Semiconductor device modeling with AMPS-1D

Lecture 3

Special Topics:
Device Modeling

Outline

- Basic concepts and physics model
- Governing equations
- Input/Output
- Brief literature survey of problems/results
- Updated features in wxAMPS
- Hands on: running standard models, creating a simple model

AMPS-1D

- A one-dimensional device simulation program for the Analysis of Microelectronic and Photonic Structures (AMPS)
- Created by the group at the Center for Nanotechnology Education and Utilization, the Pennsylvania State University (professor Stephen J. Fonash, and his group)
- To run under Windows 7/8 platform: use Windows XP mode/Virtual PC (both available from Microsoft website)
- AMPS-1D website: http://www.ampsmodeling.org ; YouTube tutorial: https://youtu.be/9jhs-UFZ_ZM

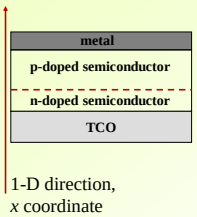
Modeled structures

- Homojunction and heterojunction p-n and p-i-n, solar cells, detectors, microelectronic (ME) structures (e.g., MIS, FET)
- Multi-junction solar cell and ME structures
- Compositionally-graded detector, solar cell, and ME structures
- Schottky barrier devices with optional back layers
- Novel device ME, photovoltaic, and opto-electronic structures

General model features

- Able to handle any defect and doping energy gap and special distribution
- Shockley-Read-Hall (S-R-H) and band-to-band recombination (no tunneling)
- Boltzmann and Fermi-Dirac statistics
- Varying material properties
- General treatment of contacts
- Ability to handle transport in devices under voltage bias, light bias, or both

Physics model

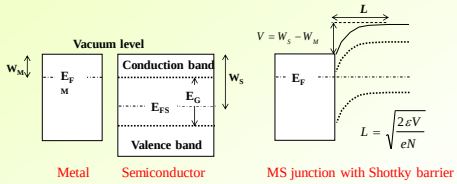


- Device is modeled in one dimension across layers, and formed junctions in physical space
- Depth is *x* coordinate
- Spatial distributions of fields, charge carriers, defects, etc.

Physics model

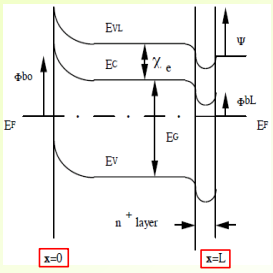
- Complete device typically consists of combination of structures
  - Shottky barrier
  - p-n homojunction or heterojunction
  - Triple and multi-junctions
- Alignment at the Fermi levels at equilibrium
  - concept of quasi-Fermi levels under bias, or light

Physics model: Shottky barrier



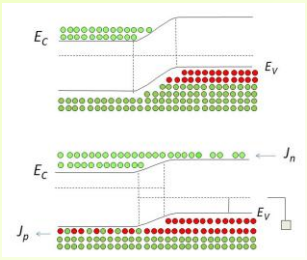
- Two materials put in contact are joint at the Fermi level on the band diagram
- Metal-semiconductor junction results in a Shottky barrier with height equal to differences in work functions Ws and Wm

Shottky barrier in AMPS



- Ψ is the position of the local vacuum level in the contact at the right hand side of any general device structure
- χ_e is the electron affinity for the layer
- Φb=Ec-Ef at each side of the device (x=0 or L)

Physics model



- P-n junction under thermal equilibrium, common Fermi level
- Same under forward bias (current Jn), showing quasi-Fermi levels

Image from:
https://nanohub.org/app/site/courses/12/3385/slides/007.01.jpg

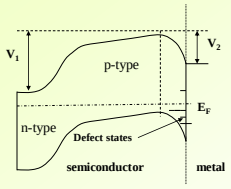
Physics model: Device description

Band diagrams for electrons

Band diagram for Si

- Conduction band Ec, electron carrier concentration Nc
- Valance band Ev, hole carrier concentration Nv
- Band gap Eg
- Fermi level Ef

Physics model: putting elements together



- Realistic p-n heterojunction with back barrier and defect states (the latter are not fully modeled, tunneling is not included)
- Thermodynamic equilibrium

