Crucial aspects for the use of silicon photomultiplier devices in continuous wave functional near-infrared spectroscopy

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Abstract: In this work, we investigate some major issues for the use of silicon photomultiplier (SiPM) devices in continuous wave functional near-infrared spectroscopy (CW fNIRS). We analyzed the after-pulsing effect, proposing the physical mechanism causing it, and determining its relevance for CW fNIRS. We studied the SiPM transients occurring as the SiPM device goes from the dark (LED in off state) to the illumination (LED in on state) conditions, and vice-versa. Finally, we studied the SiPM SNR in standard CW fNIRS operation.

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1. Introduction

Silicon Photomultiplier devices (SiPM) are very promising to advance Continuous Wave Functional Near Infrared Spectroscopy (CW fNIRS) technique for human brain cortex monitoring [1–4]. The advantages of SiPM in the CW fNIRS context come from the combination of having a high gain, of the order of 10^7, like a conventional vacuum photomultiplier, with at the same time low operation voltage, small size, high robustness and reliability, low cost, etc [5,6].

The fNIRS operates thanks to the relative transparency of human tissues in the near infrared (NIR) spectrum [7]. In this range, the light absorption is mainly due to the oxygenated and de-oxygenated hemoglobin (O2Hb and HHb, respectively) of the blood [8]. The fNIRS operation principle is based on the detection of NIR photons diffused when passing through the human tissues. The information carried out by the back-scattered photons is related to the dynamical change of O2Hb and HHb concentrations in the blood, providing relevant markers of hemodynamic and metabolic changes associated with neural activity in the brain [9–11]. The CW fNIRS operation is a cyclic measurement of light diffusion from the brain cortex with at least two wavelengths in the 700-950 nm range, generally at an overall clock frequency ranging from 1 to 100 Hz [12]. In each clock cycle, each optode (detector – optical source pair) performs a measurement of the O2Hb and HHb concentrations in a specific region of the brain cortex defined by the optode position on the scalp and the relative distances between the detector and the light source, the last providing the in-depth. To this purpose a number of light sources (generally LEDs or laser diodes) positioned on the patient head surface are alternately multiplexed, i.e., switched on and off, while the detectors collect the photocurrent due to the light back-diffused at the head surface. To suppress the ambient light noise, fNIRS operation also needs a phase in which all light sources are switched off.

We successfully integrated SiPM in an fNIRS prototype and reported an in vivo comparison with a commercial system relying on laser diodes, PMTs, and optical fibers for light probing and detection. Our prototype system provided a correct estimation of brain hemodynamics [1].

However, some artifacts were observed and, to implement a real-time SiPM based fNIRS system, these need to be carefully analyzed and understood. For this reason, in this paper we describe which artifacts are present in the transient due to the SiPM devices when the LED sources are switched on or off. In particular, we analyze and discuss major aspects to consider
when applying SiPMs to fNIRS systems, i.e. afterpulsing, device transients, and conditions to optimize the signal-to-noise ratio.

2. Experimental

Large area p-on-n SiPM detectors manufactured at STMicroelectronics clean room facilities were used for the measurements presented in this paper [13]. The SiPM structure, formed from planar p–n microcells, was fabricated onto a low doped n-type silicon epitaxial layer grown onto a highly doped n-type CZ substrate. An implanted n-layer forms an enrichment region, which defines the active area and breakdown voltage of the junction. The anode is given by the diffusion of boron from a doped in situ polysilicon layer deposited on the top of the structure. The p+ layer overlaps the enrichment region to form a virtual guard ring in order to reduce the electric field at the edge of the diode and ensure a uniform breakdown region in the central area of each microcell. The quenching resistor, made from low-doped polysilicon, is integrated on the anode of the cell itself. Thin optical trenches, filled with oxide and metal, surround the pixel active area in order to reduce electro-optical coupling effects (crosstalk) between adjacent microcells. The SiPMs used for the characterization have a total area of 4.18 × 4.68 mm² and 4871 square microcells with 60 µm pitch. The devices have a geometrical fill factor of 67.4% and are packaged in a surface mount housing (SMD) with 5.1 × 5.1 mm² total area. The SMD package is sealed by an epoxy resin transparent in the visible and near infrared wavelength ranges with a refractive index of about 1.5 at room temperature. The SiPM devices have a breakdown voltage of about 28 V at room temperature, and a photon detection efficiency (PDE) of about 12% and 8% measured at 529 nm and 700 nm and 4V-Overvoltage (OV).

