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Device simulation of the light-addressable potentiometric sensor for the investigation of the spatial resolution

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ABSTRACT

As a semiconductor-based electrochemical sensor, the light-addressable potentiometric sensor (LAPS) can realize two dimensional visualization of (bio-)chemical reactions at the sensor surface addressed by localized illumination. Thanks to this imaging capability, various applications in biochemical and biomedical fields are expected, for which the spatial resolution is critically significant. In this study, therefore, the spatial resolution of the LAPS was investigated in detail based on the device simulation. By calculating the spatiotemporal change of the distributions of electrons and holes inside the semiconductor layer in response to a modulated illumination, the photocurrent response as well as the spatial resolution was obtained as a function of various parameters such as the thickness of the Si substrate, the doping concentration, the wavelength and the intensity of illumination.

The simulation results verified that both thinning the semiconductor substrate and increasing the doping concentration could improve the spatial resolution, which were in good agreement with known experimental results and theoretical analysis. More importantly, new findings of interests were also obtained. As for the dependence on the wavelength of illumination, it was found that the known dependence was not always the case. When the Si substrate was thick, a longer wavelength resulted in a higher spatial resolution which was known by experiments. When the Si substrate was thin, however, a longer wavelength of light resulted in a lower spatial resolution. This finding was explained as an effect of raised concentration of carriers, which reduced the thickness of the space charge region.

The device simulation was found to be helpful to understand the relationship between the spatial resolution and device parameters, to understand the physics behind it, and to optimize the device structure and measurement conditions for realizing higher performance of chemical imaging systems.

1. Introduction

The light-addressable potentiometric sensor (LAPS) [1] is a surface potential sensor with an electrolyte–insulator–semiconductor (EIS) structure [2], which realizes detection and visualization of biological/biochemical events taking place at the electrolyte–insulator interface. While its precedent electrochemical sensors such ion-sensitive field-effect transistor (ISFET) and capacitive electrolyte–insulator–semiconductor (EIS) sensor measure a spatially averaged value over the sensor surface, the LAPS can acquire the local value at the measurement spot of interest addressed by illumination and generate chemical images via raster scan with a light probe. A typical LAPS setup comprises a sensor chip and a modulated light probe as depicted in Fig. 1. A DC bias voltage is applied across the EIS structure with the help of the reference electrode and the backside contact to induce a space charge region at the insulator–semiconductor interface. The surface potential relying on the local concentration of certain biochemical species will be superimposed to the bias voltage, which locally modifies the width of the space charge region.

When a part of the sensor plate is illuminated, a localized photocurrent is generated, the amplitude and the phase of which are affected by the local surface potential, and therefore, by the analyte concentration at the illuminated region. When we raster scan the sensor plate with a light probe, the spatial distribution of the surface potential can be obtained, which represents a map of the biochemical species involved [3].

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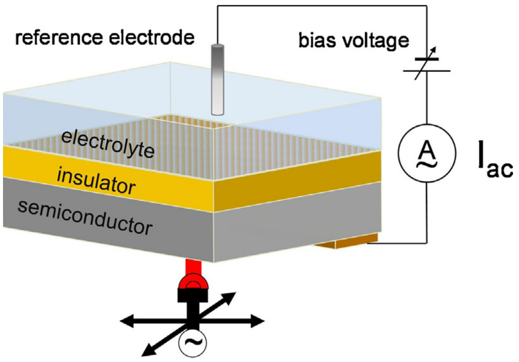

Fig. 1. Schematic of the LAPS setup.

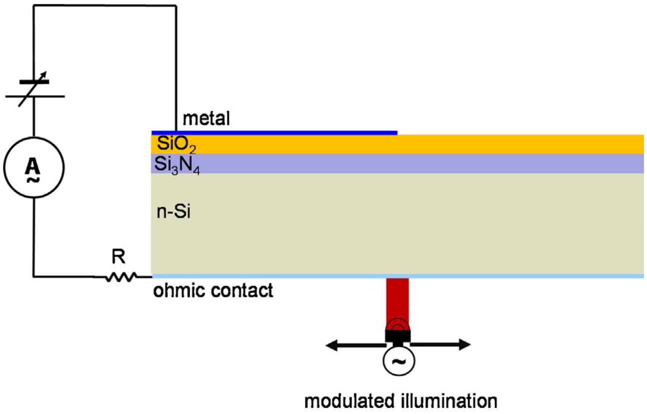

Fig. 2. One-electrode model.

