_i^*(\mathbf{x}) \zeta_{\alpha\beta\gamma}(\mathbf{x}) E_j(\mathbf{x}) \, dA.$$  

If only $E_y \neq 0$, we can write in a more compact way

$$\chi_{\text{eff}}^y(\omega) = c_i o_i(\omega),$$

$c_i$ can be derived from the experimental results.

$$n^2 = \varepsilon / \varepsilon_0,$$

$$\varepsilon = \varepsilon_0 \left[ 1 + \chi^{(1)} + 2 \chi^{(2)} E^{dc} \right].$$
COMSOL modal analysis

The waveguides show a single mode behavior but $E_z$ and $E_y$ components are not negligible compared to $E_x$ component and thus the mode is clearly not purely transverse electric. The high value of $E_z$ is due to the high index step of the waveguide.


COMSOL mechanical deformation

Silicon anisotropy described by orthotropic model and initial stress of 1 GPa


Overlap function $\chi_{y}^{\text{eff}} = c_{i} o_{i}$ 


Conclusion

- A simple model is proposed for the Pockels effect
- Design and optimization of strained silicon based device
- Other second order effect in strained silicon (e.g., Second Harmonic Generation) can be modelled
- Further investigations and experimental results are needed to evaluate all 15 coefficients
- Paper accepted on Optics Express and on arxive (http://arxiv.org/abs/1507.06589)