Combined Opto-Electronic Simulation of CCD Cell Structures by Means of Finite-Difference Time-Domain Method

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A complete opto-electronic simulation of a CCD cell structure is presented. We combined the finite-difference time-domain method for rigorous simulation of light propagation with electronic device simulation methods based on drift/diffusion charge carrier transport models.

1 Introduction

The performance of light sensitive semiconductor elements can be optimized by influencing the intensity distribution inside the structure through its optical and geometric features, such as antireflective coatings, incoupling gratings or lenses, absorbing regions, waveguide structures etc. Computer simulations can speed up the design process, however, to give useful information, need to be able to take into account all important factors that influence the device performance.

Several recent publications address the combination of device simulation with rigorous electromagnetic modelling of wave propagation effects [1, 2, 3, 4]. These effects play an important role in light sensitive as well as in miniature high-frequency devices. While feasible in principle, rigorous electromagnetic simulation still poses practical problems as far as model generation and computational effort are concerned. Therefore, exact methods are mostly used in combination with strongly simplified geometries [1].

We have combined a full wave electromagnetic simulator with electronic device simulation using drift/diffusion charge carrier transport models to simulate the behaviour of a CCD cell structure.

2 Rigorous Electromagnetic Simulation of Light Propagation

Our electromagnetics simulator EMLAB is an implementation of the finite-difference time-domain (FDTD) method [5]. This technique is becoming increasingly popular in modelling all kinds of optical structures. Recently, simulation results for light propagation in photonic crystals [6], waveguides [7], (VCSEL) laser cavities [8], integrated optics devices [9], photodetectors [2], etc. have been presented. This popularity comes, apart from the fact that the FDTD approach is completely rigorous, from the intrinsic robustness and stability of the formulation and the relative simplicity of the process of setting up a simulation model. In FDTD, Maxwell's equations are discretized both in time and space on an intertwined grid system for electric and magnetic field components, allowing a rigorous and numerically stable simulation of electromagnetic wave propagation phenomena. The discretization of complex geometries is straightforward. Areas of finite extent (open boundaries) can be handled as well as periodic structures. In addition, since FDTD is a time-domain method, it can easily be extended to handle nonlinear and signal analysis problems and coupled with other time-domain simulators.

We use this simulator to compute charge carrier generation rates within the CCD for monochromatic illumination in 2D. When light propagates in an absorbing medium with complex refractive index $n = n' + in'' = \sqrt{\epsilon}$, the corresponding $\boldsymbol{k}$-vector also becomes complex, being

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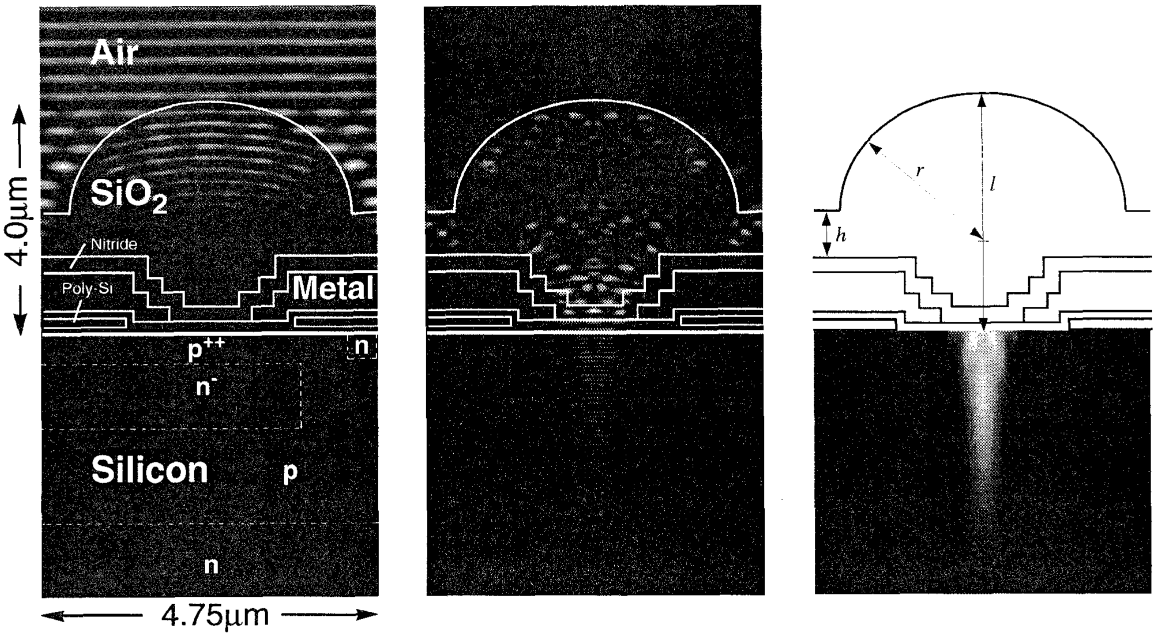

