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ABSTRACT

Photons absorbed in silicon produce electron–hole pairs, which can cause impact ionization and quantum yield larger than one. Reliable determination of quantum yield at low charge-carrier energies (<4 eV) has been challenging because photon losses due to reflectance and charge-carrier losses due to recombination affect the resulting photocurrent. Here, we present how the measurement of this fundamental characteristic of silicon crystals can be improved in the charge-carrier energy range of 1.6–4 eV by using a predictable quantum efficient detector based on induced junction photodiodes optimized for photon-to-electron conversion efficiency. The measured quantum yield values are compared with the results of theoretical calculations, revealing increased impact-ionization probabilities at 2.25 and 3.23 eV on the top of a smooth background curve calculated by a model based on free charge carriers in the silicon lattice. For the results at the lowest energies, both data and an asymptotic extrapolation model suggest that quantum yield exceeds unity by ~ 10^{-4} at 1.6 eV corresponding to a photon wavelength of 450 nm.

Silicon detectors are widely used for measurement of light and for energy conversion in solar cells. Extensive literature studies are available on analyzing the detection efficiency, including the effects of impact ionization.[1–6] Quantum yield due to impact ionization is also important in scientific applications, such as photon/particle detectors in astronomy[7–10] and primary standards of spectral responsivity.[11–14] Understanding the impact ionization processes is important for these applications as the measured signal often critically depends on quantum yield. Experimental data on impact ionization can be obtained by injecting hot charge carriers in silicon by tunneling[15] or by photon irradiation[2,7] and measuring the resulting electrical current. There are limitations on these experiments at low charge-carrier energies, where not much reliable data below 2 eV kinetic energies are available. Photon irradiation experiments[2,6,16,17] often suffer from large reflectance and charge-carrier recombination losses, which affect the measured photocurrent, while tunneling experiments[15] struggle with the determination of the exposed energy. Thus, a basic question on the location of any threshold energy of impact ionization above the indirect energy gap E_g = 1.12 eV at room temperature remains unanswered.

Here, we introduce a method that allows reliable impact ionization data in silicon to be obtained for determining quantum yield at low charge-carrier energies. The method is based on a silicon photodiode detector, which is known as a Predictable Quantum Efficient Detector (PQED), where the reflectance and charge-carrier recombination losses are made so small that they do not influence the results or any remaining losses can be corrected with low uncertainty.[11–14] Data on quantum yield above 1 are obtained between charge-carrier energies of 1.6 and 4 eV and compared with the results of theoretical calculations.

The charge-carrier recombination losses are largely eliminated by the use of *p*-type induced junction photodiodes with 5 V reverse biasing. A thick thermally grown SiO_2 layer on the top of a very lightly doped silicon substrate of impurity concentration of ~ 10^{12} to 10^{13} cm^{-3} contains trapped surface charge close to the Si/SiO_2 interface.[11] This charge generates an *n*-type inversion layer and produces a depletion region required for photocurrent generation. As there is so little impurity doping in the photodiode, the density of bulk recombination centers is reduced. Furthermore, the surface recombination velocity is also small, and the total relative losses by charge-carrier recombination are less than $1.2 \cdot 10^{-4}$ at wavelengths above λ = 400 nm,[14] as shown by the solid purple line in Fig. 1. The penetration depth in silicon reduces by one order of magnitude from 100 nm at λ = 400 to 10 nm at λ = 360 nm.[18] The relation between the penetration depth and charge-carrier recombination losses between 400 and 500 nm[14] has been used for extrapolation of losses, indicated by the dashed purple line in Fig. 1. The extrapolation assumes that the spectral shape of charge-carrier recombination losses is the same as the spectral shape of the inverse penetration depth. This assumption is approximately valid between 400 and 500 nm. The penetration depth stays constant within a factor of two between 360 and 245 nm, which leads to corresponding weak wavelength dependence also in the extrapolated charge-carrier losses in this spectral range.

