Device-level Simulation of the Light-addressable Potentiometric Sensor for High-speed and High-resolution Chemical Imaging

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Abstract

The light-addressable potentiometric sensor (LAPS) is a semiconductor-based potentiometric sensor using a light probe with an ability of detecting the concentration of bio-chemical species in a spatially resolved manner. In this work, a device-level simulation has been introduced, which enables investigation of detailed physical behavior and numerical modeling of the sensor performance. The minority carrier distribution under illumination has been obtained to lay the foundation for analyzing the spatial resolution. Moreover, the photocurrent response has been simulated to study the sensor response under different conditions, from which new findings were made. In addition to the dependence on the modulation frequency, the dependence of the sensor signal on the light wavelength was predicted.

1. Introduction

Light-addressable potentiometric sensor (LAPS) is a semiconductor-based bio-chemical sensor, which has an electrolyte - insulator - semiconductor structure. It is sensitive to the surface potential that is altered by the concentration of bio-chemical species in the liquid solution contacting the sensor surface [1]. A typical LAPS setup consists of a sensor plate biased with a DC voltage, and a modulated light probe as depicted in Fig. 1.



Fig. 1 Schematic drawing of LAPS measurement.

When a part of the semiconductor substrate is illuminated, a localized photocurrent is generated and its amplitude and phase are affected by the surface potential of the illuminated region. By scanning the sensor plate with the light probe, spatial distribution of the surface potential can be obtained, which represents a map of specific bio-chemical species. It is applicable in various aspects of the biomedical field, primarily for detecting pH and ion concentration, monitoring cell metabolism, and recording electrical signals from living cells like neurons. Therefore, much effort has been made to improve the performance of LAPS for high-speed measurement and chemical imaging at a high resolution. In addition to the experimental work, the theoretical analysis, modeling and simulation of LAPS constitute another important branch for this matter.

In this research, the idea of facilitating device-level simulation instead of an equivalent-circuit-model derivation [2] will be presented for analyzing the factors that affect the performance of LAPS. In the device-level simulation, an extensive set of models for device physics and effects in semiconductor devices can be taken into account, including optical generation and carrier transport, which enable numerical simulation of both electrical and optical behavior of LAPS. In this research, the TCAD Sentaurus tool is introduced and the operation of LAPS is modeled, simulated and characterized mainly in a 2D geometry.

2. Materials and Methods

In the constructed device model of the LAPS, various parameters listed in Table I. can be examined in order to improve the performance.

Table I. Changeable Parameters

LAPS setup	Modulated light probe
Thickness of Si substrate Thickness of insulating layer Lateral size of the sensor Dopant material Doping concentration Contact type Bias voltage	Wavelength of light Intensity of light Modulation frequency

A metal - insulator - semiconductor (MIS) structure is adopted to emulate the LAPS structure, which has an n-type Si substrate with the lateral dimension of 1 cm, thickness of 100 or 200 μ m, phosphorous doping concentration of 10^{15} cm⁻³. An ohmic contact is created on the back side of the sensor plate. The front side is coated with insulating layers of 50-nm-thick SiO₂ and 50-nm-thick Si₃N₄. The back side is illuminated through a 20- μ m-wide window with a light intensity of 6 W/cm².

3. Results and Discussion

Firstly, the distribution of the minority carriers inside the Si substrate induced by illumination is investigated, which is the determining factor of the spatial resolution, as the photocurrent is generated by separation of photocarriers within the depletion region. For example, Fig. 2 (a) shows the hole distribution induced by different wavelengths of light. To analyze the distribution quantitatively, the peak and the full width at half maximum (FWHM) values of the distribution directly beneath the depletion region are plotted in Fig. 2 (b).



Fig. 2 (a) Distribution of hole density (cm⁻³) under illumination with different wavelengths from 400 nm (top) to 1000 nm (bottom); (b) Peak and FWHM values of hole distribution directly beneath the depletion region.

At a longer wavelength, a larger amount of minority carriers arrive at the depletion region as expected from the absorption coefficient, and their distribution is more concentrated around the illuminated area. In other words, the use of a longer wavelength of light has an effect nearly equivalent to thinning the Si substrate, which can improve the spatial resolution as well as increase the photocurrent.

The LAPS can operate in both amplitude mode and phase mode [3], which use the amplitude and the phase shift of the photocurrent as the sensor signal, respectively. Hence, probing into the photocurrent response in detail is of critical significance. In this work, the dependence of the photocurrent signal on the frequency and the wavelength of illumination is investigated.



Fig. 3 Photocurrent response at different frequencies

Figure 3 illustrates the frequency dependence of the photocurrent signal induced by illumination at a wavelength of 700 nm. When the sensor is illuminated at a relatively low frequency, the period is long enough for

achieving a balance between the light-induced charging current and discharging one caused by the excess carriers within the depletion capacitor, and two opposite peaks can be observed. At a higher frequency, the light is turned on and off before achieving the balance, which leads the photocurrent to form a sinusoidal waveform. This band-pass characteristic of the amplitude and phase shift of the photocurrent must be taken into account to optimize the frequency range used for measurements.



Fig. 4 Photocurrent response for different wavelengths

Another interesting finding of the photocurrent response is the fact that it has a dependence on the wavelength as well (see Fig. 4). Due to the difference in light absorption and diffusion of carriers inside the Si substrate, charging speed of depletion capacitor varies among illumination at different wavelengths. More specifically, as is illustrated in Fig. 2, a longer wavelength of illumination was found to deliver more carriers to the depletion region, which speeds up the charging process and results in the spike-like photocurrent. At a shorter wavelength, the carriers are generated in the vicinity of the back surface and travel a longer distance. They are more likely to be lost by recombination, resulting in a smaller and more sinusoidal photocurrent signal with a smaller phase shift. These simulation results can help choose optimized light source for LAPS measurement.

4. Conclusions

In this work, a device-level simulation of LAPS has been performed. Both carrier distribution and photocurrent response have been successfully derived, furthermore, new characteristics of the LAPS have been discovered and were well explained by the theory.

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References

[1] D. Hafeman, J. Parce, and H. McConnell, Science **240**, (1988) 1182.

[2] M. Sartore, M. Adami, and C. Nicolini, Biosens. Bioelectron.7, (1992) 57.

[3] K. Miyamoto, T. Wagner, T. Yoshinobu, S. Kanoh, and M. J. Schöning, Sens. Actuators (B) **154**, (2011) 28.