# Modeling Material Susceptibility in Silicon for Four-Wave Mixing Based Nonlinear Optics

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***Abstract*—We model the third-order material susceptibility $\overleftrightarrow{\chi}^{[3]}$ in silicon waveguides for integrated optics. Analysis of four-wave mixing in these waveguides requires an in-depth study of material nonlinearity - in contrast to modeling light propagation in fibers with the optical nonlinear Schrödinger equation. We include electronic and atomic lattice (Raman) responses of the material and present a relatively easy-to-use representation of the material susceptibility.**

***Index Terms*—nonlinear optics, susceptibility, four-wave mixing, silicon photonics, integrated optics**

## I. Introduction

Optical signal processing is considered as a promising way for increasing network capacity, which is a reason why integration platforms of photonic and photo-electronic components have recently received increased attention. A key functionality of optical signal processing on integrated platforms will be wavelength conversion, where four-wave mixing (FWM) as nonlinear process is used. The choice of silicon as waveguide material leads to specific additional nonlinear effects such as Raman scattering. As a result of the high Raman gain coefficient in silicon, which is three to four orders of magnitude higher compared to silica [1], it is essential to include these effects besides the commonly considered Kerr effect. In the following, the third-order susceptibility for silicon as origin of nonlinear effects is determined.

Throughout this paper, we assume a waveguide fabricated on a (001) surface and parallel to the [110] direction. Furthermore, only the FWM processes involving one negative frequency contribution, such as optical phase conjugation (PC) and Bragg scattering (BS), will be considered.

## II. Motivation

Based on Maxwell's equations, the propagation equation of the newly generated field amplitude at frequency $f_0$ for the specific mode $a$ can be derived as

$$\begin{aligned}\frac{\partial}{\partial z}\hat{E}_a^{f_0}(z) = &-\frac{\alpha^a}{2}\hat{E}_a^{f_0}(z)\\ &- j\gamma_1^a\left(\sum_m \hat{E}_m^{f_0}(z)\,\mathrm{e}^{-j(\beta_m(f_0)-\beta_a(f_0))z}\langle Mc\rangle_m^a\right)\\ &- j\gamma_2^a\Bigg(\sum_{\substack{(\zeta,\eta,\rho)\\ \in\mathcal{S}}}\sum_{(m_1,m_2,m_3)}\langle 0\zeta\eta\rho\rangle_{m_1,m_2,m_3}^a\\ &\qquad \hat{E}_{m_1}^{f_\zeta}(z)\left(\hat{E}_{m_2}^{f_\eta}(z)\right)^*\hat{E}_{m_3}^{f_\rho}(z)\,\mathrm{e}^{-j\Delta\beta z}\Bigg),\end{aligned} \tag{1}$$

where $\mathcal{S} = \left\{(\zeta,\eta,\rho): f_0 = f_\zeta + f_\eta + f_\rho \,\middle|\, f_\zeta, f_\rho > 0, f_\eta < 0\right\}$, $\gamma_1^a = \frac{\beta_0(f_0)^2}{2\beta_a(f_0)\iint|\vec{\Psi}_a^{f_0}(x,y)|^2\mathrm{dA}}$, $\gamma_2^a = \frac{3\beta_0(f_0)^2}{8\beta_a(f_0)\iint|\vec{\Psi}_a^{f_0}(x,y)|^2\mathrm{dA}}$, $\langle Mc\rangle_m^a$ is the linear mode coupling coefficient, $\alpha^a$ the waveguide attenuation, $\beta_a$ the propagation constant of mode $a$, $\Delta\beta = \beta_{m_1}(f_\zeta) - \beta_{m_2}(f_\eta) + \beta_{m_3}(f_\rho) - \beta_a(f_0)$ the phase mismatch, $\beta_0(f_0)^2 = (2\pi f_0)^2\epsilon_0\mu_0$, and $\langle 0\zeta\eta\rho\rangle_{m_1,m_2,m_3}^a = \iint\left(\vec{\Psi}_a^{f_0}\right)^*\left(\overleftrightarrow{\chi}^{[3]}(f_0; f_\zeta, f_\eta, f_\rho)\vdots\vec{\Psi}_{m_1}^{f_\zeta}\left(\vec{\Psi}_{m_2}^{f_\eta}\right)^*\vec{\Psi}_{m_3}^{f_\rho}\right)\mathrm{dA}$ the nonlinearity coefficient with transversal field distribution $\vec{\Psi}_m^f$ and cubic fourth-rank susceptibility $\overleftrightarrow{\chi}^{[3]}(f_0; f_\zeta, f_\eta, f_\rho) \in \mathbb{C}^{3\times3\times3\times3}$. Analog equations hold for all other interacting frequencies and thus lead to a coupled system of differential equations. All susceptibilities of even order vanish in silicon [2], which turns the third-order susceptibility into the first nonlinear contribution. The $\overleftrightarrow{\chi}^{[3]}$ tensor is the origin of third-order nonlinear processes and the basis for FWM-based optics. Therefore, we derive a relatively easy-to-use model for its structure and entries.

