Thin-Film PV Technologies
Dragica Vasileska¹, Igor Sankin², Daniel Brinkman³, Christian Ringhofer¹, Bedrich Benes⁴, Dmitry Krasikov², Abdul Shaik¹ and Hao Kang⁴
¹Arizona State University, ²First Solar, ³San Jose State University, ⁴Purdue University

GOAL: To allow for predictive design of TFPV devices by eliminating the ambiguity between the observed device performance and the physical root cause.

INNOVATION: Develop advanced physical models describing capture/emission/recombination phenomena relevant to multivalent dopants, amphoteric centers, and donor-acceptor pairs. These models, incorporating grain bulk, grain boundaries, and hetero-interface properties, will be implemented in a self-contained simulation tool that will drastically reduce interpretation ambiguity and, for the first time, allow for predictive design of TFPV.

THIN-FILM PV DEVELOPMENT: NEED FOR PREDICTIVE SIMULATION

- Development targets in II–VI TFPV:
  - Graded bandgap absorber
  - High & stable P-type absorber doping
  - Long bulk lifetime & high-quality hetero-interfaces
- Traditional approach to development:
  - Empirical learning under high-level theoretical guidance
- Challenges of traditional approach:
  - High cost. Often need production line to run experiments
  - Too many knobs. Change of unit process requires up- and down-stream optimization

THIN-FILM PV DEVICE CHALLENGES: SIMULATIONS

- Multiple electrically active defect species
  - Properties and distributions cannot be measured directly
  - Not frozen in time: migrate and react (device system never equilibrates)
- Graded ternary/quaternary alloys
  - Position-dependent properties of host materials and defect species
- Grain boundaries and hetero-interfaces
  - Recomposition / charge build-up
  - Properties and composition very sensitive to process conditions

PV DEVICE: OPEN SYSTEM EXPOSED TO STRESSORS

Need coherent model to formalize complex dependencies

KINETIC MODELING OF DEFECT CHEMISTRY

- Evolution of any assembly of species in semiconductors:
  - Process, performance, metastabilities governed by same laws
  - All species including free carriers treated same way

DEFECTS EVOLUTION DURING CI TREATMENT AND Cu DOPING STAGES

- Traditional approach and the role of simulations in the VASP/Gui solar and sponge tool.

GRAIN BOUNDARIES: LEAST UNDERSTOOD PART OF THIN FILM II–VI

- GBs - Key features in thin-film absorbers
  - Dirichlet boundary conditions to grain bulk (concentrations, electrostatic potential)
  - Exchange of species between grain and surrounding
- Classical “GB segregation model” not applicable
  - Equilibrium approximation: N/A (metastabilities)
  - Boltzmann statistics (diluted concentrations): N/A
- Surface reactions - most relevant way to describe inter-grain exchange
  - Inter-grain exchange through surface transformation of species
- High degree of disorder and variety of configurations
  - Detailed 1st principle study is not possible – need effective model parameters

TWO USE CASES: “SINGLE-CRYSTAL” AND “HALF-GRAIN”

- Implementation of arbitrary GBs in 2D is very costly in terms of mesh points
- Based on learned lessons, we simplified definition of generic use cases
  - Orthogonal interfaces only; one vertical interface at most.

MESH IN 2D IMPLEMENTATION

- Each grid point is the center of a rectangular finite volume
- Allows multiple grain structures
- Rectangular mesh greatly simplifies numerical implementation
- Easy to refine mesh near GBs
- Can easily define and change parameters for any grain or layer
- Continuous flux is guaranteed by averaging:

\[
\frac{\partial N}{\partial t} = \frac{D_{cc}}{\varepsilon_{HH}} \frac{N}{\varepsilon} + (R_a + R_c)
\]

\[
V \cdot A - \frac{\partial N}{\partial t} = 0 \quad \sum_i N_i
\]

Simulation challenges in graded alloys:

- Graded alloys are present in high performing CdTe based solar cells
- Position dependent properties of species and reactions are needed

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GUI DEVELOPMENT:

- Cross-platform application & GUI framework
- Object oriented Design  •  High performance & stability

NUMERICAL ENGINE DEVELOPMENT:

- Algorithmic:
  - New Splitting Algorithm developed to handle fast reactions
  - Simultaneous reaction solver implemented for 0D, 1D and 2D
  - Improved efficiency for all cases. (27x for base 0D case)
- Task Manager / Numerical Engine interface defined and implemented
- 2D Prototype developed

Flexible Class Interfaces work for problems in any dimension

- Processed reaction operator as:

\[
R(U) = U \cdot \eta \cdot (1 + \frac{P}{K})
\]

Then the full reaction operator is given as:

\[
\eta \cdot (1 + \frac{P}{K})
\]

Using this we can write the Jacobian as:

\[
J = \frac{\partial R(U)}{\partial U} = \eta \cdot (1 + \frac{P}{K})
\]

- Interface variables are visible to numerical engine and solver classes.
- Abstract solver classes for reaction, diffusion and Poisson equation.
- Each numerical algorithm for a solver will be an inherited class to these abstract classes.
- Currently supports simultaneous reactions; Slotboom diffusion solver and Scharfetter-Gummel diffusion solver; standard, linearized, and DAE Poisson solver.

27x speed-up