Thin-Film PV Technologies

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

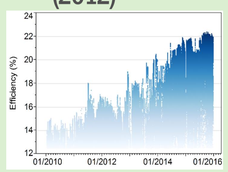
INNOVATION: Develop **advanced** physical models describing capture/emission/ recombination phenomena relevant to multivalent dopants, amphoteric centers, and donor-acceptor pairs. These models, incorporating grain bulk, grain boundaries, and hetero-interface properties, will be implemented in a **self-contained 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 nobs. Change of unit process requires up- and down-stream optimization

(FSLR)

19% (2012) ➤➤➤ 22% (2015)

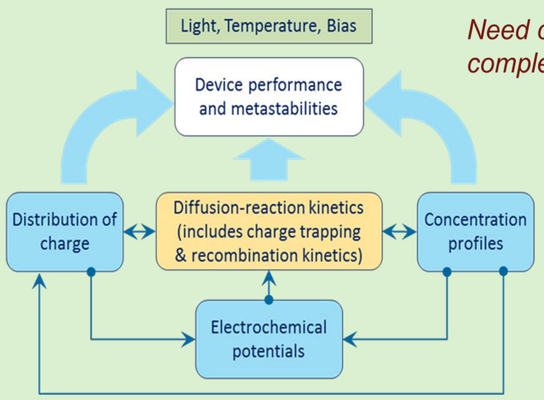


- 13,500,000 IV Sweeps
- 40,000 MA Request
- 650,000 Man Hours

THIN-FILM PV DEVICE SIMULATION: CHALLENGES

- 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 tenant defect species
- Grain boundaries and hetero-interfaces
  - Recombination / 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 ensemble of species in semiconductors:

Numerical engine

$$\begin{cases} \dfrac{d[\mathbf{X}]}{dt} = \nabla\left(\dfrac{\mathbf{D_X}}{E_{TH}}[\mathbf{X}]\nabla\boldsymbol{\mu}_\mathbf{X}\right) + \mathbf{R_X} \\ \nabla\varepsilon\nabla V = -\dfrac{q}{\varepsilon_0}\sum\boldsymbol{\theta}_\mathbf{X}[\mathbf{X}] \end{cases}$$

$[\mathbf{X}]$: Concentrations of all relevant species (free carriers, intrincic and extrinsic defects and complexes, etc.)

Defect chemistry

$\mathbf{D_X}$: Diffusivities

$\boldsymbol{\mu}_\mathbf{X}$: Chemical potentials of species

$\mathbf{R_X}$: Net production rates in chemical reactions

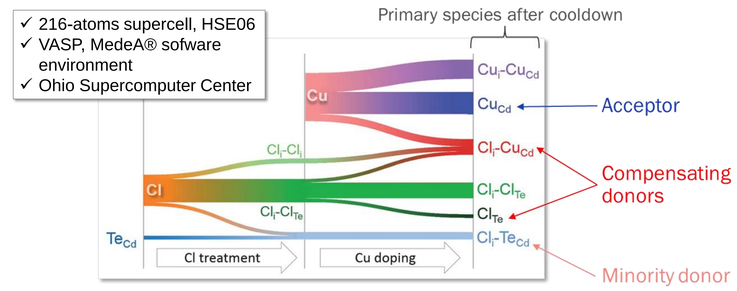
$\boldsymbol{\theta}_\mathbf{X}$: Charges carried by species

- ✓ *Process, performance, metastabilities governed by same laws*
- ✓ *All species including free carriers treated same way*

Da Guo, Daniel Brinkman, Abdul R. Shaik, I. Sankin, D. Krasikov, Christian Ringhofer and Dragica Vasileska, "Modeling Metastability in CdTe Solar cells due to Cu Migration", Springer, Book Ed. by Roderick Melnik, in press (22 pages).

DEFECTS EVOLUTION DURING Cl TREATMENT AND Cu DOPING STAGES

D. Krasikov and I. Sankin, "Defect interactions and the role of complexes in the CdTe solar cell absorber", *J. Mater. Chem. A*, 2017, Vol. 5, pp. 3503-3513



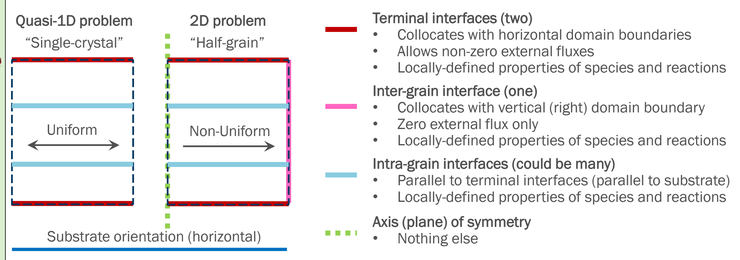
- *Realistic initial conditions - most critical aspect.*
- *Simulation of complete fab. process required to simulate field performance and metastabilities.*

