Currently, AdaptUSim is implemented using devsim[1], [2] and the following formalism following the conventional Scharfetter-Gummel stable differences approximation[3] with some relationships and non-idealities obtained from other publications[4]–[9]. We will solve for the electrostatic potential , and the hole and electron densities , and .

# Continuity Equations

The electron and hole continuity equations are

Where and refer to electron and hole densities respectively, is the current density, is the fundamental charge, is the net generation-recombination rate, is the spatially and field dependent mobility, is the quasi-Fermi level potential. Limiting to non-degenerate doping cases we use the Boltzmann relation

Such that is the electrostatic potential, is the electron affinity, is the thermal potential with the Boltzmann constant, and the absolute temperature in Kelvin. By starting with these relations after some algebraic manipulation we arrive at a finite differences relationship which is suitable for numeric simulation. We consider two adjacent nodes at position on a given mesh, location and and the current between them defined at . Namely,

Yet for small changes in potential across nodes, , care must be taken to evaluate, thus we refactor the expression as

Defining for convenience and evaluating it piecewise based on the magnitude of for numerical stability:

In this piecewise definition for expanding out , precision is maintained for 16 digits of z and obviates risks of numerical overflow. Similarly we define the current density for holes as

# Poisson’s Equation

The third equation that we must simultaneously solve is Poisson’s equation at each gridpoint node. That is

Where is the effective density of ionized donors and is the effective density of ionized acceptors, as the density of trap states with charge , and with being the dielectric constant of the material. Ionized doping level can be inferred directly from the density of dopants and the dopant energy level

With g as the degeneracy of the dopant state. (Sze pg. 23) Using the above definitions of current we introduce the displacement field and electric field as approximated by

Requiring that

With as the density of conduction band states, the density of valence band states, being the bandgap between the conduction and valence band edge, as the intrinsic carrier concentration, and as the intrinsic fermi level potential derived from the conduction and valance band potentials.

This formalism then requires we specify the net generation-recombination rate . For this term, defects may be specified with particular energy levels, densities, effective charges, and capture cross sections. In this way a host of behavior can be simulated by using known realistic defect energies.

Now introducing the thermal voltage from the effective mass .

# References

[1] J. E. Sanchez, G. Bosman, S. Member, and M. E. Law, “Two-Dimensional Semiconductor Device Simulation Noise Under Periodic Large-Signal Conditions and Its Use for Developing Cyclostationary Circuit Simulation Models,” *IEEE Trans. Electron Devices*, vol. 50, no. 5, pp. 1353–1362, 2003.

[2] J. M. Sanchez and R. D. Sacks, “Development of a multibed sorption trap, comprehensive two-dimensional gas chromatography, and time-of-flight mass spectrometry system for the analysis of volatile organic compounds in human breath.,” *Anal. Chem.*, vol. 78, no. 9, pp. 3046–54, May 2006.

[3] D. L. Scharfetter and H. K. Gummel, “Large-signal analysis of a silicon Read diode oscillator,” *IEEE Trans. Electron Devices*, vol. 16, no. 1, pp. 64–77, Jan. 1969.

[4] R. Stangl, C. Leendertz, and J. Haschke, *Numerical Simulation of Solar Cells and Solar Cell Characterization Methods : the Open-Source on Demand Program AFORS-HET*, no. February. 2010.

[5] S. M. Sze and K. K. Ng, *Physics of Semiconductor Devices*. Hoboken, NJ, USA: John Wiley & Sons, Inc., 2006.

[6] D. K. Schroder and L. G. Rubin, “Semiconductor Material and Device Characterization,” *Phys. Today*, vol. 44, no. 4, p. 107, 1991.

[7] G. Groesenken *et al.*, “Physics-Based Mathematical Conditioning of the MOSFET Surface Potential Equation,” vol. 51, no. 7, pp. 1196–1200, 2004.

[8] a. M. Itsuno, J. D. Phillips, and S. Velicu, “Design and Modeling of HgCdTe nBn Detectors,” *J. Electron. Mater.*, vol. 40, no. 8, pp. 1624–1629, Apr. 2011.

[9] W. L. Engl, H. K. Dirks, and B. Meinerzhagen, “Device modeling,” *Proc. IEEE*, vol. 71, no. 1, pp. 10–33, 1983.

[10] J. Nielsen and R. L. Mack, “Heuristic evaluation,” in *Usability Inspection Methods*, B., New York, New York, USA: Wiley, 1994, p. 142.

[11] J. Nielsen and R. Molich, “Heuristic evaluation of user interfaces,” in *Proceedings of the SIGCHI conference on Human factors in computing systems Empowering people - CHI ’90*, 1990, pp. 249–256.

[12] A. Schenk and U. Krumbein, “Coupled defect-level recombination: Theory and application to anomalous diode characteristics,” *J. Appl. Phys.*, vol. 78, no. May 2011, pp. 3185–3192, 1995.

[13] D. Rosenfeld and G. Bahir, “A Model for the Trap-Assisted Tunneling Mechanism in Diffused n-p and Implanted n + -p HgCdTe,” vol. 39, no. 7, 1992.

[14] A. M. Itsuno, J. D. Phillips, and S. Velicu, “Design and Modeling of HgCdTe nBn Detectors,” *J. Electron. Mater.*, vol. 40, no. 8, pp. 1624–1629, Aug. 2011.

# Functionality

With the above formalism in place and implemented, [] lists the number of supported features and the roadmap of future feature additions planned.

Table . List of Adaptusim features both implemented and planned.

|  |  |  |
| --- | --- | --- |
| **Name** | **Implemented** | **Comments** |
| 3D mesh support | Yes | Devsim feature |
| Spatially dependent recombination with deep and shallow charge states | Yes | [5] |
| Spatially, thermally and doping dependent bandgap | Yes | Pseudo-bulk |
| Thermionic emission and Anderson model heterojunctions | Yes | [4] |
| Field-dependent mobility including scattering processes | Yes | Analytic expression |
| Simulated electrical cross-talk | Yes | Devsim feature |
| Optical generation rates | Yes | Beer’s law absorption |
| Classes and scripting interface | Yes |  |
| Graphical Interface | Planned | [10], [11] |
| Band-to-Band tunneling | Planned |  |
| Trap-assisted tunneling | Planned | [12], [13] |
| Barrier tunneling | Planned | [14] |
| Surface recombination | Planned |  |
| Interfacial trap states and charge | Planned | Devsim feature |
| Time-dependent signal analysis (CV, noise) | Planned | Devsim feature |