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# Advances in second order nonlinear effect in Silicon

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**Abstract:** In this work, we present a theoretical model to determine the second order nonlinear coefficient under strain gradient in silicon. Furthermore, carrier effect due to applied electric field has also been taking into account to analyze the obtained experimental phase variation.

#### I. INTRODUCTION

Silicon-based photonics has generated a strong interest in recent years, mainly for optical communications and optical interconnects in CMOS circuits. The main motivations for silicon photonics are the reduction of photonic system costs and the increase of the number of functionalities on the same integrated chip by combining photonics and electronics, along with a strong reduction of power consumption<sup>1</sup>. However, one of the biggest constraints of silicon as an active

photonic material is its vanishing second order optical susceptibility, the so called  $\chi^{(2)}$ , due to the centrosymmety of the silicon crystal. Without any second order nonlinear phenomena, fast and low power consumption optical modulation based on Pockels effect and wavelength conversions based on Second Harmonic Generation (SHG), other strategies, mainly based on either plasma dispersion effect in silicon<sup>2</sup> or electro-absorption in bulk Ge and Ge/SiGe quantum wells<sup>3</sup>, have been developed for modulation. Even, impressive results have been obtained in terms of speed and efficiency; the power consumption is still too high for the next generation of photonic circuits. Indeed, the fact, not to have the possibility to exploit nonlinear effects in silicon for modulation is a very limiting factor when we expect silicon to be part of a solution to high performances and highly energy efficient devices. To overcome this limitation, strain ( $\varepsilon$ ) has been used as a way to deform the crystal and destroy the centrosymmetry which inhibits  $\chi^{(2)}$ . In fact, over the last few years Pockels electro-optic modulation and SHG have been claimed and been demonstrated in devices where the silicon active region is strained by a stress overlayer, usually made of SiN<sup>4-10</sup>. This is the very motivation to the development of *strained silicon* devices for optical modulation: the prospect of a high speed, low loss, compact, low power consumption, with large optical bandwidth and silicon compatible modulator. The paper present the recent advances in the development of nonlinear is this exciting topic including discussions from fundamental origin of Pockels effect in silicon until its implementation in a real device.

#### **II. THEORITICAL MODEL**

We start our analysis to strained silicon by studying how strain affects the silicon crystal structure to understand how  $\chi^{(2)}$  effects can be generated. To achieve that, we developed an original theoretical model based on the *Bond Orbital Model*, which is a quantum mechanical theory that describes the electrons in the bonds between the silicon. By using that approach together with symmetry arguments, we found that the spatial distribution of  $\chi^{(2)}$  in the crystal can be given by

$$\chi^{(2)}_{ijk} = \Gamma_{ijk,lmn} \, , \, \eta_{imn} \, , \qquad (1)$$

where  $\eta_{lmn}$  is a *strain gradient* component defined by :

$$\eta_{ijk} \equiv \frac{\partial \varepsilon_{ij}}{\partial x_k} \,. \tag{2}$$

This means that  $\chi^{(2)}$  is defined by the contribution of all strain gradients, weighted by the  $\Gamma$  coefficients. The values of  $\Gamma$  can be uniquely determined by the Bond Orbital description, which defines  $\Gamma$  as a function of only two parameters  $\alpha$  and  $\beta$ . In fact, being a tensor characteristic of the crystal,  $\Gamma$  depends on the crystal orientation and from our model, we could deduce the most relevant components of  $\Gamma$  in a [010] silicon wafer as a function of the angle  $\phi$  ( $\phi = 0$  corresponds to [110] and  $\phi = \pi/4$  corresponds to [100] directions) as follows:

$$\Gamma_{xxy,xxy}(\varphi) = \frac{d^{6}K}{27\epsilon_{0}} \left[ (5\beta - 3\alpha - (\alpha + \beta)\cos(4\varphi)) \right]$$
  
$$\Gamma_{xxy,yyy}(\varphi) = -\frac{d^{6}K}{27\epsilon_{0}} \left[ 2(\alpha - 3\beta) \right] .$$
(3)

The only two unknowns in the previous set of equations are the constants  $\alpha$  and  $\beta$  to be determined experimentally.

