

FREQUENCY DEPENDENCE OF THE MIS SPV RESPONSE OF p-Si EMPLOYED TO CHARACTERIZE SURFACE DEFECTS

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SUMMARY OF THE ABSTRACT

The modulated surface photovoltage (SPV) experiment in metal-insulator-semiconductor configuration (MIS) uses application of a chopped light beam upon the surface of a sample. The induced variation of the surface potential is recorded by a transparent conductive probe placed on top of the sample. We investigate the impact of the light modulation frequency on the response of untreated p-type silicon, used as a model system. Due to the absence of buried heterojunctions in the sample, we assume that the SPV response originates at the Si surface due to the presence of a defect-induced space charge region (SCR). Experimentally, we observe an increase of the phase shift of SPV with respect to the incoming beam, and a reduction in the SPV amplitude, when we increase the modulation frequency from 29 to 494 Hz. This trend is qualitatively explained by the timescale of charge carrier trapping and detrapping at the surface of the sample. We have employed drift-diffusion simulations to quantitatively evaluate the impact of key surface defects' properties, and to show the power of frequency modulation in the MIS-SPV technique. Following the Shockley-Read-Hall non-radiative recombination mechanism [1,2], parameters such as defect density and carrier capture cross sections have been evaluated. From our preliminary results, a large asymmetry in the role of the electron and hole capture cross sections arise. This can be ascribed to the doping nature of the semiconductor. Under illumination, photogenerated electrons are driven towards the surface, where they subsequently trap, with a speed which depends on the electron capture cross section. During the dark semi-period, these electrons are released by recombining with holes in the valence band, a process which mainly depends on the hole capture cross section. On the one hand, dynamics under light are impacted by the large photogenerated carrier density, which increases the electron trapping rate on the surface. On the other hand, during the dark semi-period, the hole density at the surface quickly decreases. This translates into a much higher impact on the SPV phase shift of the hole capture cross section, with respect to the electron one.

TOPIC 2 : Thin Films and New Concepts

Sub-topic 2.3 (New Modeling and Characterization Techniques)

Justification : This paper reports experimental and theoretical progress on the promising technique of surface photovoltage spectroscopy for analysis of materials and devices in PV and information on transport and defect properties.

EXPLANATORY PAGES

AIM AND APPROACH

Surface photovoltage is a widely employed technique for the study of photovoltaic materials, since it allows to probe light absorption and carrier extraction capabilities of semiconductors. In its declinations, such as transient or modulated photovoltage, it can yield important information about carrier dynamics, unveiling the presence of defects, selective interfaces and electric fields across the layer stack under study.

We here concentrate on a well-studied system, namely boron-doped crystalline silicon (250 μm – thick) to demonstrate the characterization capabilities of a coupled experimental and modelling work. We have simulated the SPV response of p-type silicon to modulated illumination employing the drift-diffusion equations, which are solved by a commercial software (Atlas from Silvaco Inc.). In our experiment and in our simulations, the modulation frequency of the incoming light has been varied between 29 to 494 Hz, and the impact of some key material parameters has been evaluated by comparing the outcomes of the simulations to the experimental trend. A Matlab routine has been set to control the input parameters of the model, from the light beam parameters (wavelength, intensity and modulation frequency) to the material parameters.

SCIENTIFIC INNOVATION AND RELEVANCE

Surface photovoltage (SPV) detects the change in the surface potential of a sample induced by illumination. The SPV arises due to generation and subsequent redistribution of photocarriers under the presence of an electric field at the surface or at the buried interfaces. Buried heterojunctions can also be the source of the SPV.

In the metal-insulator-semiconductor (MIS) operation mode, the surface of the semiconductor is separated from the top electrode by inserting a thin insulating layer (thus forming a MIS structure). The top electrode is chosen transparent, so that the semiconductor can be illuminated from the top through this electrode. Photogenerated carriers are separated by the built-in electric field at the semiconductor surface or at buried interfaces and this gives rise to the measured photovoltage. In the AC MIS-SPV, the light impinging the sample is periodically modulated, and the generation of excess carriers and their subsequent redistribution periodically change the surface potential, V_s , thus inducing a periodic surface photovoltage. The changes in V_s produce corresponding changes of the probe potential. Thus, an ac voltage on the probe proportional to the change in V_s is generated [3] and measured usually by means of a lock-in technique.