In the PQED, two 11 × 22 mm^2 induced junction photodiodes of SiO_2 layer thicknesses of 220 and 300 nm are combined as a wedge trap detector,[11] where the outcoming light beam is strongly attenuated by several reflections inside the detector (Fig. 2). The reflectance of the PQED can be determined either by calculation according to the geometry and the refractive indices of SiO_2[19] and silicon[18] or by measuring the relative intensity of the outcoming beam. The reflectance of the trap is smaller than $5 \cdot 10^{-3}$ in the visible wavelength range (Fig. 1). The spectral responsivity of the PQED in the units of A/W is

$$R(h\nu) = \frac{e}{h\nu}(1 - \rho(h\nu))(1 - \delta(h\nu))(1 + g(h\nu)), \quad (1)$$

where $e/(h\nu)$ is the responsivity of an ideal quantum detector expressed by the elementary charge e and the photon energy $h\nu$. Parameters $\rho(h\nu)$ and $\delta(h\nu)$ describe the losses by spectral reflectance and recombination of charge carriers, respectively, and $1 + g(h\nu)$ is the quantum yield. Quantum yield may be larger than one, and here, it is defined as the average number of electrons per absorbed photon in the photodiode, caused by impact ionization in silicon. Equation (1) neglects any losses due to transmission through the photodiode because the light penetration depth in silicon is less than 2 μm at the wavelengths used in this work.[18]

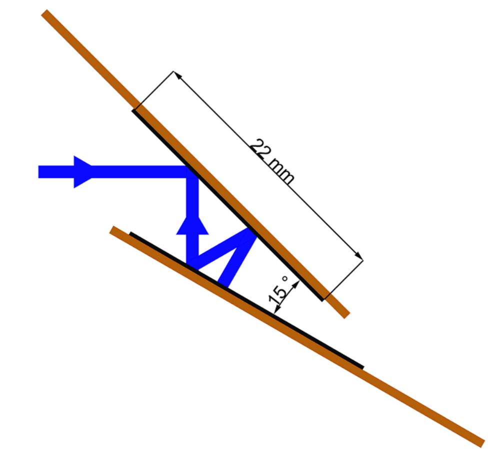

FIG. 2. Photodiode alignment in a wedge trap configuration with the light path for the 7-reflection PQED.

Our measurement setup consists of a xenon light source, grating monochromator, PQED under test, broadband wire-grid polarizer for producing light with different polarization states, and reference pyroelectric radiometer calibrated for measurement of optical power. The photocurrent signal from the PQED was divided by the optical power obtained from the pyroelectric radiometer to determine the measured spectral responsivity $R(h\nu)$ of Eq. (1). To reduce noise in the data, measurements were repeated several times and then averaged. Results with p- and s-polarized incident light are displayed in Fig. 3.[20] The relative expanded uncertainty of these data is 1%.

Impact ionization causes the measured spectral responsivity in Fig. 3 to deviate in the ultraviolet region from the ideal responsivity

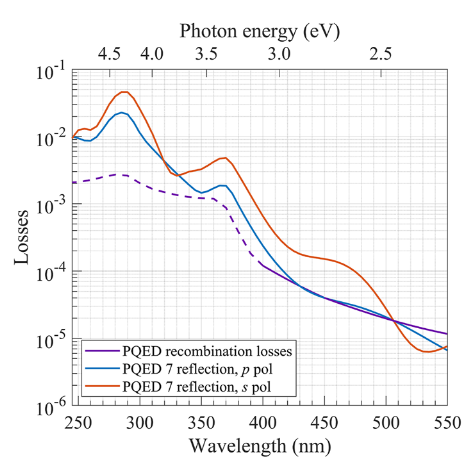

FIG. 1. Simulated charge-carrier recombination losses in PQED photodiodes from Ref. 14 (purple curve) and calculated reflectance losses of a 7-reflection PQED with p-polarized (blue curve) and s-polarized light (orange curve). The dashed purple curve represents extrapolation (see the text for details).

