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Letter to the Editor

Electron–hole pair creation energy and Fano factor temperature dependence in silicon

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Abstract

The energy to create an electron–hole pair and the Fano factor in silicon have been evaluated as a function of the temperature by means of a full Monte Carlo simulation.

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Keywords: Silicon detector; Electron–hole pair creation energy; Fano factor

Recently a measurement of the energy to create an electron–hole (e–h) pair and its temperature dependence in the range between 80 and 270 K has been performed using an Si PIN diode with 5.9 keV X-rays [1]. A value of 3.73 ± 0.09 eV with a gradient of $-0.0131 \pm 0.0004\%\,\mathrm{K}^{-1}$ was found. A Fano factor of 0.118 ± 0.004 in the temperature range between 110 and 235 K was also found. The mean energy for the generation of one pair was also measured with synchrotron radiation with energies between 300 and 1400 eV at room temperature and at 140 K [2]. Experimental results show that the energy to create an e–h pair in silicon depends both on the photon energy and on the temperature.

In this paper the energy $W(E,T)$ to create an e–h pair and the Fano factor $F(E,T)$ in silicon as a function of the photon energy and their temperature dependence are evaluated by means of a full Monte Carlo simulation. The charge carriers are produced both in the primary collision (e.g. when a photon is absorbed) and by the subsequent energy losses of the secondary e–h pairs. The absorption of photons and the subsequent relaxation of the excited atoms yield the photo-electrons, the Auger and Coster–Kronig primary electrons and the corresponding primary holes in the valence band. All primary electrons and holes lose part of their kinetic energy by phonon scattering and another part by impact ionizations, producing secondary e–h pairs [3].

In this Monte Carlo the generation of secondary e–h pairs is simulated following the prescriptions of [4,5], where a simple band-structure model is assumed and the random-k approximation to the transition rate for impact ionization is used for both electrons and holes. The ratio of phonon emission with respect to the impact ionization is the same for both electrons and holes, and depends on the energy gap, on the phonon energy and on parameter that is assumed independent on the particle energy and invariant for electrons and holes, and for the temperature. The relaxation process following the photo-absorption in the silicon shells produces electrons and vacancies in the shells according to the relaxation trees and probabilities that have been taken from Refs. [6,7].

The temperature dependence of W and F are evaluated by assuming a temperature dependence of the energy gap in silicon $E_{\mathrm{g}}(T)$ given by the Varshni equation [8]:

$$E_{\mathrm{g}}(T) = E_{\mathrm{g}}(0) - \frac{\alpha T^2}{T+\beta} \tag{1}$$

where $E_{\mathrm{g}}(0) = 1.17$ eV is the energy gap at the temperature $T = 0$ K, $\alpha = 4.73 \times 10^{-4}$ eV/K and $\beta = 636$ K. The parameters of Eq. (1) are taken from the Ioffe Institute

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database [9] and they are slightly different from the results published in Ref. [10]. Another expression for the dependence of the energy gap with temperature can be found in Ref. [11]. The energy of the optical phonon E_0 is set to a constant value of 0.063 eV in the calculation.

Fig. 1 shows the energy to create an e–h pair as a function of the temperature for incident photons of 5.9 keV energy. The pair creation energy W is given by

$$W(E,T) = \frac{E}{n(E,T)} \tag{2}$$

where E is the photon energy and $n(E,T)$ is the number of total pairs, that takes also into account the primary e–h pairs (e.g. the photo-electron, the Auger electrons and their vacancies) [3]. The W value is evaluated as the average value from a sample of 10,000 simulated events for each temperature value from 10 to 460 K. The energy to create an e–h pair slightly decreases with the temperature, from about 3.73 eV at 10 K to about 3.57 eV at 460 K. The e–h pair creation energy gradient is of order of 10^{-4} eV/K, even though the energy to create a pair is not linear with the temperature. The Fano factor for the pair number distribution is almost constant with small fluctuations around the value of 0.117.

Fig. 2 shows the energy to create an e–h pair as a function of the temperature in the range from 50 to 400 K evaluated at four different photon energies in the region around the Si L-shells, i.e. 50, 125, 200 and 500 eV. The e–h pair creation energy gradient is still of order of 10^{-4} eV/K for these photon energy values.