Roithner LaserTechnik SMC700 and SMC830 AlGaAs LEDs in SMD ceramic package emitting respectively at 700 nm and 830 nm wavelengths, was used as optical light sources. The LEDs have an area of 2 × 2 mm², viewing angle of ± 55°, average spectral bandwidth of 20 nm and 35 nm at 700 nm and 830 nm emission wavelengths respectively. The average power emission ranges from 0 to at most 3 mW and 10 mW, for 700 nm and 830 nm, respectively, in the standard LED operation range. We also used an Osram LT M673 InGaN LED at 529 nm wavelength with a luminous intensity from 0 to 160 mcd. Further features are the average spectral bandwidth of 33 nm and a viewing angle of ± 60° in standard LED operation range.

LEDs were biased using a Tektronix AWG2005 programmable voltage function source with a time resolution of 20 MS/s, 12-Bit (1/4096) Vertical Resolution. LED rise and fall times are of some tens of ns, up to about 100 ns. Such times are close to the rise and fall time of the AWG2005 programmable voltage function source, and we have verified that in all the cases the overall LED plus function generator switch on or off times are well below 200 ns. The time scales of the phenomena investigated here are much longer, above 0.5 µs, so they are not influenced by the LED rise and fall times.

Fig. 1. Scheme of the experimental set-up used to measure SiPM after-pulsing, SiPM temperature transients and signal-to-noise ratio. The distance D was about 10 cm for the first two measurements and about 80 cm for the SNR.
The SiPM current transients were measured in a Tektronix DPO7104, 1 GHz analog bandwidth digital Phosphor Oscilloscope with up to 20 GS/s real-time sample rate on one channel.

We focused our attention on various aspects of SiPM operation in typical CW fNIRS conditions. In particular, we have performed measurements on after-pulsing effects, SiPM thermal transients, and signal-to-noise ratio (SNR). Figure 1 reports the scheme of the experimental set-up used to measure such characteristics. The distance D was about 10 cm for after-pulsing and thermal transient measurements and about 80 cm for measuring the SNR.

SiPM devices were contacted in a Cascade Microtech probe station equipped with an ERS Electronic AC3 thermal chuck. The device temperature was controlled by the thermal chuck, and since the SiPM is in package, its temperature was evaluated through the measurement of the I-V characteristics. In the case of forward bias the SiPM temperature can be evaluated by considering that the SiPM current grows as $\exp(qV/nk_BT)$ where $q$ is the elementary charge, $V$ is the voltage, $n$ is the ideality factor, $k_B$ is the Boltzmann constant, and $T$ is the device temperature. In reverse bias in Geiger mode, the SiPM temperature was estimated by the temperature dependence of the dark current, as described in the following section.

3. Results and discussion

3.1. After-pulsing

The first source of artifacts when using SiPM in CW fNIRS is the SiPM after-pulsing phenomenon. It has been from long time recognized as a major problem for the application of SiPM and SPAD devices in measurement systems. Therefore, large efforts were spent to characterize this parameter, to understand the physical mechanisms underlying this phenomenon, and reduce or possibly suppress this spurious noise effect [14–16].

The afterpulsing is attributed to defects, which trap carriers produced by the avalanche, and release them with delay triggering correlated avalanches [6].

Figure 2 reports the SiPM transient after the LED switch-off averaged on 500 traces with a 100 MHz sampling frequency. Both red (700 nm) and a green (529 nm) LED sources are compared. In both cases, when the LED is in the on state, the optical power incident on the SiPM under test was of about 60 nW. After 700 nm illumination, three peaks at about 1, 1.5, and 4.5 µs delay are clearly visible. Results similar to those obtained at 700 nm were collected at 830 nm, hence we will not show them for brevity. After 529 nm illumination, only one peak at about 1 µs is detected. These peaks are detectable after the LED is switched OFF, with an intensity considerably lower with respect to the ON state photocurrent one. They are attributed to an after-pulsing / delayed detection effect.

Fig. 2. SiPM transient after 529 nm and 735 nm wavelength LED switch-off, averaged on 500 traces, 100 MHz sampling frequency
It is important to underline that the time scale of the peaks observed here (1-10 µs) completely rules out a mechanism involving the diffusion of photons. In 1 µs a photon in Si travels to a distance of about 85 m, much larger than both the SiPM device size and the light absorption length, being the last of the order of a few microns. Therefore, to explain their presence we need to consider other mechanisms.

