Diffusion-Reaction Modeling of Cu Migration in CdTe Solar Devices

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In this work, we report on development of one-dimensional (1D) finite-difference and two-dimensional (2D) finite-element diffusion-reaction simulators to investigate mechanisms behind Cu-related metastabilities observed in CdTe solar cells [1]. The evolution of CdTe solar cells performance has been studied as a function of stress time in response to the evolution of associated acceptor and donor states. To achieve such capability, the simulators solve reaction-diffusion equations for the defect states in *time-space domain* self-consistently with the *free carrier transport*. Results of 1-D and 2-D simulations have been compared to verify the accuracy of solutions.

Evolution of concentration profile for an arbitrary defect C is simulated by solving reaction-diffusion equation [2]

$$\frac{dC}{dt} = -\frac{dJ_C}{dx} - R_C \qquad (1)$$

In (1), R_C represents the net reaction rate of the defect C, and for the case of Cu is calculated based on the main reactions responsible for p-type doping formation in CdTe [3]:

$$Cu_i + Cd_{Cd} \Leftrightarrow Cu_{Cd} + Cd_i \qquad (2)$$

$$Cu_i + V_{Cd} \Leftrightarrow Cu_{Cd} \qquad (3)$$
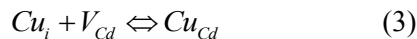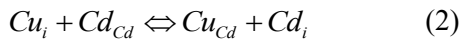
In reaction (2), also known as the knock-off reaction, forward and backward rates are calculated as

$$\begin{cases} R_f = K_f C_s [Cu_i] \\ R_b = K_b [Cu_{Cd}][Cd_i] \end{cases} \qquad (4)$$

In (4), C_S stands for the concentration of cation sites in CdTe, while K_f and K_b represent temperature-dependent rate constants. The expression describing the flux of species C in the gradient of its electrochemical potential is given below.

$$J_C = -D_C \left\{ \frac{[C]}{kT} \nabla \left(G_F + \theta\varphi \right) + \nabla [C] \right\} \qquad (5)$$

In (5), diffusivity of the defect C is given by D_C, θ is the amount of carried charge, G_F is the free energy of formation, and the electrostatic potential is provided by φ. Due to very high diffusivities of free carriers, we considered them reaching steady-state concentrations at every time step when solving (5) for much slower ionic species.

In our 2D FEM scheme, anisotropic diffusion model for a single grain boundary of width δ located at x=0 is utilized, and is given by

$$\frac{dC}{dt} = \frac{d(D\,d[C]/dx)}{dx} + \frac{d(D\,d[C]/dy)}{dy} \qquad (6)$$

where $\quad D = \begin{cases} D_{gb}, & |x| < \delta/2 \\ D_g, & |x| \geq \delta/2 \end{cases} \qquad (7)$

For a finite difference mesh with size h=δ and a symmetric grain boundary, this model gives identical discretization to the traditional Fisher model [4].

In summary, the diffusion-reaction model has been applied to *Cu*-related defects in *CdTe* PV devices. The simulation results from this study give us a deeper understanding of the role of *Cu* on the performance of *CdTe* solar cells. The 1D diffusion-reaction code is installed on nanoHUB.org.

REFERENCES

[1] K. D. Dobson, I. Visoly-Fisher, G. Hodes, and D. Cahen, "Stability of CdTe/CdS thin-film solar cells," *Solar Energy Materials and Solar Cells,* vol. 62 (2000).
[2] P. M. Fahey, P. B. Griffin, and J. D. Plummer, "Point defects and dopant diffusion in silicon," *Reviews of Modern Physics,* vol. 61 (1989).
[3] S. Hu, "Nonequilibrium point defects and diffusion in silicon," *Materials Science and Engineering: R: Reports,* vol. 13 (1994).
[4] J. C. Fisher, "Calculation of diffusion penetration curves for surface and grain boundary diffusion," *Journal of Applied Physics*, vol. 22 (1951).
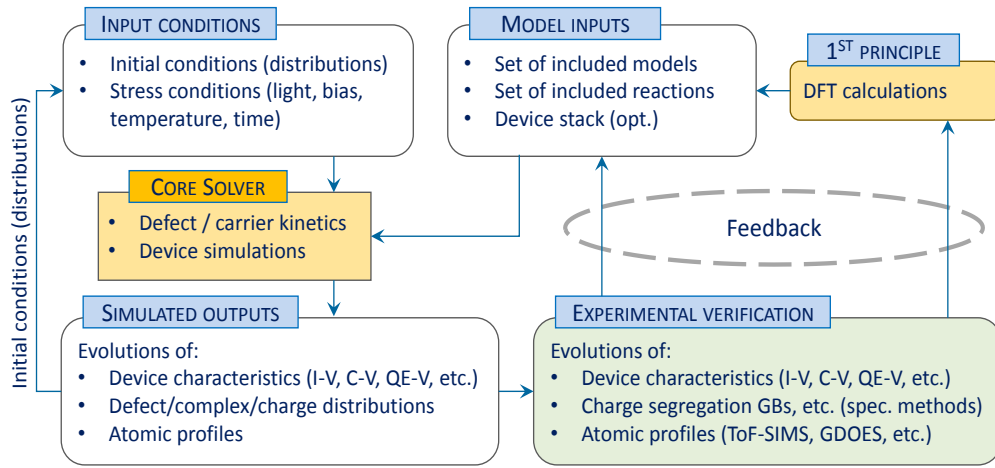
Fig. 1. Unified diffusion-reaction/device solver – multi-scale computation with feedback (https://nanohub.org/tools/predicts1d/).
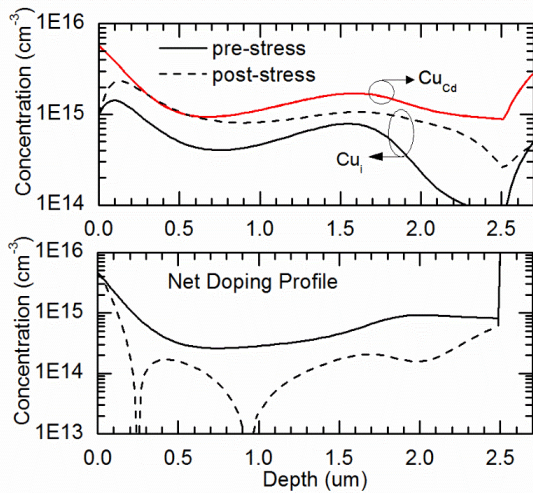

