

Modeling of light soaking effect in CdTe Solar Cells

Da Guo and Dragica Vasileska

School of Electrical, Computer and Energy Engineering
Arizona State University, Tempe, AZ 85287, USA
e-mail: vasileska@asu.edu

Abstract— In this work, a diffusion-reaction model was employed to study Cu’s role in light soaking effect of CdTe solar cells. Our simulation shows that both passivation of Cu dopants and Cu migration under light soak could cause device performance enhancement. The simulation result also suggests that 10^{-13} cm²/s diffusivity of Cu interstitials could explain the 10-hour long light soaking effect at 65°C.

Introduction:

Nearly all PV technologies exhibit changes in device performance under extended illumination, or “light soaking”, although the magnitude and the trend of these changes are not always the same among different technologies. Experiments on both commercial modules and research cells based on CdTe technology have shown improvement of cell performance under light soaking conditions for up to 20 hours [1]. Many accredited such phenomena to the passivation of traps and migration of Cu ions. In this work, we employed a self-consistent one-dimensional (1D) diffusion-reaction simulator to study the migration and passivation of Cu related dopants in CdTe solar cell as a function of soaking conditions.

Physical Models:

The employed 1D simulator was originally developed to study the incorporation of Cu and compensating mechanisms among Cu dopants in CdTe material [2]. It solves diffusion-reaction equations both for the free carriers and the point defects in time-space domain self-consistently with global Poisson equation [2], [3]. It should be noted that reaction-diffusion equations describing evolution of ionic species have same form as those describing evolution of free carriers. Namely, the diffusion-reaction equation for species X (target defect) is of the form

$$J_X = D_X \left(\frac{d[X]}{dx} + \frac{[X]}{kT} \frac{d[q\phi + G]}{dx} \right) + R_X \quad (1)$$

where D_X is the diffusivity, q is the charge of the defects, kT is the thermal energy, ϕ is the electrostatic potential and G is the spatially dependent formation energy of the defects and R_X is the net production rate of each defect. In this work, we are primarily interested in the interactions between free carriers and major Cu dopants such as $Cu_i(+)$ donors and $Cu_{Cd}(-)$ acceptors:



Rate Law is applied to calculate the reaction rate. Details of the calculation of reaction rate can be found in [2], [3].

Simulations:

A simplified dopant compensation picture is employed in this work. Namely, 10^{16} cm⁻³ $Cu_{Cd}(-)$, 0.4×10^{16} cm⁻³ $Cu_i(+)$ and 0.5×10^{16} cm⁻³ background donor is assumed as the initial defect distribution in our simulation, resulting in 10^{15} cm⁻³ hole concentration in the CdTe absorber layer, which is a typical doping concentration in poly-crystalline CdTe solar devices. A standard ZnTe/CdTe/CdS structure with common electronic properties is employed in our simulation.

Since light soaking is usually conducted after dark storage of the solar devices, we first simulate the equilibrium of the defect system in CdTe cells under dark without any bias as an original point of our light soaking simulation. Figure 1 shows the equilibrium distribution of Cu_i and Cu_{Cd} as well as the band diagram of the solar cell under dark soak at 65°C. Due to the built-in potential of the p-n diode, most of $Cu_i(+)$ is pushed away from the depletion region, resulting in more net acceptor in the junction area. 10% of Cu_{Cd} is deionized while most of Cu_i is charged in the neutral region of p-type layer due to lack of electrons. On the other hand, few $Cu_{Cd}(0)$ are present in the depletion region, due to low density of holes in that area.