The inspection of Fig. 2 clearly indicates the presence of numerous peaks after 700 nm illumination, while only one peak is observed, at the shortest delay (about 1 µs), after the 529 nm LED illumination. Such circumstance suggests that the observed peaks are due to emission of minority carrier (holes) from defects located at large depths in the device. Such holes travel by diffusion to the surface reaching the multiplication region and triggering the avalanches, thus producing a time-delayed detection.

We now discuss some arguments in favor of the above hypothesis. The SiPM is a p-on-n device illuminated from the front side, i.e. from the p + anode side, hence, the light penetrates quite deeply in the detector. The absorption coefficient ($\alpha$) is $\sim 3 \times 10^3$ and $\sim 8 \times 10^2$ cm$^{-1}$ at 529 and 700 nm [17], corresponding to absorption lengths of $\sim 3.3$ and $\sim 12.5$ µm, respectively. Since 95% of the light is absorbed within a $3/\alpha$ thickness, we estimate that the “illuminated” region, i.e. the detector absorption region, is about 10 µm and 37.5 µm at 529 nm and 700 nm, respectively. Therefore, when the LED is ON, the SiPM device contains minority carriers (holes) in the n-region, which diffuse towards the multiplication region, where they have a high probability to trigger the avalanche. For p-on-n SiPMs this is the “normal” detection mechanism, which requires holes diffusion. It is a quite slow mechanism, but for the CW fNIRS application, where the device speed is not a crucial feature, SiPMs can still be used. The results are, indeed, excellent, since the gain due to the avalanche allows a very large device responsivity. In addition to the “normal” mechanism, we propose a parallel one, involving defects located at large depths, tens of microns, responsible for a delayed detection/afterpulsing effect. We propose that such defects can trap some minority carriers (holes) and release them with a delay. Like in the normal detection mechanism, holes will travel by diffusion to the multiplication region and trigger the avalanche. We propose that the peaks shown in Fig. 2 are, then, due to the time needed by the minority carriers to diffuse from the defect location to the avalanche region. The presence of peaks can be ascribed to the fact that defects are present only starting from certain depths. In fact, if the light has an absorption length able to reach such depths, the defects will then emit minority carriers, but it will be required some time for such carriers before they can actually reach the multiplication region near the surface. So for “deep” defects, i.e. located at large depths, and not close to the surface, a delay has to be observed. It should be reminded that the same conclusion drawn for 700 nm can be extended to 830 nm illumination.

At 700 nm the peaks are at $t = 1, 1.5$ and 4.5 µs, which correspond to depths, estimated as $\sqrt{(D \times t)/3}$ where $D$ is the hole diffusivity, of 20, 25, and 43 µm, respectively. In fact, the holes are emitted at the depth at which the defect are located, and then such emitted carriers, to be detected, have to reach the multiplication region of the SiPM, located near the surface. The diffusion is isotropic, so we can write $Dt = \sigma_x^2 = \sigma_y^2 + \sigma_z^2 = 3\sigma_z^2$, since $\sigma_x = \sigma_y = \sigma_z$, where $\sigma_x^2, \sigma_y^2$, and $\sigma_z^2$ are the total variance and the variances in the x, y, and z directions. The $\sigma_z$ values (equal to $\sqrt{(D \times t)/3}$), i.e. 20, 25, and 43 µm, are perfectly compatible with the “illuminated” depth, estimated as $3/\alpha$, equal to 37.5 µm at 700 nm. On the other hand, at 529 nm wavelength, the “illuminated” depth is shallower, i.e. 10 µm, and it is consistent with the presence of only a single peak at the shortest delay, about 1 µs, with a $\sqrt{(D \times t)/3}$ of 20 µm.

Such depths correspond to the n + CZ substrate, where the presence of defects is likely since there are high P and O concentrations and, consequently, a large probability of generating impurity complexes and precipitates [18–20].
By changing temperature, all the peaks at 700 and at 529 nm are still well visible, as shown by the data reported in Fig. 3. This is well explained by the proposed mechanism, since the holes diffusivity has a relatively weak temperature dependence in the investigated range.

In ref [21], time constants of the same order of magnitude are observed, though no peaks are found. This suggests that in the SPADs studied in ref [22], similar defects are present but they are uniformly distributed in depth.

3.2. Thermal transients

In Fig. 2, after the regions of the peaks, we still see a current transient, whose duration is of the order of a few hundreds of microseconds. These transients are quite visible in Fig. 4(a) and (b), where a linear time scale is used.