Fig. 2. Defect profiles and corresponding doping profiles simulated after a 200ºC 220s anneal and two-hour open circuit stress in a standard CdS/CdTe solar cell. Extra Cu_i moved into CdTe layer due to small built-in electric field under OC condition, which reduced the p-type net doping during the stress.
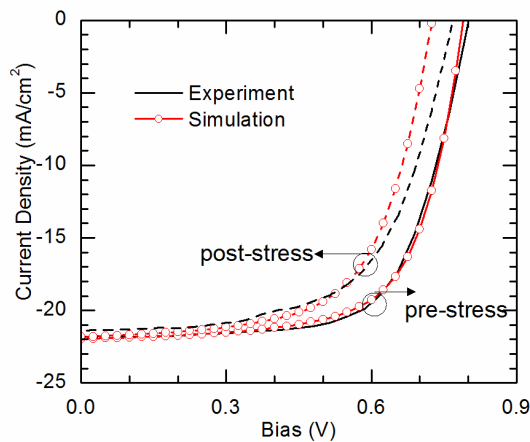

Fig. 3. Comparison between simulated and experimental IV curves of the CdTe solar cell before and after the stress. Loss in p-doping caused the reduction of V_{OC}, hence the conversion efficiency.
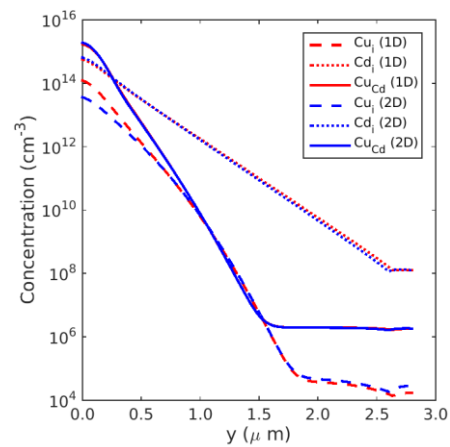

Fig. 4. Comparison of the concentration of Cu_i, Cd_i and Cu_{Cd} for the 1D finite-difference scheme and the 2D finite-element method scheme finished by a standard 200ºC 220s anneal from a finite Cu source. Although the time step employed for the 2D case is 100 times larger than the 1D time step, the difference between these profiles is negligible.
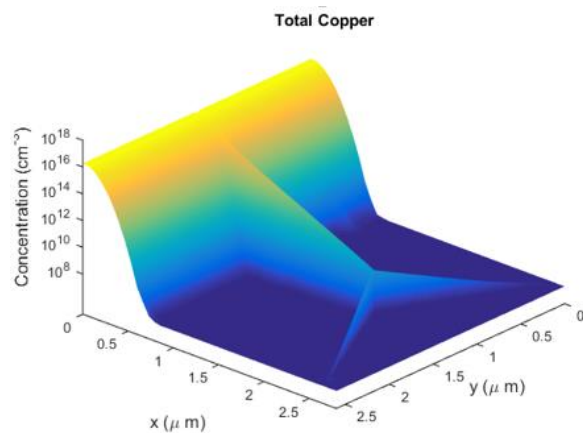

Fig. 5. The 2D FEM scheme allowed the inclusion of grain-boundary enhanced diffusion of Cu in the simulation. A fork-shaped grain-boundary was assumed in this 2D simulation. Clear segregation of Cu along the boundary was achieved.