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A method to overcome the time step limitation of PC1D in transient excitation mode

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Abstract

This paper presents a method to overcome the time step limitation of PC1D in the transient excitation mode without changing the source code of PC1D. By comparing the results obtained from PC1D using the proposed method with results obtained from a finite element analysis, the correctness of the method is confirmed. The proposed method allows simulations over long times with high time precision, which is currently not possible in PC1D in transient excitation mode.

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Keywords: PC1D; transient; time step limit

1. Introduction

PC1D is a computer program used for modelling crystalline semiconductor devices, with emphasis on photovoltaic devices [1]. It is widely used as a simulation tool for photovoltaic research and industry, not only helping users to understand the fundamental mechanism and operation of solar cells, but also efficiently giving reliable and predictable results for research purposes [2-4]. However, one limitation of PC1D is that the number of time steps in transient excitation mode is limited to 200 [5]. As a result, if long duration simulations are required, big time steps should be chosen. Conversely, if small time steps are desired, only short duration simulations can be achieved. It is impossible for users to perform simulations that require both long duration and small time steps. This is a limitation within the PC1D source code set by the size of the cache memory at the time the program was written

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and compiled. In this paper, we will present a method which overcomes the time step limitation of PC1D without changing the source code of PC1D.

2. Approach

A straightforward method to overcome the time step limitation imposed by PC1D would be to store the final solution of a given simulation and then load it back as the initial condition for a subsequent simulation. Since this is not possible in PC1D, we devise a method which relies on storing data of the final transient simulation, process this data and then load the processed data back into PC1D to allow it to restart a simulation based on the conditions of the previous simulation.

To achieve this, we investigate the mechanism of how PC1D performs a transient simulation. The first two steps of a transient simulation find the thermal equilibrium and steady-state solutions. Taking advantage of this, by forcing the steady-state solution to be equal to the final solution of a previous transient simulation, a subsequent transient simulation can be continued from where the previous one ends. The required steady-state solution can be achieved by using an external depth-dependent photogeneration profile (specified by an external ASCII file with suffix GEN [5]). This profile can be calculated based on the final solution of the transient simulation. What remains is to load the calculated GEN file to create an initial condition for the second step of a transient simulation and then remove this file to allow the transient simulation to continue with the transient conditions of interest. In this paper, we demonstrate the method using a transient primary time-dependent illumination intensity (specified by an external ASCII file with suffix LGT [5]), but it could be equally used with any other time-dependent variations of external voltage and excitation wavelength.

For computing the external depth-dependent photogeneration profile, we employ the minority carrier density, the current density, and carrier recombination solutions obtained from PC1D. Taking p-type silicon as an example, we have the following continuity equation [6]

$$\frac{dn}{dt} = \frac{1}{q}\frac{dJ_e}{dx} + G - U \tag{1}$$

where n is the electron carrier density, t is the time, q is the electron charge, J_e is the electron current density, x is the depth into the silicon sample. G and U are the depth-dependent carrier generation and recombination rate, respectively.

As the GEN file we need to compute is assumed to be a steady-state condition, we make $dn/dt = 0$. Therefore, G is given by

$$G = U - \frac{1}{q}\frac{dJ_\mathrm{e}}{dx} \tag{2}$$

By integrating both sides of Eq. (2) with respect to x, we have

$$G_\mathrm{cum} = U_\mathrm{cum} - \frac{1}{q}J_\mathrm{e} \tag{3}$$

J_e and the depth-dependent cumulative recombination, U_cum, can be directly output from PC1D. As the depth-dependent cumulative carrier generation, G_cum, is required for the GEN file, we can simply use Eq. (3) to create an ASCII file that would become the GEN file of interest.