Clearly, the presence of current transient during SiPM operation has an impact in the fNIRS application and requires a detailed understanding. The first possible explanation is the emission of the trapped holes, which follows an exponential behavior with a characteristic time \( \tau \). According to the Shockley-Read-Hall (SRH) model, \( 1/\tau \) is equal to \( \gamma T^2 \sigma \times \exp(-E_T/kT) \), with \( \gamma \) an universal constant, \( T \) the absolute temperature, \( \sigma \) the hole trap cross section, \( k \) the Boltzmann constant, and \( E_T \) the trap energy, i.e. the distance in energy between the valence band edge and the trap energy. Therefore, by increasing the temperature, according to the SRH model, the emissivity \( 1/\tau \) should increase. To verify this point, we studied the temperature dependence of the SiPM photocurrent transients after the LED switch off. The results are summarized in Fig. 4(c). A negligible temperature dependence is observed, allowing us to conclude that \( E_T \) should be essentially zero. In such hypothesis, \( 1/\tau \) should be equal to \( \gamma T^2 \sigma \). Therefore, by considering a typical value of \( \sigma = 1 \times 10^{-15} \text{ cm}^2 \), \( E_T = 0 \text{ eV} \), the SRH model would predict that \( \tau \) should be of the order of 10 ps, i.e. about 7 orders of magnitude faster than what it is observed. Then, we can rule-out an explanation based on the SRH model for the slow part of the transient.

To summarize, the observed after-pulsing peaks observed at times in the range 1 – 5 \( \mu \)s are due to defects in the \( n^+ \) CZ substrate which emit holes, the estimated distance traveled by the holes before triggering the avalanche is 20 \( \mu \)m or more. The defects must be shallow in terms of \( E_T \), since a negligible temperature dependence is observed for the emission transient.

The slow transient, well visible in Fig. 4(a) and (b) is not related to the holes emission from the defects. We believe it is a thermal effect: when the SiPM device switches off, the temperature decreases and the SiPM current decreases too. To estimate the SiPM temperature decrease, we must consider the temperature dependence of the SiPM leakage current. From
Figs. 4(a) and (b), we observe that the current transients at the LED switch-off correspond to a decrease of a factor 2 – 3 for chuck temperatures in the range 25 – 50 °C.

Fig. 4. (a) averaged SiPM response after 700 nm LED switch off (500 traces, 100 MHz sampling rate); (b) averaged SiPM response after 529 nm LED switch off (500 traces, 100 MHz sampling rate); (c) Normalized SiPM switch off transient (after 700 nm LED switch off) at various temperatures. The figure legends indicate the SiPM device temperatures measured in forward bias, see experimental section for further explanation.

When we consider the temperature dependence of the steady-state SiPM dark current (Fig. 5), we observe that a change of the SiPM current of a factor 2 – 3 corresponds to a change of device temperature of about 10 – 20 °C.

Fig. 5. SiPM Dark Current temperature dependence (V bias = 32.5 V).

Therefore, the SiPM current transients at the LED switch-off may be explained in terms of a device cooling of 10 – 20 °C when the LED is switched off. In fact, when the LED is on, for the SiPM illumination conditions used in the experiments here reported, the power dissipated in the SiPM is of about 0.4 W, in the presence of an optical pump power of about 60 nW. By switching off the LED, the dissipated power becomes suddenly small, a thermal transient
takes place, and SiPM temperature decreases of 10 – 20 °C. Such explanation is well sup-
ported by considering the thermal resistance expected for a device of about 20 mm² in an SMD
package, as we have. In such a case, the thermal resistance \( R_T \) is expected to be in the range
10 – 100 °C/W [22], and therefore the expected device temperature change \( \Delta T \) is \( 0.4W \times R_T \)
= 4 – 40 °C, i.e. a temperature variation in good agreement with our conclusions.

According to the above explanation, the exact opposite thermal effect, i.e. a SiPM warm-
ing, should take place when we switch on the LED. In this case, the power dissipated in the
SiPM goes from almost zero to some tenths of Watts, according to the optical signal level we
used, in the range from 20 nW to 60 nW. This should increase the SiPM temperature in the
same time scale, i.e., in some hundreds of microseconds.

![Graph](image)

**Fig. 6.** (a) SiPM dissipated power as the 700 nm LED is switched on at various levels of LED
illumination. When the LED is switched on, the SiPM current and dissipated power rise to a
level (L1), and then slowly increase to a steady state level (L2); (b) reports the temperature rise \( \Delta T \) as
function of steady state SiPM power dissipation (SiPM biased at 30.5 V). \( \Delta T \) can be estimated
from the difference L2-L1, since \( \Delta T \) is expected to be an increasing function of L2-L1. Figure
6(b) reports the difference L2-L1 as a function of the steady-state dissipated power L2. By
considering the temperature dependence of the SiPM dark current reported in Fig. 5, and by
assuming the same temperature dependence for the SiPM current under illumination, we can
also evaluate the corresponding temperature change in °C, and this is reported on the right ax-
is.