While SPV has been widely employed and analysed using simplified analytical approaches based on approximations, only few works have been analysing the measurements using a full numerical modelling. The drift-diffusion model is a powerful tool to study the electronic properties of semiconductors employed for photovoltaic applications. Being physics-based, the outcomes of the regression of experimental data (i.e. the model parameters) can be directly exploited to evaluate the “quality” of the structures impacting charge carrier generation, separation and collection.

RESULTS (OR PRELIMINARY RESULTS) AND CONCLUSIONS

On one hand, we measured and simulated the SPV response of p-type crystalline silicon under chopped monochromatic light, at a wavelength of 850 nm and at frequencies ranging from 29 Hz to 494 Hz.

On the other hand, in our model, in order to generate an SCR, we placed a layer of electronic traps that are present at the silicon surface, and down to 1 nm depth. These consist of two levels located at 50 meV above and 50 meV below the intrinsic Fermi level, respectively of donor and acceptor type. This is carried out to mimic the defective silicon surface, which is known to possess amphoteric traps related to dangling bonds [4]. To realize equilibrium, these traps exchange carriers with the bulk silicon layer, creating a surface SCR. We here investigate the impact of surface defects' properties on the frequency dependence of SPV. We have varied the defect density (for acceptors and donors simultaneously) and the carriers' capture cross sections.

We represent experimental data with black dots in Figure 1. The data is plotted as modulated SPV amplitude (detected at the light modulation frequency) as a function of the detected SPV phase shift with respect to the input light beam.

While the bulk Si material parameters have been taken from the literature (www.ioffe.ru), we fixed the bulk doping to $1.5 \times 10^{16} \text{ cm}^{-3}$, as indicated in the sample datasheet. Starting defects parameters, such as capture cross section for electrons ($\sigma_e = 10^{-16} \text{ cm}^2$), holes ($\sigma_h = 10^{-16} \text{ cm}^2$), and defect density ($N_S = 2.4 \times 10^{11} \text{ cm}^{-2}$) have been set to qualitatively match the range of measured SPV amplitude and phase. A sweep of these values around these starting points has been performed to evaluate the sensitivity of the model.

We start by discussing the impact of the asymmetry in capture cross section in Figure 1a-b. Here we highlight that the two simulated trends are very different. The surface SCR electric field drives photogenerated electrons toward the surface, which then recombine with holes during the dark semiperiod. This creates an asymmetry between hole and electron dynamics. While the impact of varying only σ_e on the phase shift is very low, a decrease of the SPV amplitude can be obtained for very low values of σ_e (Figure 1a). On the other hand, σ_h radically influences both SPV amplitude and phase (Figure 1b). For the largest values of σ_h we considered, the SPV rise and decay are nearly instantaneous and the phase shift tends to 180° . For values on the other end of the range, nearly 100° phase shift is obtained, and the signal becomes strongly triangular. Being p – type doped and under low injection, holes dynamics in the Si sample dictate the timescale of the trapping – detrapping phenomena.

Looking at Figure 1c, we notice that very low or very high values of σ for both electrons and holes simultaneously are not feasible, and a mean value of 10^{-16} cm^2 seems to be the most realistic. Values below 10^{-16} cm^2 would generate almost instantaneous SPV response, denoted by a phase shift which approaches 180° . Values above 10^{-17} cm^2 increase the SPV amplitude, but generate an amplitude(phase) trend which is not seen in experimental data.

From Figure 1d, we highlight that N_S values larger than $2.4 \times 10^{11} \text{ cm}^{-2}$ would allow the trend to better match the experimental data by increasing the amplitude(phase) slope, but an adjustment of the other parameters would be needed to reduce the SPV amplitude to the measured range of values.

