PC1D VERSION 5: 32-BIT SOLAR CELL MODELING ON PERSONAL COMPUTERS

Donald A. Clugston and Paul A. Basore
Photovoltaics Special Research Centre
University of New South Wales, Sydney 2052, Australia

ABSTRACT

The computer program PC1D is widely used for modeling crystalline solar cells. This paper describes a new version of the program which takes advantage of the latest graphical environments of personal computers to offer improved visualization of cell design and operation, simpler comparison of experimental data with simulation results, greatly increased calculation speed, and improved models for generation and recombination effects. We demonstrate the use of some of these features to explore the importance of trap-assisted tunneling at heavily doped junctions in material with low carrier lifetime, as is often encountered in thin polycrystalline silicon cells.

INTRODUCTION

It is important for any simulation program to keep pace with new developments in experimental work and theoretical models, and in available computer working environments. PC1D is the simulation program in most widespread use among the photovoltaic community. Over the past year, PC1D was cited at least twenty times in refereed journals [1]. Hence, it is particularly important that rapid development of the program be continued.

PC1D version 5 uses the 32-bit environment of Windows 95 to provide improvements in accuracy, speed, and convenience. Firstly, the program introduces new physical models, thus extending the domain over which simulation results are valid; secondly, the speed of the program has been dramatically increased; and thirdly, enhancements have been made to the user interface to make the program easier to use, and make parameter entry less error-prone.

As innovative new cell designs are explored, simulation programs are being required to operate outside of their usual regime. Some new designs are exposing inadequacies in the existing models. In particular, additional physical effects become important with heavy doping. Previous versions of PC1D [2-5] did not include these degradation mechanisms, making heavy doping misleadingly attractive. PC1D Version 5 incorporates improved models for two such heavy-doping effects: free-carrier absorption and trap-assisted tunneling.

The new free-carrier absorption model has already been discussed in a journal publication [6], where its significance for spectral analysis of cells is discussed. An additional consequence of this research, not mentioned in that paper, is that improving the light-trapping of near-bandgap wavelengths is far less beneficial than previously predicted.

Trap-assisted tunneling is implemented in PC1D using the field-enhanced recombination model proposed by Hurkx et al. [7]. To overcome objections that the Hurkx model overestimates trap-assisted tunneling [8], the parameters in the model have been made user-adjustable in PC1D.

PC1D FOR WINDOWS 95

In the interval between the last PVSC conference and the present time, Microsoft Windows 95 has become the dominant operating system on personal computers. It was clear to the authors that the next major release of PC1D should be a Windows 95 version, to harness the substantial benefits obtainable with this 32-bit operating system. In addition to the ability to cope with long filenames and other benefits of the Windows 95 operating system, PC1D Version 5 introduces several enhancements to the user interface. The new version makes extensive use of tabbed dialog boxes to make the program simpler and more convenient to use. The menu structure has been greatly simplified. The graphics code has been modified to eliminate annoying screen flicker during simulation runs.

The Windows environment encourages the use of intuitive, highly visual programs. The exploration of new cell designs is greatly simplified by the use of good visualization tools. In contrast, traditional numerical simulators describe a cell via a textual listing of parameters. This becomes cumbersome when complex designs are used. It is easy to make mistakes when entering parameters, and such errors can be difficult to trace. To aid in visualizing the cell structure being simulated, the Parameter View of PC1D now includes a device schematic (Fig. 1). As texturing, doping, and external elements are added, the schematic changes to reflect the new design. This instantaneous feedback helps users to ensure that they are performing the simulation which they intended. If the device is defined using multiple regions, each composed of a different

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material, the schematic display is segmented to clarify the size and properties of each region separately.