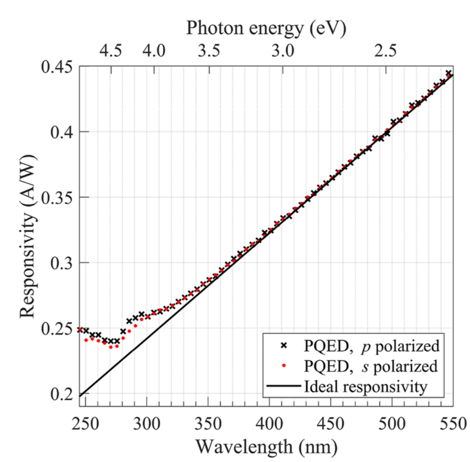

FIG. 3. Measured responsivity for the 7-reflection PQED at p-polarization (black crosses) and s-polarization (red dots) from Ref. 20 and ideal responsivity $e/(h\nu)$ of the silicon photodetector (solid line).

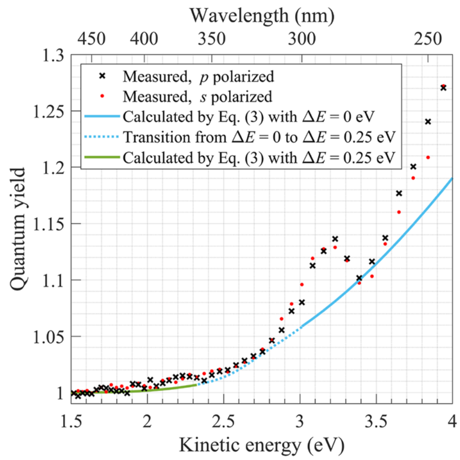

FIG. 4. Quantum yield measured with p (black crosses) and s (red circles) polarizations. The solid line is calculated by Eq. (3) with $\Delta E = 0$ for $E > 3$ eV (blue) and $\Delta E = 0.25$ eV for $E < 2.3$ eV (green). The blue dotted line represents the transition from $\Delta E = 0$ to $\Delta E = 0.25$ eV.

of the quantum detector indicated by the solid line. The responsivity for s-polarized light is lower than that for p-polarized light at wavelengths of 250–310 nm because reflectance of the former is larger in that spectral range, as seen in Fig. 1. In addition, it is seen that the reflectance is larger than the recombination losses. With known values of $e/(h\nu)$, $\rho(h\nu)$, and $\delta(h\nu)$, the measured quantum yield corresponding to $1 + g(h\nu)$ is obtained from Eq. (1) and shown in Fig. 4 as a function of the charge-carrier kinetic energy $E = h\nu - E_g$. Above kinetic energy $E = 1.6$ eV, the experimental quantum yield starts to get values above 1, reaching 1.3 at 4 eV.

We next compare the measured quantum yield with theoretical results. A straightforward calculation of quantum yield assumes that the charge-carrier density of states can be described by that of free carriers, while more detailed derivations consider the energy band structure in the silicon lattice.[1,4,10] According to those calculations, the excess number of electron–hole pairs per absorbed photon as a function of photon energy $h\nu > E_g$ is given by

$$g(h\nu) = \int_0^{h\nu - E_g} P(h\nu, E)N(E)\mathrm{d}E, \tag{2}$$

where $P(h\nu, E)$ is the probability distribution of generating a hole or electron of kinetic energy E and $N(E)$ is the average number of electron–hole pairs produced by impact ionization by a carrier with the initial energy E above the energy gap E_g. The maximum energy available for a charge carrier is $h\nu - E_g$.

