# The lateral photovoltage scanning method (LPS): Understanding doping variations in silicon crystals

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***Abstract*—The lateral photovoltage scanning method (LPS) can be used to detect undesired impurities which appear in silicon crystals during growth. Our goal is to make a digital twin of the LPS method. To this end, we replace inflexible blackbox code with a physics preserving finite volume discretization, confirming three theoretical results via a new simulation strategy. By making the simulation transparent, it becomes easier to trace intermediate results and gain theoretical insights.**

## I. Introduction

It is impossible to measure the temperature distribution within a crystal during growth. Yet, to improve crystal growth this is paramount. Due to temperature fluctuations, microscopic variations appear in the doping concentration. These *striations* follow the solid-liquid interface [1] and can be measured even in the cooled-down crystal, see Figure 1. Traditional techniques to measure striations have a poor spatial resolution, take long time or are inherently destructive. To overcome these limitations, the *lateral photovoltage scanning* method (LPS) has been proposed [2]. This opto-electrical measurement procedure detects doping inhomogeneities at wafer-scale and room temperature in a non-destructive fashion, see Figure 2. The LPS method excites the semiconductor crystal with a laser, creating a voltage difference $u_{LPS}$ at the sample edges which is proportional to the local doping variation [3]

$$u_{LPS} \sim \nabla N_D. \tag{1}$$

After integration one obtains from the $u_{LPS}$ signal, the doping profile. However, from a mathematical point of view one has to solve an inverse problem. An efficient solution of this inverse problem – a long-term and difficult task – requires a fast and reliable solution of the *forward* problem (where the voltage difference enters as a boundary condition). For this reason, we focus on the forward problem here.

## II. LPS model

The van Roosbroeck is the standard drift-diffusion model for semi-classical transport of free electrons and holes due to a self-consistent electric field in a semiconductor device. The stationary model (excluding boundary conditions) is given by:

$$\begin{aligned} -\nabla\cdot(\varepsilon_r\nabla\psi) &= q\Big(p - n + N_D(\mathbf{x})\Big) \\ \mp\frac{1}{q}\nabla\cdot\boldsymbol{J}_{n,p} &= G(\mathbf{x}) - R, \end{aligned} \tag{2}$$

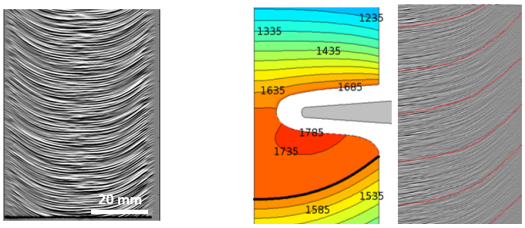


Fig. 1. Striations from LPS measurement (left); temperature field simulation of floating zone silicon crystal as well as striations (right). Here the black line represents the solid-liquid interface at 1687 K, leading to striations (tracked red line). Temperature field simulation by Robert Menzel (IKZ).

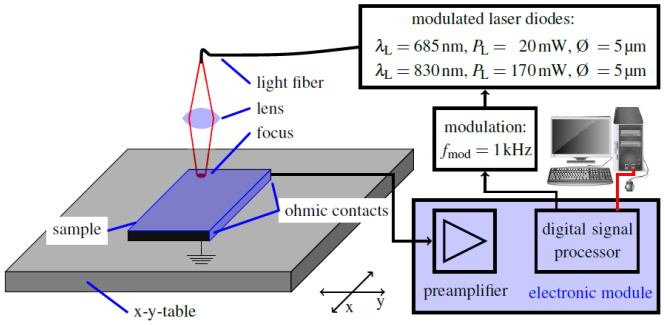


Fig. 2. LPS measurement setup.

where $q$ denotes the elementary charge, $\varepsilon_r$ the dielectric permittivity, $G$ the generation and $R = R(\psi, \varphi_n, \varphi_p)$ the recombination. Due to the growth process the donor concentration takes a sinusoidal form with a given wavelength $\lambda$ along the $x$ axis: $N_D(\mathbf{x}) \sim \sin(2\pi x/\lambda)$. The current densities for electrons and holes are given by $\boldsymbol{J}_n = -q\mu_n n\nabla\varphi_n$ and $\boldsymbol{J}_p = -q\mu_p p\nabla\varphi_p$. The set of unknowns is expressed by the electrostatic potential $\psi$ and the quasi-Fermi potentials for electrons $\varphi_n$ and holes $\varphi_p$.

The densities for electrons and holes are given by $n = N_c\exp[(q(\psi-\varphi_n) - E_c)/(k_BT))]$ and $p = N_v\exp[(q(\varphi_p - \psi) + E_v)/(k_BT)]$. Here, we have denoted the conduction and valence band densities of states with $N_c$ and $N_v$, the Boltzmann constant with $k_B$ and the temperature with $T$. Furthermore, $E_c$ and $E_v$ refer to the conduction and valence band-edge energies, respectively, and $\mu_n$ and $\mu_p$ to the mobilities.

