

Impurity-to-Efficiency Simulator for Sentaurus TCAD

User Manual

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I. User Audience

The MIT PVLab and Synopsys, Inc. jointly developed and are freely and publicly distributing the Impurity-to-Efficiency (I2E) Simulator models written in the Alagator scripting language. Details about I2E are found in [1]. An online applet version of I2E and more information about the tool can be found at [2]. The Alagator scripting language is used to specify partial differential equations and boundary conditions for use with diffusion simulations in the TCAD tool Sentaurus Process [3]. This version of the I2E simulator was announced and applied in a recent publication [4].

This brief instruction guide is written for users who have access to and are already familiar with Sentaurus TCAD, including Sentaurus Process, Sentaurus Device, and Sentaurus Structure Editor [2]. We provide scripts that are designed to run from the command line, but they can also be adapted for use with Sentaurus Workbench.

[1] Hofstetter et al., “Impurity-to-efficiency simulator: predictive simulation of silicon solar cell performance based on iron content and distribution”, Prog. Photovolt: Res. Appl., 2010, n/a doi: 10.1002/pip. 1062.

[2] <http://pv-i2e.mit.edu>

[3] See Sentaurus TCAD User Guides.

[4] A.E. Morishige, H. Wagner, J. Hofstetter, I. Avci, C. del Cañizo, T. Buonassisi, “Combined Effect of Heterogeneous Lifetime and Gettering on Solar Cell Performance,” Proceedings of the 5th International Conference on Crystalline Silicon Photovoltaics in Energy Procedia (2015).

II. Overview of Provided I2E Alagator Scripts

Here we provide several scripts for running I2E in Sentaurus TCAD, including:

- 1) I2E Model file (I2E_Models_SentaurusTCAD.tcl)
- 2) 1D command file that calls the I2E Model file (I2E_1D_SentaurusTCAD.cmd)
- 3) Flexible dimensionality (can be adapted for 1D, 2D, or 3D) version of the command file that calls the I2E Model file (I2E_SentaurusTCAD.cmd)
- 4) Command file that suppresses some default parameters and turns AdvancedCalibration off (mySuppressDefaults.tcl). This file is called right before the I2E Model file is called.

To download the scripts, go to <http://pv.mit.edu/home/resources>, scroll down to “Impurity-to-Efficiency Simulator for Sentaurus TCAD”, and click on the “Download Scripts” button.

The 1D command file runs as provided. Copy the file to the server where you are running Sentaurus, and In the command line, type “sprocess I2E_1D_SentaurusTCAD.cmd”. The flexible dimensionality version requires you to define your own device structure. Consult the Sentaurus Process User Guide, Chapter 6: Alagator Scripting Language for more details and examples.

III. Example Workflow

Here we outline the workflow that we use to run the Impurity-to-Efficiency Simulator for Sentaurus TCAD.

We use Microsoft Excel to define parameters for multiple simulations. Inputs to sprocess include (but are not limited to) the initial impurity point defect concentration (in cm^{-3}), initial precipitated impurity concentration (in atoms/cm^3), initial impurity precipitate spatial density (precipitates/ cm^{-3}), peak phosphorus concentration, and time-temperature profile parameters. Inputs to sdevice include (but are not limited to) the wafer doping level, the unit cell width, contact metallization dimensions, bulk lifetime, surface recombination velocities, and any dopant, impurity, or lifetime profiles generated by the sprocess simulations.

We then use MATLAB to read in the parameters from Excel to generate a batch of Sentaurus command files.

We upload the generated command files to the server where we run Sentaurus and run the Sprocess command files. For example, `"sde -e -l 1_I2E_sde.cmd; sprocess 1_I2E.cmd; sprocess 1_I2E_1D.cmd"` generates a simulation structure, runs a 2D process simulation that outputs post-processing impurity distributions, and then generates the doping profiles in 1D.

We store the final interstitial iron concentration (FI) as a PMIUserField in the .tdr file to pass it to Sentaurus Device, where we model the recombination activity due to point defects as traps.

We store the final precipitate-related carrier lifetimes that we calculate in SProcess as "eLifetime" (electron lifetime) and "hLifetime" profiles in the .tdr file, and those profiles are called by the keyword "Lifetime" in the "File" section of the sdevice command file as described in the Sentaurus Device User Guide.

Note that in 1D the user can view profiles at text in .plx files, and in 2D or 3D, the user can view outputs in .tdr files using the Sentaurus svisual program.

We then copy the .plx files (Emitter.plx and Precipitates.plx) that came from the 1D simulation back to the local machine and generate the appropriate dopant concentration to be used in the device simulation from those profiles.

We then generate the batch of sdevice command files for our solar cell architecture and upload those files and any additional parameter files to the server and run the commands. For example, `"sde -e -l 1_sde.cmd; sdevice 1_dark_des; sdevice 1_rampLight_des; sdevice 1_des."`

Finally, we copy the .plt files back to the local machine and analyze the solar cell device performance.