Physics model and governing equations

- Governing semiconductor device equations: Poisson equation, free electron, and hole continuity equations

$$\frac{d}{dx}\left(\varepsilon(x)\frac{d\Psi}{dx}\right) = q\cdot\left[p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)\right]$$

$$\frac{1}{q}\left(\frac{dJ_n}{dx}\right) = -G_{op}(x) + R(x)$$

$$\frac{1}{q}\left(\frac{dJ_p}{dx}\right) = G_{op}(x) - R(x)$$

p,n – free carrier concentrations
$N^{\pm}_{DA}$ – charged dopants
p_t,n_t – defect concentrations
Jn, Jp – the electron and hole current densities
R(x) is the net recombination rate;
G(x)- the optical generation rate

Physics model and governing equations

- Transport theory allows for the electron and hole current density J_n, and J_p to be expressed as

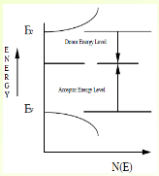
$$J_n(x) = q\mu_n n\left(\frac{dE_{Fn}}{dx}\right)$$

$$J_p(x) = q\mu_p p\left(\frac{dE_{Fp}}{dx}\right)$$

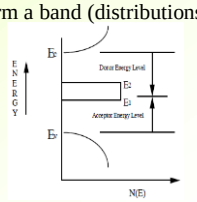
- Here $\mu_{n,p}$ are corresponding electron/hole mobilities
- Obtain equations for $E_{Fn,}$ E_{Fp} - the quasi-Fermi level positions

Physics model: dopants

- Dopants are purposely present
- Localized dopants ($N^{\pm}_{D,A}$) can be discrete gap states, and/or gap states that form a band (distributions)



Discrete dopant levels



Band of dopant states

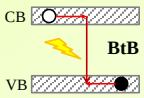
Physics model: defects

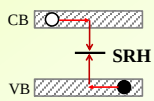
- Defects are inadvertently present due to imperfections in crystal structure (e.g., grain boundaries), and impurities
- As with localized dopants, discrete, banded, and continuous defect states are allowed
- For the donor-like states, we need the number of these states per volume that have lost an electron or, equivalently, have trapped a hole (visa-versa for acceptor-like states), p_t, and n_t

Physics model: generation

- When a semiconductor is subjected to an external source of illumination and $hv>E_{gop}$ at some point x (termed the optical bandgap at x), free electron-hole pairs are produced
- This is the process encompassed by the generation term G_{op}(x) in the continuity equation

Physics model: recombination





- Direct band-to-band
  - Between the occupied states in the CB and the vacant states in the VB
- Indirect, or Shockley-Read-Hall
  - Through a defect state in the gap
- Auger recombination not included
  - Involves three carriers: after recombination, the energy is given an electron in the conduction band (as opposed to emission as a photon or phonon)

Boundary conditions

- AMPS solves these three coupled non-linear differential equations, each of which has two associated boundary conditions, at x=0 and x=L

$$\Psi(0) = \Psi_0 - V, \quad \Psi(L) = 0$$

$$J_p(0) = -qS_{p0}\left(p_0(0) - p(0)\right), \quad J_p(L) = -qS_{pL}\left(p_0(L) - p(0)\right)$$

$$J_n(0) = -qS_{n0}\left(n_0(0) - n(0)\right), \quad J_n(L) = -qS_{nL}\left(n_0(L) - n(0)\right)$$

- $S_{p,n}$ – surface recombination velocities (adjustable parameters)
- At x=0 in thermodynamic equilibrium, potential is set to Ψ_0
- $\Psi(0)$ becomes Ψ_0-V if a voltage bias, light bias, or both exist

Solution of governing equations

- For numerical solution definition domain, and equations must also be discretized
- At the discretion of the user a non-uniform grid spacing is usually adopted

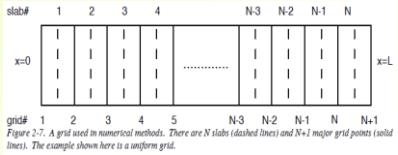


Figure 2-7. A grid used in numerical methods. There are N slabs (dashed lines) and N+1 major grid points (solid lines). The example shown here is a uniform grid.