## III. The Tensor Nature of the Suscepetibility in Silicon

In silicon, there are two main parts that account for nonlinear processes, namely the electronic contribution ($e$) due to bound electrons and the Raman contribution ($R$) stemming from atomic lattice vibrations. Hence, it is reasonable to split the third-order nonlinear susceptibility tensor into its main parts, i.e., $\overleftrightarrow{\chi}^{[3]} = \overleftrightarrow{\chi}_e + \overleftrightarrow{\chi}_R$, and investigate each part separately [3].

### A. Electronic Susceptibility in Frequency Domain

Due to spatial symmetry, only 21 out of 81 entries of $\overleftrightarrow{\chi}_e$ are nonzero, of which only four are independent of each other [2]. If only wavlengths $\lambda > \lambda_{\min} = 1.10\,\mu\mathrm{m}$ are considered, the Kleinmann condition is satisfied and three of the four independent elements can be approximated to be equal [3], [4], [5]. Usually the electronic susceptibility is considered as nearly constant, since variations of the interacting frequencies lead to only small fluctuations of $\overleftrightarrow{\chi}_e$. For a wavelength range including the commonly used optical bands from O to L, the spacing between interacting frequencies is small enough to treat nonlinearity caused by the electronic contribution as being indepent of the interacting frequencies, i.e. $\overleftrightarrow{\chi}_e(f_0; f_\zeta, f_\eta, f_\rho) \approx \overleftrightarrow{\chi}_e(f_0)$. With this assumption and for $\lambda \in [1.2\,\mu\mathrm{m}, 2.4\,\mu\mathrm{m}]$ (also inlcuding bands O to L), the last two independent entries of $\overleftrightarrow{\chi}_e$ can be related to each other

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as well [6]. Furthermore, the real and imaginary part of the last independent entry is linked to the Kerr coefficient $n_2$ and the two-photon absorption coefficient $\beta_{\text{tpa}}$, respectively. Altogether, this leads to the 21 nonzero elements

$$\begin{aligned}
\chi_e^{xxxx} &= \Re\{\chi_e^{xxxx}\} + j\Im\{\chi_e^{xxxx}\} \\
&= \chi_e^{yyyy} = \chi_e^{zzzz} \\
\frac{\chi_e^{xxxx}}{2.36} &= \chi_e^{xxyy} = \chi_e^{zzyy} = \chi_e^{yyzz} = \chi_e^{zzxx} = \chi_e^{xxzz} \\
&= \chi_e^{yyxx} = \chi_e^{xyxy} = \chi_e^{zyzy} = \chi_e^{yzyz} = \chi_e^{zxzx} \\
&= \chi_e^{xzxz} = \chi_e^{yxyx} = \chi_e^{xyyx} = \chi_e^{zyyz} = \chi_e^{yzzy} \\
&= \chi_e^{zxxz} = \chi_e^{yxxy} = \chi_e^{xzzx},
\end{aligned} \tag{2}$$

with $\Re\{\chi_e^{xxxx}\} = 2.3482 \cdot n_2(f_0) \cdot \epsilon_0 \cdot c_0 \cdot n^2(f_0)$, $\Im\{\chi_e^{xxxx}\} = \frac{1.1741}{2\pi f_0} \cdot \beta_{\text{tpa}}(f_0) \cdot \epsilon_0 \cdot c_0^2 \cdot n^2(f_0)$ [5], [7], where the characteristics of $n_2$ and $\beta_{\text{tpa}}$ can be found in [4].