This is what we do observe: Fig. 6(a) reports SiPM photocurrent transients as the LED is
switched on, at various levels of LED illumination. When the LED switches on, at \( t = 0 \) in
Fig. 6, the SiPM current and power increase to a high level (L1), but then there is a slow fur-
ther increase to a steady state level (L2), in some hundreds of microseconds. The difference
of dissipated power L2-L1 is an increasing function of the final temperature increase reached
by the SiPM, while the steady-state power L2 is proportional to the illumination level. The
plot of L2-L1 as a function of L2 is reported in Fig. 6(b). A nice linearity is clearly observed.
We can also estimate the temperature rise \( \Delta T \), by considering the temperature dependence of
the SiPM dark current reported in Fig. 5, and by assuming the same temperature dependence
for the SiPM current under illumination. Through this hypothesis, we evaluate the corre-
sponding SiPM temperature change in °C, and this is reported on the right axis of Fig. 6(b).

### 3.3. Signal-to-noise ratio measurements

The Signal-to-Noise ratio (SNR) is evaluated by performing measurements of the SiPM pho-
tocurrent signal under LED illumination [23,24,2] with a square wave of 17 Hz and 50% duty
cycle. The signal (S) is the difference of the average photocurrent when the LED is on and the
average dark current when the LED is off, while the noise (N) is the root-mean-square (RMS)
of the photocurrent, thus, since the signal we measured is a voltage difference (current
through a resistor), the SNR in dB is defined as \( 20 \log_{10} (S/N) \). The signal is an average of
10 cycles, acquired by the oscilloscope with a constant sampling frequency of 1 MHz, and
integrated in a time range going from 100 µs (corresponding to an effective sampling frequency of 10 kHz) to 10 ms (corresponding to an effective sampling frequency of 100 Hz). The minimum optical power delivered to the SiPM by the LED sources was, both at 700 nm and 830 nm, of about 1 nW.

Figures 7(a) and (b) report the data of SiPM SNR as a function of the SiPM bias at two LED wavelengths, 700 and 830 nm, typical of fNIRS operation. As the effective sampling frequency decreases, or equivalently as the integration time increases from 100 µs to 10 ms, an evident improvement of the SNR is observed. The largest SNR is found at voltages of about 31.5 V, i.e. for ~3 V overvoltage.

![Graph](image1)

Fig. 7. Signal to Noise Ratio as a function of bias voltages of the SiPM. Photocurrent measured under LED illumination with a square wave of 17 Hz and 50% duty cycle; (a) 700 nm LED; (b) 830 nm LED. (c) SNR at 31.5 V bias voltage measured (dots) and extrapolated (lines, linear fit) as function of the effective sampling frequency.

Figure 7(c) reports the measured SNR at 31.5 V as a function of the effective sampling frequency. At 100 Hz, the SNR is above 80 dB, and the extrapolated SNR at 10 Hz is close to 100 dB, both at 700 and 830 nm.

4. Conclusions

SiPM devices are very promising for CW fNIRS since they allow very high responsivity and SNR. After-pulsing effects, related to defects located in the n+ CZ substrate, produce negligible problems for the CW fNIRS application since they only cause small after-pulsing / delayed detection effects in the 1-5 µs time range, i.e., in a time domain not relevant for CW fNIRS. A more important effect to take into account is the temperature change (rise and fall) as the SiPM device goes from the dark condition (LED in off-state) to the illumination condition (LED in on-state), and vice-versa. In this paper we show that (a) such temperature change produces transients in the SiPM current of a few hundreds of µs, (b) the temperature change is of the order of 10 – 20 °C, and (c), the temperature can be reduced by reducing the
LED power in on-state, since we noticed that the optical power required in an fNIRS application with this kind of detectors can be set in the range of 10 – 50 nW. Another crucial aspect to consider in the fNIRS application is the presence of the thermal transient described above. It is therefore very important in our opinion in the fNIRS application to use an appropriate electronic time gating to filter out the transient period in which the SiPM temperature changes because of the LED switch on or switch off. Finally, we measured that the SiPM devices exhibit a high SNR in standard CW fNIRS operation, of about 60-70 dB at 1 kHz and extrapolated a value close to 100 dB at 10 Hz.

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