Solution of governing equations

- Obtain a set of three unknown state variables at each point in the device: the electrostatic potential Ψ, the hole quasi-Fermi level E_{Fp}, and the electron quasi-Fermi level E_{Fn}
- Once the state variables are determined for a given set of biasing conditions (voltage, light, or both) and temperatures, the current density-voltage (J-V) characteristics for these conditions can be generated

Solution of governing equations

- Newton-Raphson method is used in AMPS to solve this set of 3(N+1) algebraic equations
  - write the 3 governing differential equations in terms of differences in the state variables at the grid points defining these slabs (N-1 for each governing equation)
  - add 6 BC equations
- Since it is a method that iteratively finds the roots of a set of functions fi, fei, and fhi, adequate initial guess for the roots is crucial

Input

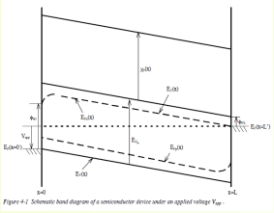


Figure 4-1. Schematic band diagram of a semiconductor device under an applied voltage V_{bi}.

- Input for 3 types of parameters
  - Parameters describing entire device, particular region (layers, surfaces), and those that define the illuminating spectrum
- There are five separate dialog boxes for inputting voltage biases, illumination conditions, operating temperature, and front and back contact data

Physics model

- DOS (density of states) model: details of recombination traffics, trapping and the charge state of the defects are fully accounted for
  - Input energy gap distribution of the defects, their spatial variation, capture cross section information
- Lifetime model: a simplification (linearized lifetime picture), does not account for the details of recombination, provides quick answer
  - Input lifetime values

Standard AMPS models

- Originally developed for crystalline Si, GaAs, others; multiple models are available
- Later standard models for polycrystalline devices at the level of best efficiencies were developed
  - CdTe
  - CuIn(Ga)Se_2, or CIGS
  - a-Si
- Shared as *.AMP files

Output

- Capable of calculating:
  - band diagrams
  - current components, current-voltage characteristics
  - recombination, generation profiles
  - electric field as a function of light intensity, voltage, temperature
- Output: plots of the above functions

Output: Example

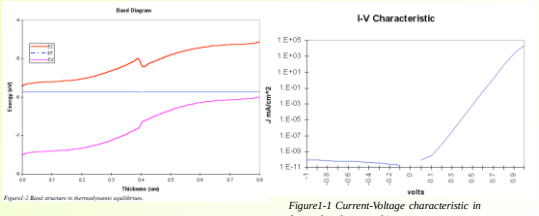


Figure1-1 Current-Voltage characteristic in forward and reverse bias

RT current-voltage characteristic in forward and reverse bias and the band structure in thermodynamic equilibrium for an $Al_{0.3}Ga_{0.7}As$/GaAs p-n heterojunction diode. The doping levels taken to be 10^{16} cm^{-3} in both layers

Output: Example

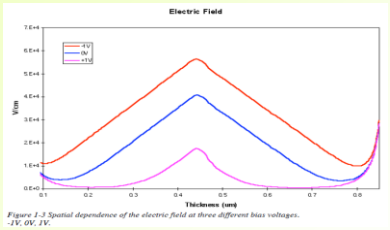


Figure 1-3 Spatial dependence of the electric field at three different bias voltages. -1V, 0V, 1V.

- The space charge at -1, 0, and +1 volts (i.e., forward, 0, and reverse biases)
- This example demonstrates how AMPS can be used to determine the amount of charge transfer in the space charge regions of heterojunction structures and the widths of these space charge layers as a function of bias

AMPS-1D

BRIEF LITERATURE SURVEY OF PROBLEMS AND RESULTS

Numerical modeling of CIGS and CdTe solar cells: setting the baseline

M. Gloeckler, A.L. Fahrenbruch, and J.R. Sites, Proceedings of 3rd World Conference on PV, Osaka, Japan, 2003

- Numerical modeling of devices in general, and polycrystalline solar cells in particular, must be done with only partial knowledge of input parameters
- The paper provided baseline parameters leading to the best solar cell device performances at the time:
  - CIGS at the efficiency of 17.7% (close to NREL record)
  - CdTe at the efficiency of 16.4% (NREL)