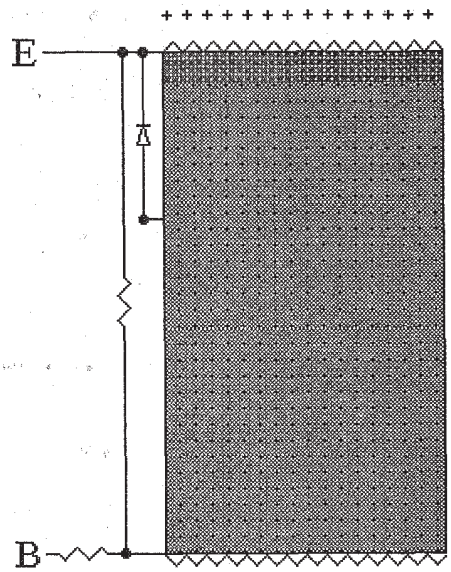

Fig. 1 Typical device schematic displayed by PC1D, showing dopant type, texturing, front-surface charge, electrical contacts, shunt and series elements.

The core of the program, a matrix inversion scheme, has been implemented in very fast assembler code. Further enhancements of the program have resulted in a huge increase in calculation speed. It is now approximately 2.2 times faster than Version 4†. This makes it feasible to perform calculations with a large number of time steps and/or a large number of finite elements.

PC1D is commonly used for interpreting experimental data to determine the structure of a device. For example, by matching a simulated IQE curve to an experimental one, several important device parameters can be determined. In previous releases of PC1D, performing such a match was tedious. Version 5 provides the ability to display experimental data and simulation results on the same graph within PC1D, enabling rapid comparison. An example is shown in Fig. 2, in which it is clear that the PC1D model needs to use a higher value for the rear optical reflectance to match the experimental data at near-bandgap wavelengths, and a lower front-surface recombination velocity to match the experimental data at the blue end of the spectrum. An iterative approach can be followed until an accurate fit is obtained.

† When both programs are running on Windows 95. This excludes improvements due to the operating system itself. Version 5 on Windows 95 is about 3.5 times faster than version 4.6 running on Windows 3.1.

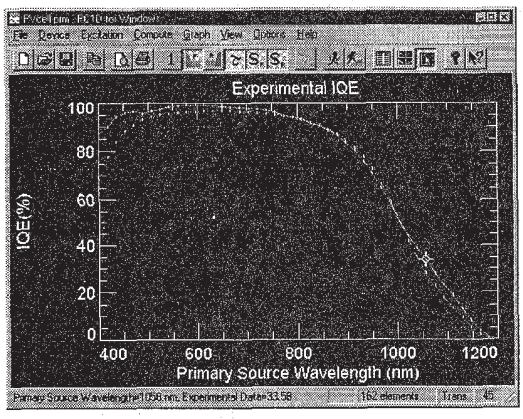

Fig. 2 Experimental IQE data displayed in PC1D together with the simulated IQE curve for easy comparison.

IMPROVED CONVERGENCE

There are some types of problems which PC1D is unable to solve. With releases of PC1D prior to version 4, convergence problems were difficult to diagnose. New features were added to allow non-convergent problems to be investigated. An option was added to the program to update the output graphs after each iteration, and a single-step facility was created to allow thorough investigation of all of the solution variables at the end of each iteration. The value of this approach was enhanced by adding an additional "Convergence Error" graph to the program, which shows the convergence error for each point across the device, for each iteration. This shows how far each mesh point is from satisfying the equations. It was discovered that the difficulty is often localized, being caused by a large change in one of the quasi-Fermi potentials across a single solution element.

A 'dynamic renoding' scheme was introduced to the program starting with version 4.2. The program searches for mesh points that are likely to cause difficulties. It subdivides these elements so that changes in the potentials are less severe. This new technique expanded the range of solutions which PC1D can solve, particularly situations involving large reverse bias.

FREE-CARRIER ABSORPTION

Free-carrier absorption can be a significant parasitic optical process in solar cells. This effect was incorporated starting with version 4.3 of PC1D, and it is described in detail in a recently published article [6]. The impact of this process on the performance of single-crystal silicon solar cells is only important when one or more layers are doped more heavily than 10 Ω/□. However, it does have enough of an effect on the near-bandgap spectral response to influence the determination of device parameters from this portion of the spectrum.

As an example involving application of the free-carrier absorption model, the internal quantum efficiency was calculated using PC1D for a textured silicon solar cell

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with an emitter doped to 50 Ω/□ that has a good rear-surface reflectance of 95% and a diffusion length equal to the device thickness of 300 μm. Fig. 3 illustrates the calculated result both with and without free-carrier absorption enabled.