#### **III. FABRICATION AND CHARATERIZATION**

The silicon waveguide requires two main features: a source of strain and a source of electrostatic field. The former is achieved by placing a layer of straining material, under high internal stress ( $\sigma_0$ ), on top of the waveguide. This highly

stressed layer strains the waveguide underneath, creating the strain gradients required to generate  $\chi^{(2)}$  in the waveguide. The stress layer we used was a SiN thin film, deposited by PECVD whose internal stress  $\sigma_0 = 1.2$  GPa compressive stress. The electrostatic field is created by placing electrodes on top of the waveguide which are activated by the application of a voltage difference  $V_s$ . The cross-section of the final structure we designed is shown in Fig. 1



Fig. 1 : Schematic view of modulator based on Pockels effect including a stress layer and electrodes.

However, silicon is a semiconductor and its free-carrier concentration and distribution is dependent on the applied electric field (F)<sup>11</sup>. Therefore, there are two electro-optic effects that take place in the waveguide when an electric field is applied to the waveguide: the plasma- dispersion effect, an effect that corresponds to a variation of refractive index of silicon due to a variation of free-carrier concentration; and the Pockels effect, an effect that depends on the interaction of the electric field inside the waveguide and the strain gradients. These two effects, however, are deeply connected: the application of an electric field induces a change in free-carrier distribution, that in turn affects the electric field distribution inside the waveguide, which influences the Pockels effect. Furthermore, the SiN stress layer required to induce strain in the waveguide, is usually characterized by a considerable positive charge distribution (Q f) which also affects the free carrier concentration in the waveguide. Therefore, in order to study Pockels effect in strained silicon, we must include the study of the free-carriers inside the silicon waveguide together with the charging effects of the cladding and the strain effects. The final electro-optic effect is then a combination of the plasma dispersion effect ( $\Delta n_{eff-e}$ ) and Pockels effect ( $\Delta n_{eff-e}$ ), which can be reduced to:

$$\Delta n_{eff} = \Delta n_{eff_c} + \Delta n_{eff_P} =$$

$$= \Delta n_{eff_c} + \Gamma_{xxy,xxy} \left( \widehat{\eta_{xxy}^{xxy}} + \zeta \widehat{\eta_{yyy}^{xxy}} \right)$$
(4)
where  $\zeta = \Gamma_{xxy,xxy} / \Gamma_{xxy,yyy}$ 

Both  $\Delta n_{effc}$  and  $\Delta n_{effP}$  are voltage dependent and their values as a function of Vs are determined by simulating the structure using COMSOL multiphysics, which combines elasticity, optical and semiconductor effects in a single simulation. Furthermore, it is difficult to dissociate both effec

There are two main differences between both electro-optic effects: Pockels effect is a very fast effect limited only at the THz range, whereas plasma-dispersion effect can be limited at the GHz range. Furthermore, Pockels effect depends on the crystal orientation whereas carriers are not sensitive to crystallographic directions. To detect these two differences experimentally, we designed, fabricated and characterized Mach-Zehnder Interferometers compatible with RF electro-optical modulation and with the waveguides orientation. The fabrication of the devices was successfully performed in the Centre Technologique Universitaire (CTU) by using a wide range of techniques: e-beam lithography,

ICP etching, silicon thermal oxidation, PECVD, e-beam evaporation, among others. Obtained results will be discussed during the presentation and compared t the theoretical considerations.

#### **IV. CONCLUSIONS**

To sum up, we developed a new theoretical model to explain the origins of strain-induced  $\chi^{(2)}$  in silicon which related the electro-optic effect with strain gradients. We used these concepts to simulate the electro-optic effects in an approach that includes semiconductor, strain and optical effects. Lastly, we designed, fabricated and measured some samples under several bias voltages. A discussion on the different effects involved in strained silicon as a function of the frequency and device geometry will be presented during the talk.

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