Following is the flow chart of the procedures required by this method:

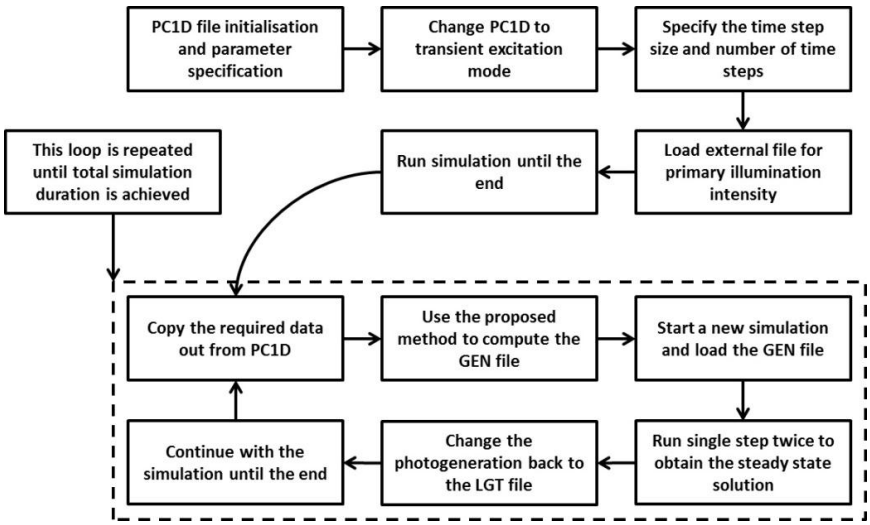

Fig. 1. Flow chart of the procedures required by the proposed method

3. Discussion

In order to verify the validity of the method, we simulate a periodic square wave (on and off) of a monochromatic light to illuminate a silicon sample. As revealed by a finite element analysis (FEA) [7], under such periodic signal, the excess minority carrier density will undergo accumulation and decay process when the signal is on and off, respectively (as shown in Figure 2(a) for the first 5 illumination oscillations). After a sufficient number of illumination oscillations, the minority carrier density distribution will eventually change in a periodic manner, which is referred as a "stabilised" condition (as shown in Figure 2(b) for the 10^{th} and 11^{th} illumination oscillations).

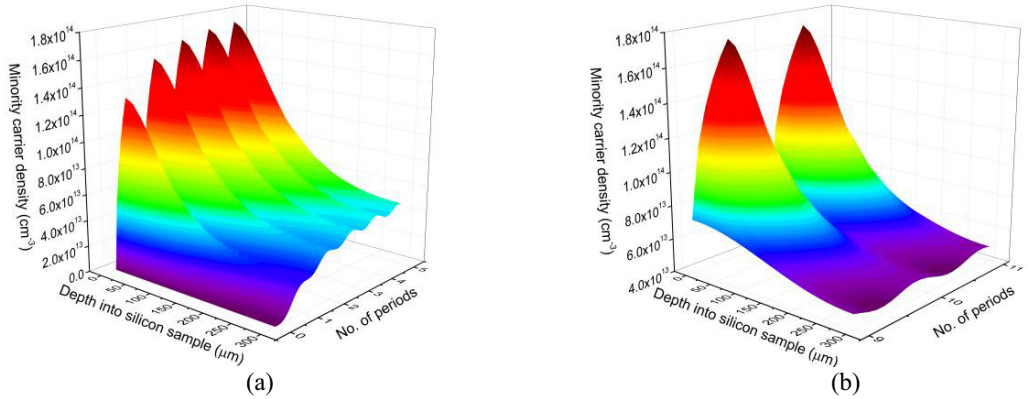

Fig. 2. The minority carrier density distribution along depth into silicon sample with a periodic square wave monochromatic light illumination (a) minority carrier density distribution builds up before getting stabilised (b) periodically stabilised minority carrier density distribution (obtained using TPL1D [8]). Parameters used are as follows: Wavelength of the monochromatic light is 900 nm. The period of the square wave is 8 μs and it has a duty cycle of 50%. When the signal is on, its intensity is 0.1 W/cm^2, which corresponds to a photon flux of approximately 4.525×10^{17} #/cm^2/s. The silicon sample is selected to be a 300 μm thick p-type semiconductor with a background doping density of 1.5×10^{16} #/cm^3. The bulk minority carrier lifetime is set to 10 μs and the silicon surfaces are assumed to be perfectly passivated (surface recombination velocity is zero).