CIGS and CdTe solar cells baseline

General Device Properties		
	Front	Back
Φ_b [eV]	Φ_{bn} = 0.0	Φ_{bp} = 0.2
S_n [cm/s]	10^7	10^7
S_p [cm/s]	10^7	10^7
Reflectivity R_f [1]	0.05	0.8
Layer Properties		
	ZnO	CdS	CIGS
W [nm]	200	50	3000
$\varepsilon/\varepsilon_0$ [1]	9	10	13.6
μ_n [cm^2/Vs]	100	100	100
μ_p [cm^2/Vs]	25	25	25
n, p [cm^{-3}]	n: 10^{18}	n: 10^{17}	p: $2x10^{16}$
E_g [eV]	3.3	2.4	1.15
N_C [cm^{-3}]	$2.2x10^{18}$	$2.2x10^{18}$	$2.2x10^{18}$
N_V [cm^{-3}]	$1.8x10^{19}$	$1.8x10^{19}$	$1.8x10^{19}$
ΔE_c [eV]	- 0.2		0.3
Gaussian (midgap) Defect States			
	ZnO	CdS	CIGS
N_{DG}, N_{AG} [cm^{-3}]	D: 10^{17}	A: 10^{18}	D: 10^{14}
E_a, E_D [eV]	midgap	midgap	midgap
W_G [eV]	0.1	0.1	0.1
σ_n [cm^2]	10^{-12}	10^{-12}	$5x10^{-13}$
σ_h [cm^2]	10^{-15}	10^{-12}	10^{-15}

CIGS parameters

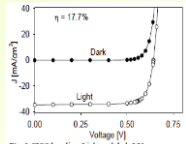


Fig. 1 CIGS baseline: Light and dark J-V

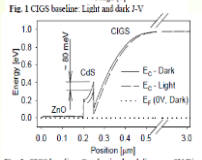


Fig. 3: CIGS baseline: Conduction band diagram - 0V Bias

CIGS and CdTe solar cells baseline

General Device Properties		
	Front	Back
Φ_b [eV]	Φ_{bn} = 0.1	Φ_{bp} = 0.4
S_n [cm/s]	10^7	10^7
S_p [cm/s]	10^7	10^7
Reflectivity R_f [1]	0.1	0.8
Layer Properties		
	SnO_2	CdS	CdTe
W [nm]	500	25	4000
$\varepsilon/\varepsilon_0$ [1]	9	10	9.4
μ_n [cm^2/Vs]	100	100	320
μ_p [cm^2/Vs]	25	25	40
n, p [cm^{-3}]	n: 10^{17}	n: 10^{17}	p: $2x10^{14}$
E_g [eV]	3.6	2.4	1.5
N_C [cm^{-3}]	$2.2x10^{18}$	$2.2x10^{18}$	$8x10^{17}$
N_V [cm^{-3}]	$1.8x10^{19}$	$1.8x10^{19}$	$1.8x10^{19}$
ΔE_c [eV]	0		-0.1
Gaussian (midgap) Defect States			
	SnO_2	CdS	CdTe
N_{DG}, N_{AG} [cm^{-3}]	D: 10^{17}	A: 10^{18}	D: $2x10^{14}$
E_a, E_D [eV]	midgap	midgap	midgap
W_G [eV]	0.1	0.1	0.1
σ_n [cm^2]	10^{-12}	10^{-17}	10^{-12}
σ_h [cm^2]	10^{-15}	10^{-12}	10^{-15}

CdTe parameters

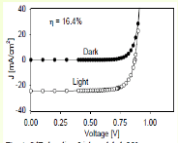


Fig. 4: CdTe baseline: Light and dark J-V

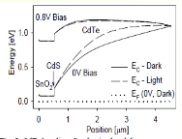


Fig. 5: CdTe baseline: Conduction band diagram

The relationship of CdS/CdTe cell band profiles to J-V characteristics and bias-dependent quantum efficiency, A.L. Fahrenbruch, 2006 IEEE 4th World Conference on Photovoltaic Energy Conference, Waikoloa, HI

- AMPS models of two extreme profiles are discussed: an n/i/p junction, where V_{bi} is mainly supported by charge at the contacts, and an n/p junction, where V_{bi} is supported by charge in the bulk CdTe within the absorber
- Effects of various model parameters on the CdTe device efficiency are presented for both models
- Apparent Quantum Efficiency (AQE) and some transient behavior is analyzed

CdS/CdTe cell band profiles

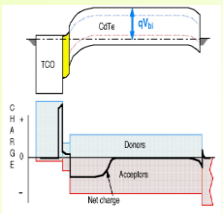


Fig. 1. Schematic of an n/p junction, based on AMPS simulation. (V_{bi} is approximate, assuming that Ef is close to the CB in the TCO).