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"

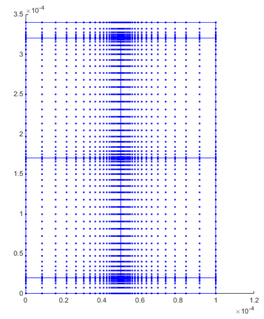
- Implementation of arbitrary GBs in 2D is very costly in terms of mesh points
- Based on learned lessons, we simplified definition of generic use cases
  - ✓ *Orthogonal interfaces only; one vertical interface at most.*



MESH IN 2D IMPLEMENTATION

- Each grid point is the center of a rectangular *finite volume*
- Allows multiple grain structures
- Rectilinear 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:

$$\bar{D} = \frac{2}{\frac{h^+}{D^+} + \frac{h^-}{D^-}}$$



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
- Lattice sites no longer assigned to specific elements.

(***invited talk at Spring MRS Meeting 2017***) Igor Sankin, Dmitry Krasikov, Andenet Alemu, Christian Ringhofer, Da Guo, Daniel Brinkman, Dragica Vasileska, Markus Gloeckler, "Comprehensive Solution for Defect Chemistry in II-VI Photovoltaics".

(***contributed talk at Spring MRS Meeting 2017***) Dmitry Krasikov, I. Sankin, A. Alemu, "Influence of Defects Interactions on the Properties of CdTe:Cl,Cu Solar Cell Absorber".

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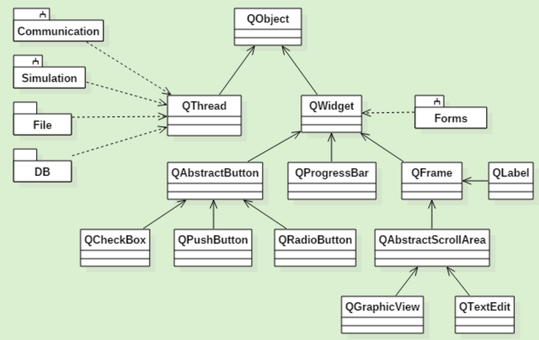
GUI DEVELOPMENT:

- Successfully developed and tested data communication between C++ program and Matlab code/C++ Dynamic-link library (DLL)
- Created a working prototype of the GUI
- Set up the project database, and connected to GUI prototype

Qt Framework for GUI Development

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

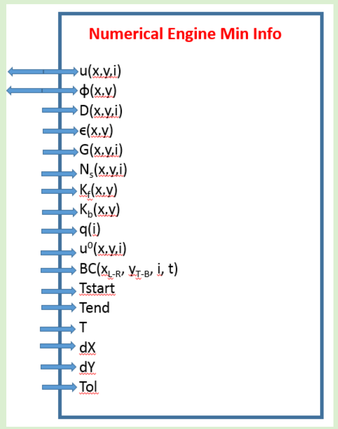


NUMERICAL ENGINE DEVELOPMENT:

- 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

- Fixed the d*ata standard* between numerical engine and task manager.
- Task manager is a black box to numerical engine and vice versa.
- Supports parallel development of task manager infrastructure and numerical engine algorithms.
- All the interface data variables are 2D arrays for language flexibility.



- Interface variables are visible to numerical engine and solver classes.
- Abstract solver classes for reaction, diffusion and Poisson equation.
- Each numerical algorithms 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.

- Formulated reaction operator as:

$$\boldsymbol{R(U) = U^T Q U + P U + K}$$

- Solved using implicit Euler method with Newton iteration.
- Reactions solved for 0D improved efficiency.

0D Reaction Solver	Time [s]
PREDICTS	17.61
PVRD	0.637

27x speed-up

To determine the arrays **Q**, **P**, **K** we first write the reaction rate equations as

$$\frac{du_i}{dt} = \sum_j^N \sum_k^N a_{jk}^i u_j u_k + \sum_j^N b_j^i u_j + c^i$$

Then the NxNxN **Q** array elements are given as

$$q(i,j,k) = q(i,k,j) = \begin{cases} \frac{a_{jk}^i}{2} & if\ a_{jk}^i \neq 0 \\ 0 & otherwise \end{cases}$$

The NxN **P** array elements are given as

$$p(i,j) = \begin{cases} b_j^i & if\ b_j^i \neq 0 \\ 0 & otherwise \end{cases}$$

The N-dimensional **K** array elements are given as

$$K(i) = \begin{cases} c^i & if\ c^i \neq 0 \\ 0 & otherwise \end{cases}$$

Using this we can write the Jacobian as

$$J = (Q + Q^T)U + P$$

(***invited talk at Spring MRS Meeting 2017***) Dragica Vasileska, Igor Sankin, Da Guo, Daniel Brinkman, Christian Ringhofer, Andrew Moore, James Sites, "Metastability and Reliability of CdTe Solar Cells"