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PC1Dmod 6.1 – state-of-the-art models in a well-known interface for improved simulation of Si solar cells

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ABSTRACT

In this paper, we present a new, updated version of the commonly used semiconductor device simulator PC1D named PC1Dmod 6.1. The new program is based on the previously published command line version cmd-PC1D 6.0, which has implemented several new options related to the device physics, but now uses an updated version of the original PC1D graphical user interface. The program thus provides the possibility for using Fermi–Dirac statistics and a selection of state-of-the-art models for crystalline silicon, including injection-dependent band gap narrowing, carrier mobility and Auger recombination, in a familiar setting.

Version 6.1 also has implemented the recently published band gap narrowing model by Yan and Cuevas, which is based on empirical studies of a large selection of both n^+ and p^+ emitters, in addition to Schenk's model. It has also implemented the mobility model for compensated material by Schindler et al. Finally, the maximum number of nodes, time steps and wavelengths have been increased in order to reduce unnecessary constraints on simulations and external files.

The results from the PC1Dmod 6.1 simulations have been compared with those of other simulation tools and with previously published data to verify the correct implementation of the new models. Emitter saturation currents calculated using PC1Dmod 6.1 showed an excellent agreement with those obtained using the emitter recombination calculator EDNA 2, and the new program was able to successfully reproduce previously published experimental data and previous implementations of the models. Both PC1Dmod 6.1 and the command line version cmd-PC1D 6.1 are open source software, and are freely available for download.

1. Introduction

PC1D is an efficient, one-dimensional semiconductor device simulator which has strongly influenced the solar cell research community [1,2]. The program uses a finite-element numerical method for solving the coupled nonlinear equations for carrier generation, recombination and transport in the device. It can be applied both for simulation of device performance and as a tool for new users to understand the fundamentals of solar cell physics. The main advantages of PC1D include a high calculation speed, an intuitive user interface and an extensive list of material and physical parameters. By varying the applied bias or the wavelength of the excitation light source, PC1D can calculate both current–voltage characteristics and the spectral quantum efficiency of the solar cell, but it also has a large number of other options for output data, both in the spatial domain and in the time domain.

The carrier statistics in PC1D is based on the Boltzmann approximation, and several PV-specific models have been developed for use in this framework. However, since electrons are Fermions, they obey Fermi–Dirac (F–D) statistics. F–D statistics should therefore generally be used (together with a correct description of the band structure and the density of states) to obtain correct simulation results. Recently, we developed a modified version of the program called cmd-PC1D 6.0, which extends the original program by implementing F–D statistics [3]. Furthermore, models for various properties of crystalline silicon (c-Si) have been refined and improved since the latest official release of PC1D in 1997. We therefore also implemented several advanced Si-specific models into cmd-PC1D 6.0 in order to improve the accuracy of simulations of c-Si devices. An update that was of particular importance was the model for band gap narrowing (BGN), as the effect of carrier degeneracy at high doping levels (which is not accounted for by Boltzmann statistics) was previously included into an *apparent*

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BGN model. A list of the currently implemented state-of-the-art models for c-Si is provided later in this paper (Section 3).

For practical reasons, the changes to the device physics have previously been implemented in a simplified, command line version of PC1D which gives additional possibilities for scripting simulations. However, this flexibility comes with a requirement of a certain degree of programming skills for the user, or alternatively, the need to use a compiled Matlab program as an alternative graphical user interface, which was also provided [4]. As a response to several requests from the solar cell research community, we now present a new version of the program called PC1Dmod 6.1, which implements the new physical models into an updated version of the original GUI. Additionally, new Si models for BGN in highly doped regions, mobility in compensated material and position-dependent Shockley–Read–Hall recombination have been added, in addition to some numerical improvements.

The present paper is organized as follows. In Section 2 we give a short overview of the F–D implementation and the new physical models which were introduced in cmd-PC1D.6.0 [3]. In Section 3 the models newly introduced in this work (version 6.1) are described. In Section 4 we verify that the latest models have been correctly implemented by comparing the results to other well-accepted simulation tools and previously published data. In Section 5 we provide some details on the changes made to the user interface and on the configuration of physical models, as well as changes to the c-Si material files and to the numerical constraints of the program. The key results and suggestions for further work are given in Section 6.