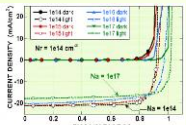
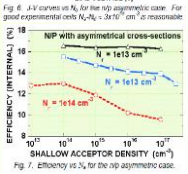


Fig. 6. J-V curves vs N_A for the n/p asymmetric case. For good experimental cells N_D-N_A ~ $3x10^{14}$ cm^{-3} is reasonable



Nr – donor-like recombination center

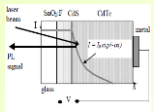
Fig. 7. Efficiency vs N_A for the n/p asymmetric case.

External bias effect on junction photoluminescence in CdS/CdTe solar cells, D. Shvydka, A.D. Compaan, V.G. Karpov, IEEE 2002

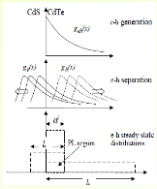
- Study photoluminescence (PL) from the CdS/CdTe solar-cell junction region
- We observed that applied external bias V does not change the spectral shape of the PL signal, but significantly affects the integral PL intensity I(V)
- The observed phenomena is attributed to the field-induced separation of the light-generated e-h
- AMPS modeling was used to find values of electric field at each bias point

Bias-dependent PL in CdS/CdTe solar cells

PL geometry



General model



Experimental results

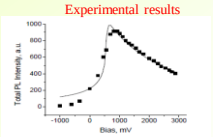


Fig. 3. The measured PL intensity in a wide range of applied biases for an unstressed device. Solid line represents analytical fit by Eq. (2)

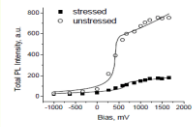


Fig 4. Bias-dependent PL data (points) under 20-sun laser beam and theoretical fits (curves) by Eq. (2)

Bias-dependent PL in CdS/CdTe solar cells

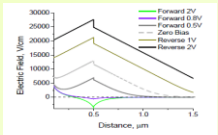


Fig. 6. AMPS-1D generated simulation of the electric field in the junction region.

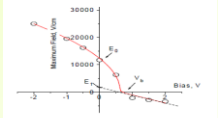
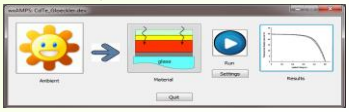


Fig. 7. AMPS-1D simulated data on the field-bias dependence for a CdTe/CdS solar cell (dots) in comparison with the piece-wise approximation in Eqs. (3) and (4) (solid line).

- Data consistent with the model where PL is suppressed by two competing mechanisms: field induced spatial separation of charge carriers and their non-radiative recombination; we have observed the crossover between the two mechanisms
- Developed a semi-quantitative model of bias-dependent PL
- The main effect of degradation is found to be a decrease in the non-radiative recombination lifetime (possibly by introducing new recombination centers)

wxAMPS

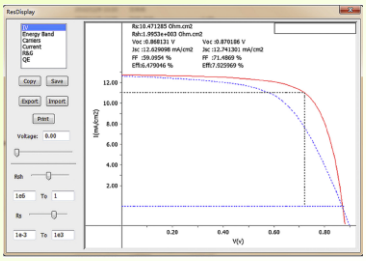
- New wxAMPS is available through university of Illinois (Angus Rockett group)
- Executable and supporting files for Windows 7/8
- Beyond the original AMPS kernel, wxAMPS incorporates two tunneling models
- Based on the option for an unlimited number of layers in the simulation, modeling graded solar cells can be implemented easily in wxAMPS



wxAMPS: updated features

- User interface: 5 separate input windows are combined into one for quick editing and viewing
- Two tunneling models added: trap-assisted tunneling and the intra-band tunneling (with changes to solver)
- When simulating a series of bias voltages, the solution for the previous voltage is used as the initial guess for the next voltage calculation thus reducing the iteration times and significantly improving convergence

wxAMPS: updated features



Result display window

Summary

- AMPS-1D is one of the oldest modeling packages for semiconductor devices
- With standard models available is useful for a number of problems
- Somewhat complicated installation
- Resent updates should help with making it more user-friendly

References

- A manual for AMPS-1D, The Center for Nanotechnology Education and Utilization, The Pennsylvania State University
- Y. Liu, Y. Sun, and A. Rockett, "A new simulation software of solar cells--wxAMPS", Solar Energy Materials and Solar Cells, 2012.
- Other references given in slides