Figure 1: FDTD simulation of light propagation in a CCD cell. A plane quasimonochromatic, TM polarized wave with $\lambda = 550\,\text{nm}$ and intensity $I_0 = 3.77 W/m^2$ is incident from the top. The two pictures on the left show the time dependent intensity distributions shortly after the beginning of the simulation and in the time harmonic state. The picture on the right shows the charge carrier generation rate. White corresponds to the maximum generation rate $G^{\text{opt}} = 2.0 \times 10^{19}\,/\text{cm}^3/\text{s}$.

given by

$$\boldsymbol{k}^2 = n^2 \boldsymbol{k}_0^2 = (n' + in')^2 \boldsymbol{k}_0^2 = (\epsilon' + i\epsilon'')\boldsymbol{k}_0^2 \tag{1}$$

with $\boldsymbol{k}_0$ the vacuum wavevector. To model this behaviour in EMLAB, a nonzero conductivity s has to be assigned to that medium. Since one also has

$$\boldsymbol{k}^2 = \omega^2 \epsilon\mu \left(1 - i\frac{\sigma}{\omega\epsilon}\right) = \boldsymbol{k}_0^2 \mu r \left(\epsilon_r - i\frac{\sigma}{\omega\epsilon_0}\right) \tag{2}$$

the complex refractive index is correctly modelled if one sets

$$\sigma = \frac{2\pi\epsilon_0\epsilon''}{\lambda_0 \mu r} \tag{3}$$

with λ_0 the vacuum wavelength.

The intensity distribution is given by the time averaged Poynting vector

$$\boldsymbol{S}_{\text{av}} = \frac{1}{2}\Re\left(\hat{\boldsymbol{E}} \times \overline{\hat{\boldsymbol{H}}}\right) \tag{4}$$

where the complex quantities are found from the real field values at two different times after the time harmonic state has been achieved. The power density absorbed at each point is computed as follows:

$$W = -\nabla \cdot \boldsymbol{S}_{\text{av}} = \frac{1}{2}\sigma|\hat{\boldsymbol{E}}|^2 \quad . \tag{5}$$

With the photon energy given by $E_{\text{ph}} = hc_0/\lambda_0 = \hbar\omega$ the optical carrier generation rate G_{opt} is found to be

$$G_{\text{opt}} = \eta \frac{W}{E_{\text{ph}}} \tag{6}$$

with η the quantum yield, which gives the average number of charge carriers generated by a single photon. For generation in silicon at visible wavelengths, $\eta = 1$ can be assumed [10].

3 Electric Simulation

The actual electronic behaviour of the CCD is then obtained by means of an accurate electronic simulation of the device structure. The light distribution is taken into account via the optical generation rate computed with EMLAB. We use the mixed-mode multi-device simulation program $\text{DESSIS}_{-\text{ISE}}$ to solve the semiconductor device equations for drift/diffusion charge carrier transport. Thus, the complete path from incident light to terminal currents can be simulated accurately.

4 Simulation Results

We modelled the charge carrier generation for various CCD cell structure geometries, i. e. different focal lengths

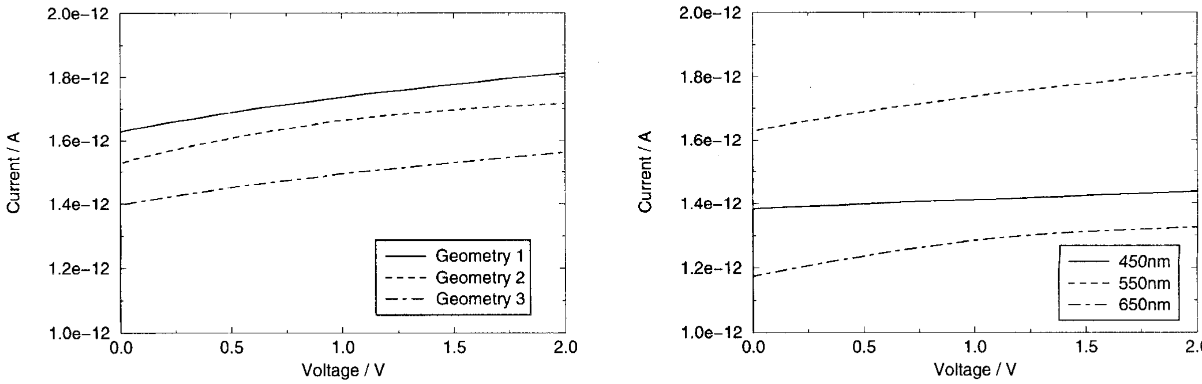

Figure 2: Quasistationary current due to photo-generated carriers at the CCD's photodiode for different geometries at $\lambda = 550$nm (left) and for Geometry 1 at different illumination wavelengths (right) as a function of the (reverse bias) voltage U applied to the n^- doping region..