The light addressability is the most important feature of the LAPS, which facilitates various applications in chemistry and biology [2–5] including monitoring of cell metabolism and detection of microorganisms. In such imaging applications, the spatial resolution is of crucial importance to realize, for example, measurement of a single cell. Therefore, extensive efforts have been put forth to study the spatial resolution of the LAPS, both experimentally and theoretically [5–15].

Experimental investigation on the spatial resolution of the LAPS is done usually by modifying the LAPS surface to generate artificial surface potential patterns, where the spatial resolution is defined as the smallest size of the structure the LAPS can resolve. Possible surface modifications include coating with dielectric materials (e.g. photoresist) and UV irradiation prior to experiments, which lead to difference in surface potentials between coated and non-coated areas, or treated and untreated areas, respectively [5,9–11]. In these methods, however, many test patterns with different sizes must be prepared to determine the spatial resolution. An alternative experimental method was performed by coating a part of the LAPS with a thin metal layer [12–14]. A bias voltage was applied to the metal, and a light probe scanned the front or back surface across the border between the metalized region and the uncoated region to measure the diffusive propagation of photocarriers.

In all these experimental investigations, however, the spatial resolution is not only determined by the intrinsic device physics involved, but also limited by the details of the experimental setup used, such as the size of the light probe and the sharpness of the mask edge, etc. To find the physical limitations and essential dependence of the spatial resolution on device parameters, theoretical and simulation study is necessary. Therefore, researchers have been seeking theoretical models to analytically study the resolution [5,8–10,12,15].

For detailed analysis of the photocurrent, the transport equations for both electrons and holes in the semiconductor must be solved. The transport equation consists of four parts, i.e., the light-induced generation, recombination, isotropic diffusion and drift in the electrical field. As it is not possible in general to solve these equations analytically, some assumptions have been made to come up with a simplified model to trace the diffusion-driven lateral spread of photocarriers in the semiconductor after an instantaneous flash of light. It was also assumed to be sufficient, as far as the spatial resolution was concerned, to take only diffusion and recombination of minority carriers into account, neglecting the drift under low injection assumption. Such a simplified model not only gives approximated values but also makes it impossible to analyze the transient photocurrent and to investigate the dependence of its amplitude and phase on various parameters.

In our previous paper, the device simulation of the LAPS was successfully performed with Sentaurus TCAD, one of Synopsys simulation tools [16], in which different device parameters were examined in order to optimize the LAPS structure and measurement parameters to realize enhanced performance such as a good signal-to-noise ratio and a high-speed measurement. In this study, the device simulation model was further extended to investigate the spatial resolution of the LAPS. Since the device simulation takes an extensive set of models for device physics into account, it makes it possible to probe into the detailed physical behavior inside the LAPS and the photocurrent response to the surface potential step.

2. Methodology

2.1. Model

The model adopts the method of generating artificial surface potential step by coating half of its front surface with a metal layer. When the uncoated region of the sensor is illuminated from the backside, most of photocarriers will not arrive at the space charge region under the metal layer and no photocurrent will flow. In contrast, there will be a photocurrent if a point under the metallized region is illuminated. The spatial resolution can be then determined by measuring the decay of the photocurrent while moving the light beam from the metallized region to the uncoated region.

As depicted in Fig. 2, the 2D physical model of the LAPS with a lateral length of 1 cm is used in this study. The insulating layers of 50-nm-thick SiO_2 and 50-nm-thick Si_3N_4 are formed on the n-type Si substrate with a thickness of 10–500 μm and phosphorus doping of 10^{13}–10^{17} cm^{-3}. Half of the front surface is coated with a metal layer and biased with a voltage of -0.1 V. An ideal ohmic contact with no barrier height for carriers is formed uniformly at the backside. To simplify the model, the metal layer and the ohmic contact are assumed to be optically transparent, which eliminates the influence of the light absorption and reflection in the metal. In experiments, the metal electrode on the front surface is replaced with a solution and it is not necessary to coat ohmic contact uniformly on the backside of the LAPS.

The light beam with a wavelength of 500–1000 nm and an intensity of 1–6 W/cm^2 is switched on and off at a pulse repetition frequency of 5 kHz, and illuminates a 20-μm-wide window on the backside of the LAPS. The modulated light probe is moved from the metallized region to the uncoated region.

2.2. Physics

When the incident light is turned on and if the photon energy is larger than the band gap of the semiconductor, electron-hole pairs are generated in the vicinity of the back surface of the LAPS, and they start to diffuse toward the front surface. Some of them will recombine during this process, and those which eventually reach