For low energy transfer, $P(h\nu, E)$ can be approximated by a sum of two delta functions of E peaked at zero and at $h\nu - E_g$.[10] As low photon energies are our primary interest here, we use the delta function approximation leading to $g(h\nu) \approx N(h\nu - E_g)$ because $N(0) = 0$. It is then assumed that the charge carrier density of states can be described by that of free carriers, which gives[1,10]

$$g(h\nu) = \left[1 + A_1\left(h\nu - E_g - E_{ph} - \Delta E\right)^{1/2} / \left(h\nu - 2E_g - \Delta E\right)^{7/2}\right]^{-1}, \tag{3}$$

where $A_1 = 105A/(2\pi) = 86.9$ eV^3 is the constant derived in Ref. 1, $E_{ph} = 0.063$ eV is the energy of the optical phonon in silicon,[21] and ΔE is an energy shift, which is nominally zero but can be used here to relax the above-mentioned assumption on the charge carrier density of states. Wolf *et al.*[5] compared the results in Ref. 1 with other experiments[3] and more realistic band structure calculations.[4] They found out that around a kinetic energy of 2 eV, the results of Refs. 3 and 4 seem to be shifted to lower energies by $\Delta E = 0.25$ eV, relative to Ref. 1.

The quantum yield calculated by Eq. (3) is shown by the solid curve in Fig. 4. It is mostly below the measured data, revealing increased impact-ionization probabilities at kinetic energies of 2.25 and 3.23 eV on the top of a smooth background curve. These peaks correspond to peaks A and C measured by Kolodinski *et al.*,[2] close to the same energies, and are caused by hot electrons and hot holes, respectively. It should also be noted that in Fig. 4, we do not see peaks B (2.64 eV) and D (3.47 eV).[2]

The quantum yield calculated with $\Delta E = 0.25$ eV, as shown in Fig. 4, is expected to be applicable at charge carrier energies of about 2 eV and below. As shown in Fig. 5, we apply those calculations to the external quantum efficiency data published in Ref. 22, after correcting for the estimated reflection and charge-carrier recombination losses. The measured and calculated quantum yield values agree well when taking into account that the simplified calculated result does not include any fitted parameters. Remarkably, both the data and calculated curve indicate quantum yield above 1 at kinetic energies of 1.6 eV. The extrapolated quantum yield curve reaches 1 at $E = 1.37$ eV corresponding to a photon wavelength of 498 nm.

Previous studies of quantum yield in silicon provide information on experimental results and calculation methods, but their main interest has been at energies corresponding to incident photons in the ultraviolet and higher energy ranges. Here, we have described how those results can be applied at short visible wavelengths. This spectral range has recently become important for quantum yield

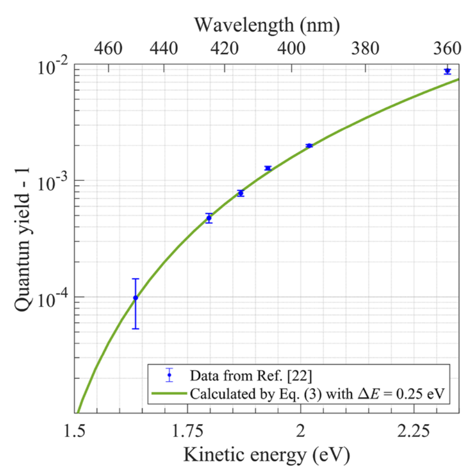

FIG. 5. Experimental quantum yield from Ref. 22 (blue dots) with a 9-reflection PQED and quantum yield calculated by Eq. (3) (green curve). Correction of internal losses[14] from Fig. 1 and reflectance correction for the 9-reflection trap structure are applied to data points. The uncertainty is given at the 1σ level.

studies because of the need to extend the predicted spectral responsivity of the PQED across the full silicon photodetector range. For the results at lowest energies, we show that the threshold kinetic energy of impact ionization is at 1.6 eV or below.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Mikhail Korpusenko: Formal analysis (equal); Investigation (equal); Methodology (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Anna Vaskuri**: Investigation (equal); Methodology (equal). **Farshid Manoocheri**: Conceptualization (equal); Validation (equal). **Erkki Ikonen**: Conceptualization (lead); Supervision (lead); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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