Alig et al. [4] inferred that the temperature dependence of the phonon energy is weak, so the contribution to the energy to create an e–h pair in silicon with the temperature due to the phonon temperature dependence is negligible. In order to evaluate this effect, the energy to create an e–h pair is evaluated assuming a linear dependence of the phonon energy from the temperature, i.e. $E_0(eV) = 0.063 + a(T(K) - 300)$. For the slope a the values of $\pm 10^{-5}$ and $\pm 10^{-4}$ eV/K have been simulated, namely 1 order of magnitude less than the energy gap temperature gradient and of the same order of the energy gap temperature gradient. The results for incident photons of 5.9 keV energy are shown in Fig. 3. For positive values of slope a the e–h pair creation energy gradient decreases, and for large positive values it becomes positive. On the other hand, for negative values of a the e–h pair creation energy gradient increases, and for large negative slope values it becomes too large with respect to the experimental results.

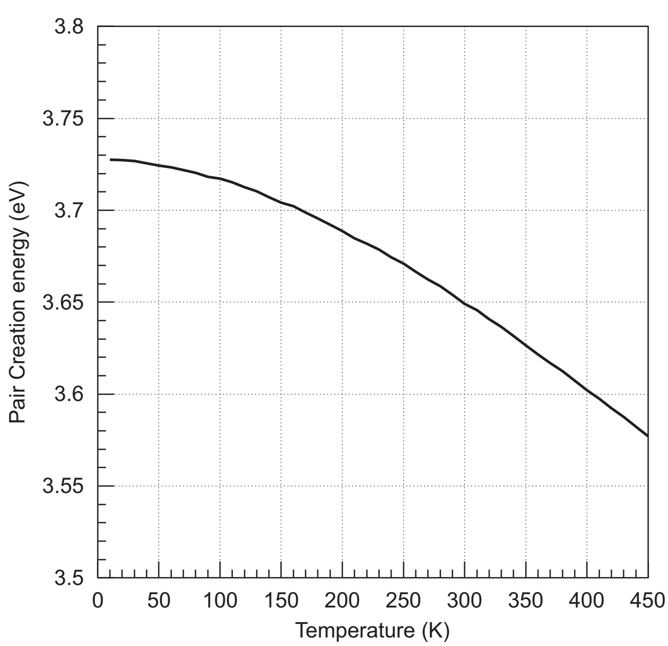

Fig. 1. Electron–hole pair creation energy in silicon as a function of the temperature for 5.9 keV incident photons.

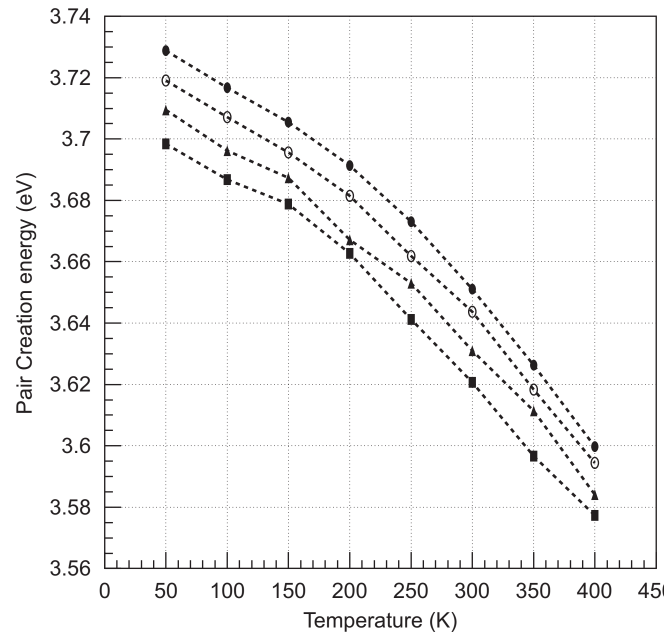

Fig. 2. Electron–hole pair creation energy (average value) as a function of the temperature at different photon energies. Full circles: $E = 50$ eV; full triangles: $E = 125$ eV; full squares: $E = 200$ eV; open circles: $E = 500$ eV. The dashed lines are drawn as a guide for the eye.

Fig. 4 shows the mean energy to produce a pair as a function of the incident photon energy, for two different temperature values, i.e. 140 and 300 K (the energy of the optical phonon is set to a constant value of 0.063 eV). The energy to create an e–h pair approaches a constant value for incident photon energies above the Si K-shell energy. The constant value is about 3.70 eV at 140 K, while decreases to about 3.65 eV at 300 K. These results are in agreement with the one shown in Refs. [2,12]. The dependence of W on the incident photon energy exhibits a discontinuity in the photon energy region around the Si L-shells (e.g. around 100 eV) (see Ref. [3] for more details). A maximum value of about 3.85 (3.80) eV is found at incident photon energy around 4.5 eV, and a minimum value of about 3.6 (3.5) eV is found at incident photon energy around 6 eV for 140 (300) K. Finally, a linear