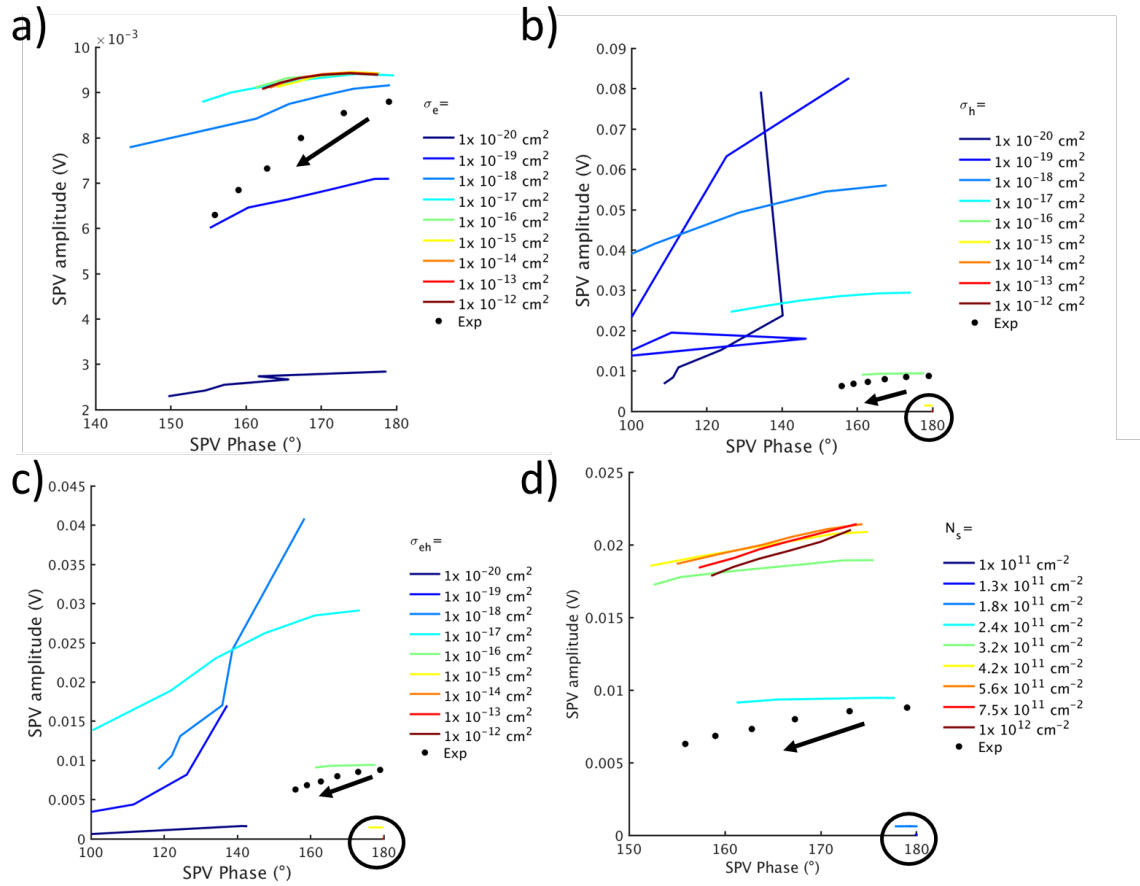


Figure 1: Modulated SPV amplitude-phase plots from experimental p-type Si data (black dots) and simulated data using SRH surface defects, as a function of defect parameters; (a): varying electron capture cross section (σ_e), while hole capture cross section is fixed at $\sigma_h=10^{-16} \text{ cm}^2$; (b): varying hole capture cross section (σ_h), while electron capture cross section is fixed at $\sigma_e=10^{-16} \text{ cm}^2$; (c) varying simultaneously the capture cross sections of electron and holes (with equal values); (d) varying the surface defect density (N_s). The default value of N_s used in (a), (b), (c) is $N_s=2.4 \times 10^{11} \text{ cm}^{-2}$. Black arrows indicate increasing light modulation frequency (29→494 Hz). Black circles highlight curves with phase shift values close to 180° .

Given the results of this analysis, we can affirm that investigating the frequency dependence of the MIS SPV with the help of the drift – diffusion model could be of great interest to study defect and interface dynamics of the materials employed in photovoltaic applications.

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