2. Fermi–Dirac statistics and physical models introduced in version 6.0

The performance of solar cells is strongly affected by carrier recombination, which again depends on the excess concentration of minority carriers. Because of this, both the pn product and the recombination processes in the device must be known precisely in order to obtain accurate simulation results. The pn product at equilibrium scales as the square of the intrinsic carrier density n_i, and at large doping densities it is also significantly influenced by degeneracy and BGN. In order to correctly account for the statistical effects of electrons being Fermions, which become particularly apparent at carrier concentrations larger than $10^{18}\,\mathrm{cm}^{-3}$, Fermi–Dirac statistics should be used [5]. F–D statistics is now used as default in PC1Dmod, using the same implementation that was introduced for cmd-PC1D 6.0. Interested readers are referred to our previous publication [3] for a more detailed description.

The models used in PC1D 5.9 have been developed for use together with Boltzmann statistics, and should therefore be re-evaluated when changing to F–D statistics. This is particularly true for BGN, as the current models used in PC1D represent the *apparent* BGN, which accounts for various effects, including degeneracy at high doping levels. Because of this we cannot apply F–D statistics together with the existing BGN models, as this would overestimate the high doping effects. Instead, the BGN is calculated using the comprehensive theoretical model for both p-type and n-type Si by Schenk [6], which is derived for the case of F–D statistics from a non-self-consistent, full random phase approximation formalism, taking both carrier–carrier and carrier–dopant interactions into account. Schenk's model also accounts for BGN in the base substrate due to injected carriers, which can have a significant effect in devices and lifetime samples at high injection conditions [7].

The Schenk BGN model takes part in a collection of state-of-the-art models for (highly doped) c-Si which were chosen for use in cmd-PC1D 6.0 [3] as suggested by Altermatt et al. [5,8]. This set of models also includes Sproul and Green's model for the temperature-dependent intrinsic carrier density $n_{i,0}(T)$ [9], which has been linearly scaled by a constant factor 0.9677 to match the latest value of $9.65\times10^{9}\,\mathrm{cm}^{-3}$ at 300 K as reported by Altermatt et al. [10], as well as the extensive and commonly used mobility model by Klaassen [11,12]. Furthermore, we have also implemented the latest parameterization of intrinsic recombination by Richter et al. [13], which was derived using F–D statistics and Schenk's parameterization for BGN, and is based on a large set of empirical data, taking the latest advances in material quality and surface passivation into account. As an alternative we have also implemented the also commonly used model by Kerr and Cuevas [14] for intrinsic recombination. The current selection of new models implemented in PC1Dmod 6.1 is given in Table 1. More details on the choice of models and their implementation can be found in Ref. [3].

Table 1
Overview of the new Si models in PC1Dmod and cmd-PC1D. (*)=New models in version 6.1.

Model	Symbol	Ref.	
Intrinsic carrier density	$n_{i,0}(T)$	Altermatt et al. (2003)	[10]
Intrinsic energy band gap	$E_{g,0}(T)$	Green (1990)	[18]
Effective density of states, conduction band	N_c	Green (1990)	[18]
Effective density of states, valence band	N_v	(adjusted to match $n_{i,0}$)	
Bandgap narrowing	ΔE_c, ΔE_v	Schenk (1998)	[6]
		Yan and Cuevas (2013)*	[15]
		Yan and Cuevas (2014)*	[16]
Carrier mobility	μ_n, μ_p	Klaassen (1992)	[11,12]
		Schindler (2014)*	[17]
Intrinsic recombination	U_{intr}	Richter et al. (2012)	[13]
		Kerr and Cuevas (2002)	[14]
Numerical approximations for:			
Fermi integral	$u=\mathrm{F}_{1/2}(\eta)$	Van Halen and Pulfrey (1985)	[19]
Inverse Fermi integral	$\eta=f_{1/2}(u)$	Antia (1993)	[20]

3. Physical models added in version 6.1

The framework for implementing new models and a simple configuration of which models and parameters to use is now in place in the PC1Dmod program, and additional options for physical models can therefore be included in a simple manner, thus meeting the needs of different users and enabling the program to follow the latest scientific progress.

A clear example of an ongoing scientific debate is the discussion of how to simulate carrier recombination in the highly doped surface regions in Si solar cells, and the role of the band gap narrowing in this regard. Recently, Yan and Cuevas have published an empirical BGN model for 300 K based on fitting of measured emitter saturation current densities for a large selection of n^+ and p^+ dopant profiles determined by electrochemical capacitance–voltage measurements [15,16]. There is an ongoing discussion in the scientific community regarding the differences in the theoretical (Schenk BGN and F–D statistics) and empirical (effective BGN and Boltzmann/F–D statistics) approach to simulate highly doped regions in silicon. In order to provide users with additional options and to improve the predictive powers of the program, the empirical model of Yan and Cuevas has now been implemented in PC1Dmod 6.1 as an alternative to Schenk's BGN model (See Table 1). The