The square wave requires abrupt changes of then generation rate when the light is switched on or off. Coarse time steps are not able to guarantee that this abrupt change can be captured (as shown in Figure 3). Therefore, we have to choose a very small time step size to ensure the numerical simulation captures this process. Considering the time step limit of PC1D in transient excitation mode, the total simulation duration is limited, within which a stabilised minority carrier density distribution might not have been achieved. Therefore, we have to use the method proposed here to extend the simulation duration until a stabilised condition is achieved.

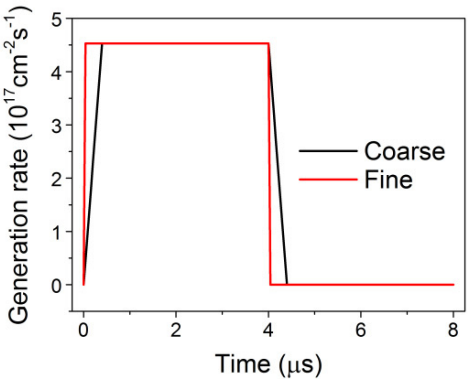

Fig. 3. Generation rate with abrupt change when coarse and fine time steps are used in PC1D. “Coarse” and “fine” refer to time steps of 500 ns and 50 ns, respectively. It is obvious that a coarse time step reduces the steepness of the generation rate.

Table 1. The external time-dependent illumination intensity specification

Time (μs)	Intensity (W/cm^2)
0	0
0.05	0.1
4	0.1
4.05	0
8	0
8.05	0.1

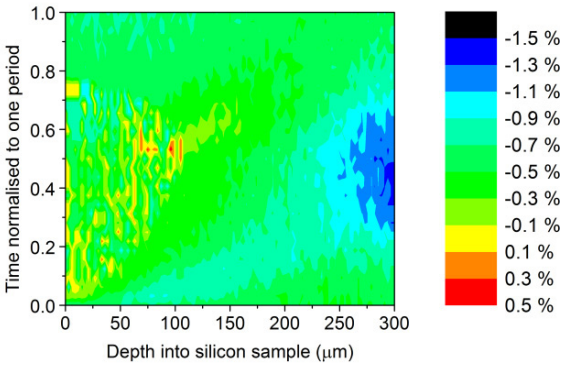

Fig. 4. Comparison of the relative difference of stabilised periodical minority carrier density obtained from PC1D and TPL1D.

For the transient excitation setting, the time step size is set to 50 ns and the number of time steps is set to 160, which would ensure the simulation of a single period of the signal each time. Same parameters are adopted for the simulation using PC1D and for other parameters, we use default settings.

The LGT file is specified with a rise and fall time of 50 ns in Table 1, which is an approximation the square wave.

By using the method proposed in this paper, we could extend the simulation duration indefinitely. In practice, we repeat the loop identified with the dotted line in Figure 1 until a stabilised excess minority carrier density distribution is obtained. In this case, 9 iterations are necessary before the stabilised excess minority carrier density distribution is found. The periodic distribution of minority carrier obtained from TPL1D [8] and the method introduced in this paper are then compared and the result is shown in Figure 4.

According to Figure 4, the results obtained from two methods coincide very well with each other, with a maximum relative deviation of about -1.5% and it mainly concentrates around 0.5%. As a result, the validity of the method proposed here has been verified.

4. Summary

In order to overcome the time step limit of PC1D in transient mode, the proposed method computes the external depth-dependent photogeneration profile from the final solution of a transient simulation. This photogeneration profile can then be input as the initial condition of the subsequent simulation, allowing us to overcome the time step limitation of PC1D and be able to do transient simulations for any length of time with an arbitrarily high time precision (limited only by the numerical accuracy of PC1D). The validity of the method is verified by comparing the excess minority carrier density obtained with result of the FEA method developed elsewhere [7]. The proposed method is particularly relevant when small time steps are required while long simulation duration is also needed. The drawback of the method is that many steps of the method need to be manually performed including copying the required data, loading the relevant photogeneration file, running the two first simulations in single step mode and then running the remaining transient simulation. These manual operations could be very time consuming if long simulation duration is required and many iterations are needed. Recently, papers have been published on a command-line version of PC1D [9,10], which enable flexibility through implementing the calculations in a scripting environment. As a result, future work will focus on merging this method into the command-line version of PC1D or modifying the source code of PC1D to overcome the time step limitation in a more efficient way.

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