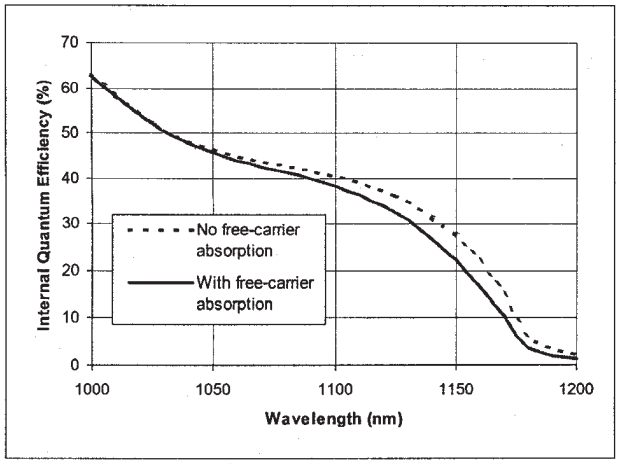

Fig. 3 Impact of free-carrier absorption on a solar cell with typical emitter doping and good rear-surface reflectance.

TRAP-ASSISTED TUNNELING

Trap-assisted tunneling becomes important as doping increases because heavy doping leads to steep gradients in the band structure at junctions. When the depletion region is very narrow, carriers can tunnel across the bandgap through intermediate trap states. Consequently, junction recombination is much worse for heavily-doped junctions than was predicted by previous versions of PC1D.

The Hurkx model [7] of trap-assisted tunneling is implemented in PC1D 5 using field-enhanced recombination. The steepness of the gradient in the band structure is directly related to the electric field strength. The standard SRH formula for recombination is used, but with the electron and hole lifetimes reduced by a factor of 1+ Γ, where Γ is a function of the electric field. The Hurkx model for Γ is:

$$\Gamma = prefactor.\frac{|F|}{F_\Gamma}\exp\left[\left(\frac{F}{F_\Gamma}\right)^2\right]$$

where $$F_\Gamma = \frac{\sqrt{24m^*(kT)^3}}{q\hbar} \qquad \text{(Eq 1)}$$

This expression can be parameterized by specifying a prefactor and the value of F_Γ at 300 K. Hurkx et al. suggest a prefactor value of $2\sqrt{3\pi}$ (=6.14) and a value for the effective electron mass of $m^*=0.25m_0$ (F_Γ =368.8 kV/cm at 300 K).

EXAMPLES USING TRAP-ASSISTED TUNNELING

To illustrate the importance of considering trap-assisted tunneling in certain cases, we studied the effect of this mechanism on junction recombination for asymmetrically doped junctions where the lifetime is low, as might be encountered in thin polycrystalline silicon material. We found that the junction recombination is determined almost entirely by the doping density in the more lightly doped side (the "base"), although the shape of the doping profile in the vicinity of the junction also has some effect. We considered the case of an abrupt junction and also a graded junction similar to that formed when a heavily doped emitter is diffused into a uniformly doped base.

The dependence of recombination on base doping density for an abrupt asymmetrical junction is illustrated in Fig. 4.

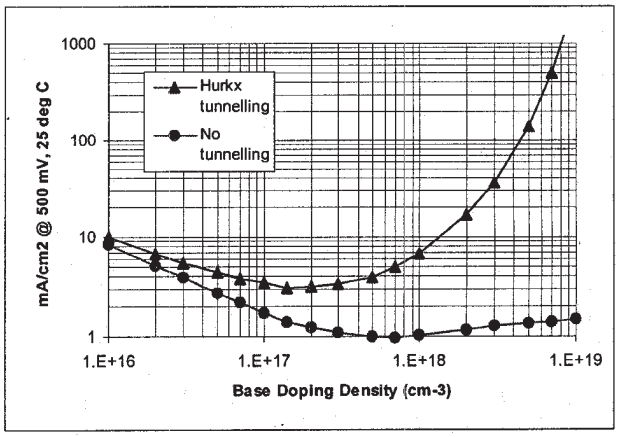

Fig. 4 Dark current for an abrupt n^+p junction in 10-ns silicon material calculated using PC1D Version 5 showing the impact of trap-assisted tunneling.