### B. Raman Susceptibility in Frequency Domain

The Raman contribution $\overleftrightarrow{\chi}_R$ emerges from the interaction of light with lattice vibrations (phonons) of the material. If the difference of two incident light waves coincides with the frequency of the lattice vibration (resonance), the atom is excited to a higher vibrational eigenstate. The susceptibility elements induced by Raman scattering can be stated as [8], [1], [3]

$$\begin{aligned}
&\chi_R^{\text{ijkl}}(f_0; f_\zeta, f_\eta, f_\rho) = \chi_R^{\text{ijkl}}(f_0; f_1, -f_2, f_3) \\
&= \frac{1}{\pi} f_v \Gamma \frac{c_0}{Z_0} \left( \chi_1^{\text{ijkl}}(f_2 - f_3) \sum_{n=1}^{3} (R_{ij})_n (R_{kl})_n \right. \\
&\qquad \left. + \chi_1^{\text{ijkl}}(f_2 - f_1) \sum_{n=1}^{3} (R_{il})_n (R_{jk})_n \right),
\end{aligned} \tag{3}$$

with $\chi_1^{\text{ijkl}}(f_2 - f_a) = \frac{n^2(f_a) g_R(f_a)}{f_a\left(\left(f_v^2 - (f_2 - f_a)^2\right) - j\Gamma(f_2 - f_a)\right)}$, $a \in \{1, 3\}$, and $i, j, k, l \in \{x, y, z\}$, where $\Gamma = 105\,\text{GHz}$ is the FWHM-bandwidth, $f_v = 15.6\,\text{THz}$ the vibrational eigenstate frequency, $Z_0 = \sqrt{\frac{\mu_0}{\epsilon_0}}$, $g_R$ the Raman gain coefficient, and $R_n$, $n \in \{1, 2, 3\}$ the three Raman matrices with $R_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & -1 \\ -1 & -1 & 0 \end{bmatrix}$, $R_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$, $R_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & -1 \\ 1 & -1 & 0 \end{bmatrix}$. Each Raman matrix corresponds to the respective displacement of the phonons along the crystallographic directions of the medium and reflects its crystal symmetry. The terms $\sum_{n=1}^{3} (R_{ij})_n (R_{kl})_n$ and $\sum_{n=1}^{3} (R_{il})_n (R_{jk})_n$ determine the 18 nonzero elements of $\overleftrightarrow{\chi}_R$. Note that all denoted frequency values apply only at room temperature, i.e., $T \approx 300\,\text{K}$. The formula and the required parameters for the approximation of $g_R$ can be found in [1], [9], [10], [11]. Equation (1) was solved with a variable-step, variable-order Adams-Bashforth-Moulton solver. The generation process of the phase-matched BS idler, based on (1) and the presented composition of $\overleftrightarrow{\chi}^{[3]}$ is illustrated in Figure 1.

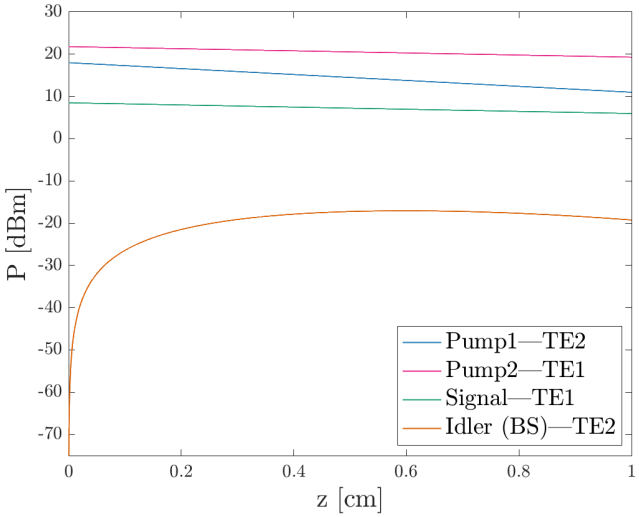


Fig. 1. Power development of input and output waves over the waveguide.

## IV. Conclusion

Numerical simulation of FWM-based signal generation necessitates thorough modeling of the material susceptibility $\overleftrightarrow{\chi}^{[3]}$. We have shown that it consists of two parts which can be calculated separately: electronic and Raman contributions $\overleftrightarrow{\chi}_e$ and $\overleftrightarrow{\chi}_R$. We linked the components of $\overleftrightarrow{\chi}_e$ to material parameters and presented a closed-form solution for $\overleftrightarrow{\chi}_R$. Although the approximations we applied limit the useable wavelength region, it includes all commonly used optical transmission bands.

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