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We measure a potential difference generated by the laser at the two ohmic contacts $\Gamma_{D_1}$ and $\Gamma_{D_2}$. Let $j_{D_i}$ be the electric current flowing through the $i$-th ohmic contact. According to the conservation of charge, the currents satisfy the relation $j_{D_1} + j_{D_2} = 0$; we define $i_D := j_{D_1} = -j_{D_2}$. We model the voltage meter as a simple circuit having only a resistance $\mathcal{R}$. The network has two nodes, in which the potentials are respectively $u_{D_1}$ and $u_{D_2}$. According to Modified Nodal Analysis (MNA), we have

$$u_{D_2} + \psi_0|_{\Gamma_{D_2}} - (u_{D_1} + \psi_0|_{\Gamma_{D_1}}) = \mathcal{R}\, i_D(u_{D_2}), \qquad (3)$$

where $\psi_0$ refers to the built-in potential. Usually one of the nodes of an electric circuit is assumed to have an electric potential equal to the ground. This means in our case that we can set $u_{D_1} = 0$. In other words, $u_{LPS} = u_{D_2} - u_{D_1} = u_{D_2}$.

Notice that (3) is an implicit equation for $u_{D_2}$ since $i_D$ depends on $u_{D_2}$ via the van Roosbroeck system (2).

## III. Simulation Setup and Strategy

We use a 2D geometry, corresponding to a cut along the $y = y_0$ plane and a laser spot position $(x_0, y_0)$ in Figure 2. The sample is $3\,\mathrm{mm}$ long ($x$ axis) and $50\,\mu\mathrm{m}$ thick ($z$ axis).

We solve the model (2) via a finite volume discretization and Newton solver embeddings with the open-source ddfermi software tool [4]. After solving for the equilibrium solution ($G = R = 0\,\mathrm{cm}^{-3}\mathrm{s}^{-1}$ and $\varphi_n = \varphi_p = 0$), we first apply a bias and then turn on the laser. Once we reach the prescribed laser power, we sweep the sample for different laser spot positions. For every laser spot position we need to ensure that (3) holds. To achieve this, we solve (3) for the LPS voltage $u_{LPS}$ via the secant method which usually converges within four iterations to a tolerance of $10^{-7}$.

Previous results [5] were obtained with a blackbox COMSOL code which lacked the now required level of flexibility. For example, it is unclear how (3) is solved.

## IV. Results

Tauc made three main theoretical predictions in [3]: First, the LPS voltage $u_{LPS}$ depends on local doping variations, see (1). Second, $u_{LPS}$ depends logarithmically on moderate laser intensities. And third, eventually $u_{LPS}$ saturates for higher laser intensities due to the screening effect.

With our computational setup we were able to qualitatively reproduce all three of Tauc' predictions. The LPS voltage does indeed vary with the gradient of the doping profile: Figure 3 shows the LPS voltage and the doping gradient with respect to the laser spot positions $x_0$, assuming the laser moves along the $x$ axis. The maxima in the LPS voltage nicely coincide with the maxima in the doping gradient. Using a commercial tool, similar behavior has been observed [5].

Moreover, our simulation confirms the logarithmic dependence on moderate laser intensities as well as the eventual saturation for higher laser intensities, see Figure 4.

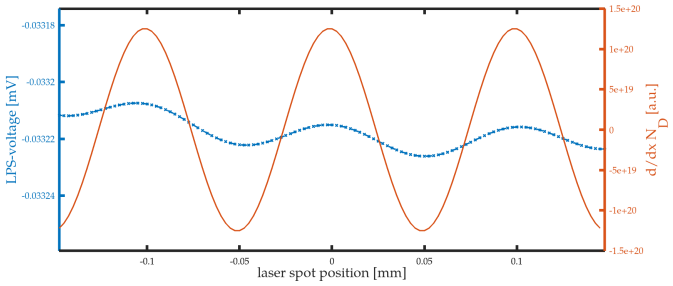


Fig. 3. Alignment between gradient of doping concentration and LPS voltage for a laser beam sampling along the $x$ axis.

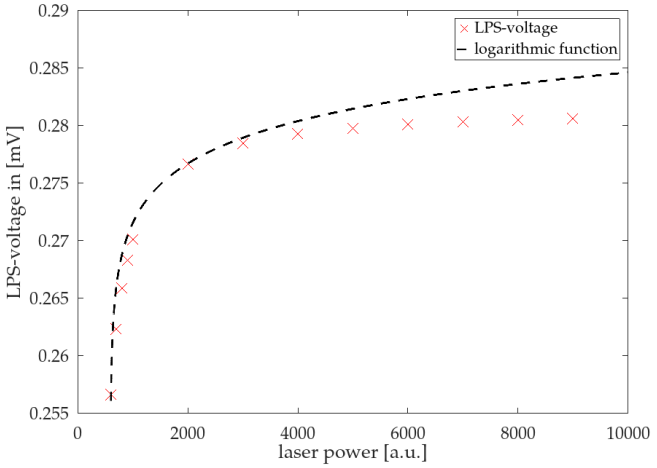


Fig. 4. Logarithmic behavior of LPS voltage as a function of the laser power. Our simulation matches the theoretic predictions made by Tauc [3].

## V. Conclusion

To improve predictions regarding the temperature field during silicon crystal growth, we simulated the lateral photoscanning method. With a flexible open-source software tool we were able to verify theoretical observations made by Tauc.

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