Fig. 4 was calculated for an abrupt junction formed into a p-type base using an n-type emitter with a doping concentration of 3.5×10^{19} cm^{-3} and a thickness of 0.2 μm (100 Ω/□). The current shown in the figure is the dark current at 500 mV forward bias for a 1-μm-thick device having zero surface recombination velocity and electron and hole lifetimes both equal to 10 ns. Virtually all of the current under these conditions is due to recombination within the junction space-charge region. In the absence of trap-assisted tunneling, the recombination decreases initially with increasing doping density as the width of the depletion region is reduced, but begins to climb again as bandgap narrowing takes hold above 10^{18} cm^{-3}. With trap-assisted tunneling enabled, recombination is higher at all doping densities investigated, but is particularly significant for heavy base doping. At the optimum doping density of 1.4×10^{17} cm^{-3}, trap-assisted tunneling increases the recombination current by a factor of 2.2. If this were the dominant recombination mechanism in a solar cell, inclusion of trap-assisted tunneling in the model would decrease the estimated cell voltage by 40 mV for the conditions simulated here (n=2).

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The dependence of recombination on base doping density for a graded junction typical of a doped emitter is illustrated in Fig. 5.

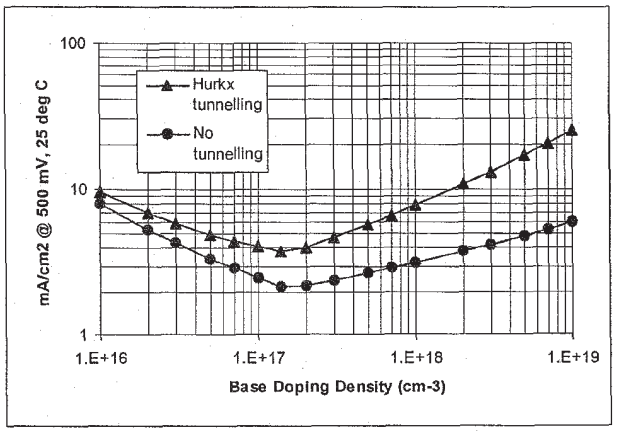

Fig. 5 Dark current for a graded n^+p junction in 10-ns silicon material calculated using PC1D Version 5 showing the impact of trap-assisted tunneling.

Fig. 5 was calculated for a junction formed into a p-type base using a gaussian n-type emitter with a surface concentration of 3.5×10^{19} cm^{-3} and a depth factor of 0.2 μm (100 Ω/□). As in the previous example, the current shown in the figure is the dark current at 500 mV forward bias for a 1-μm-thick device having zero surface recombination velocity and electron and hole lifetimes both equal to 10 ns. Again, virtually all of the current under these conditions is due to recombination within the junction space-charge region. At the optimum doping density of 1.4×10^{17} cm^{-3}, trap-assisted tunneling increases the recombination current by 75%, somewhat less than for the abrupt junction. If this were the dominant recombination mechanism in a solar cell, inclusion of trap-assisted tunneling in the model would decrease the estimated cell voltage by 30 mV.

In summary, trap-assisted tunneling causes abrupt junctions that are doped above 10^{19} cm^{-3} on both sides to have extremely high recombination, and this needs to be avoided in practice. For graded junctions the impact is somewhat reduced, but trap-assisted tunneling still increases the junction recombination by a significant factor. Although an optimized abrupt junction has less recombination than an optimized graded junction, the difference when trap-assisted tunneling is included is much less. PC1D 5 can be used to evaluate cells in which these effects are important.

PROGRAM AVAILABILITY

PC1D version 5 is available from the Photovoltaics Special Research Centre at the University of New South Wales in Australia for a fee of 150 Australian dollars (approximately US$100). Request an order form via e-mail to pc1d@unsw.edu.au. The program is provided on a single 3.5-inch diskette. The license allows you to run the program on multiple computers or on a local-area network, as long as all of the computers are under the control of a single licensed individual.

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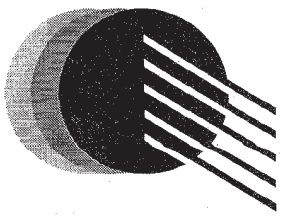

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