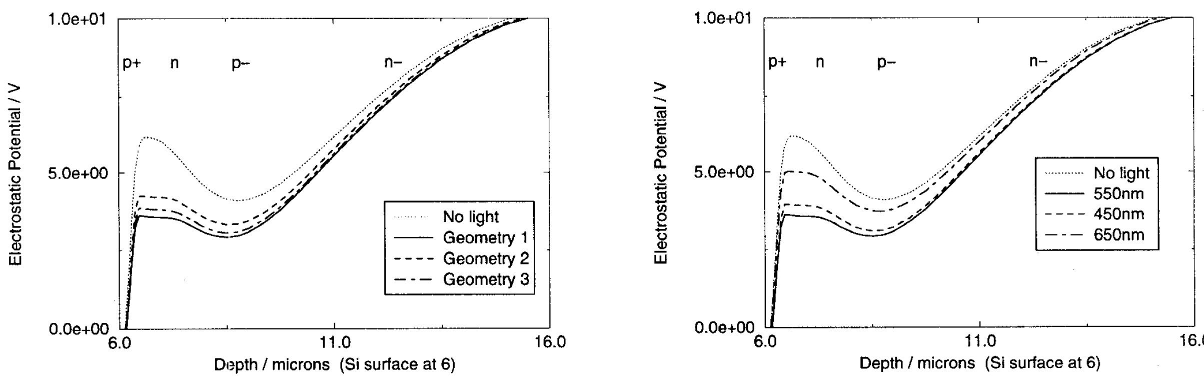

Figure 3: Transient electrostatic potential reduction due to photo-generated carriers in the CCD geometries at $\lambda = 550$nm (left) and for Geometry 1 at different illumination wavelengths (right).

of the microlens on top, under quasimonochromatic illumination at different wavelengths. For this purpose, we assumed that a plane wave is perpendicularly incident on top of the structure. FDTD simulation was carried on until a time harmonic state was reached. The intensity distribution and charge carrier generation rates were then computed. Fig. 1 shows the geometry, the doping and the results of the FDTD simulation for one of the CCD cell structures under consideration. In what follows this structure will be referred to as Geometry 1. For this structure, the front vertex of the microlens is $l_1 = 4.0\mu$m above the silicon substrate. The radius of curvature is $r_1 = 2.0\mu$m and the planar portion of the SiO_2 layer has a thickness of $h_1 = 0.75\mu$m. To examine the effect of the microlens focal length, this structure was compared to two alternative structures. The two other structures, referred to as Geometry 2 and Geometry 3, have their front vertices $l_2 = 5.0\mu$m and $l_3 = 6.7\mu$m above the substrate and have curvatures of $r_2 = 2.5\mu$m and $r_3 = 3.2\mu$m and SiO_2 layer thicknesses of $h_2 = 2.75\mu$m and $h_3 = 4.75\mu$m, respectively. Assuming that $n_{SiO_2} = 1.5$, the resulting focal lengths in SiO_2 are $f_1 = 6.0\mu$m, $f_2 = 7.5\mu$m and $f_3 = 9.6\mu$m.

For the electrical analysis of the CCD cell, two different simulations were performed. In a first step, the CCD's photodiode was modelled in steady state. Fig. 2 shows the quasistationary current due to the optically generated charge carriers as a function of the voltage applied to the n^- doping region in reverse bias for a number of structure geometries and for Geometry 1 at different wavelengths. In a second step, a transient simulation of the charging of the floating n-region (Fig. 1) were carried out. For the transient simulation the n region was depleted, resulting in a potential of approximately 7V. The n-type substrate was kept at a constant voltage of 10V. The optical generation was applied for 1ms resulting in the potential distributions shown in Fig. 3.

The results obtained can be used to optimize the geometry of the CCD cell to achieve the maximum sensitivity for a given wavelength. Alternatively, a geometry can be chosen that minimizes the wavelength dependency in order to get a maximum uniformity of the wavelength response.

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