Figure 2 shows the equilibrium defect distribution and band diagram of the solar cells under 1 Sun illumination with 0.8V forward bias (maximum power point) at 65°C. Comparing to the previous dark storage condition, a couple of difference is presented here: (1) $Cu_i(+)$ moves deeper into the junction area due to the forward bias, reduces acceptor density in the depletion region, (2) light-generated excess electrons passivate $Cu_i(+)$, thus increasing the hole concentration in the

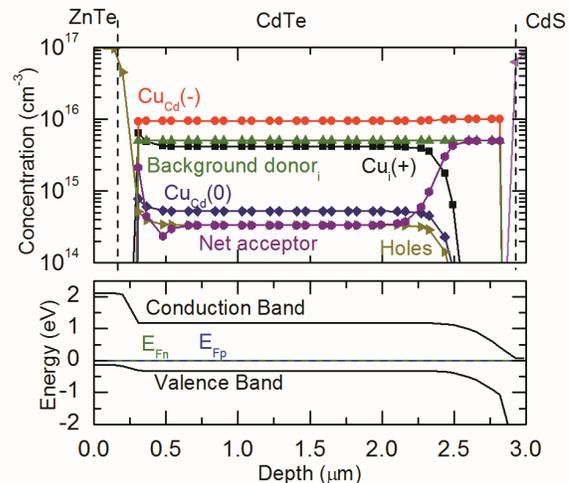


Figure 1 Equilibrium of the solar cell under dark.

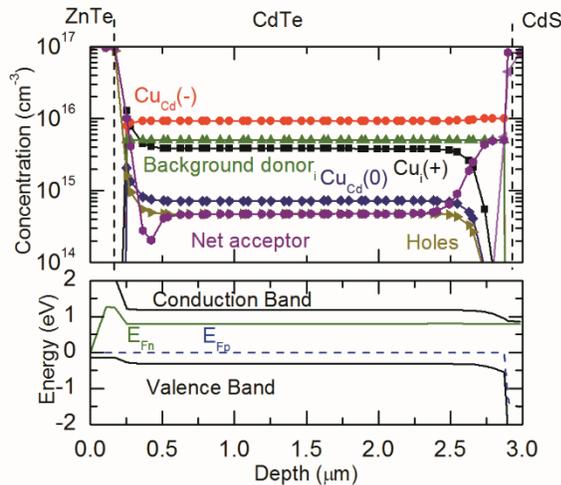


Figure 2 Equilibrium of the solar cell under light soaking with V_{mp} applied.

absorber layer, (3) more $Cu_{Cd}(0)$ is present, as a result of more holes passivating acceptors (4) the depletion region width should be increased after the light soak as lower doping is achieved in the junction area. Since first-principle calculated fast diffusion coefficient ($9 \times 10^{-10} \text{ cm}^2/\text{s}$ at 65°C) is assumed [4], only 0.03 hour of light soaking could drive the device into equilibrium (see Soak A of Figure 3).

We further simulate different soaking conditions to isolate the effect from passivation caused by excess carriers and migrations related to external voltage bias on CdTe cells. Table I lists the soaking conditions and the corresponding mechanisms potentially caused the performance changes. Figure 3 shows the efficiency changes of the solar cells as a function of soaking time with different modes. Both Soak A and C experienced similar device performance enhancement as a result of external bias while soak B & D barely changed the solar cell efficiency regardless of the presence of excess electrons. An additional simulation of light soaking with voltage bias (Soak E) is performed without the migration part of Cu defects. Smaller increment in device performance is achieved as a result of excess holes passivating $Cu_{Cd}(-)$ in the junction area within 0.01 hour of light soaking. Thus, we could conclude that both $Cu_i(+)$ migration towards the junction area and excess holes injected in the depletion region can cause the enhancement of device performance commonly observed from CdTe photovoltaic devices. Soaks F & G are

TABLE I
LIST OF SOAKING CONDITIONS

Soak	Illumination	Voltage Bias	Mechanism
A	1 Sun	0.8 V	Both
B	1 Sun	0 V	Passivation
C	Dark	0.8V	Migration
D	Dark	0 V	None
E	1 Sun	0.8 V	No Migration
F	1 Sun	0.8 V	$10^{-12} \text{ cm}^2/\text{s}$
G	1 Sun	0.8 V	$10^{-13} \text{ cm}^2/\text{s}$

Soak A is the light soaking presented in Figure 2.

Soak D is the dark storage presented in Figure 1.

Soak E & F are simulated with smaller Cu_i diffusivity.

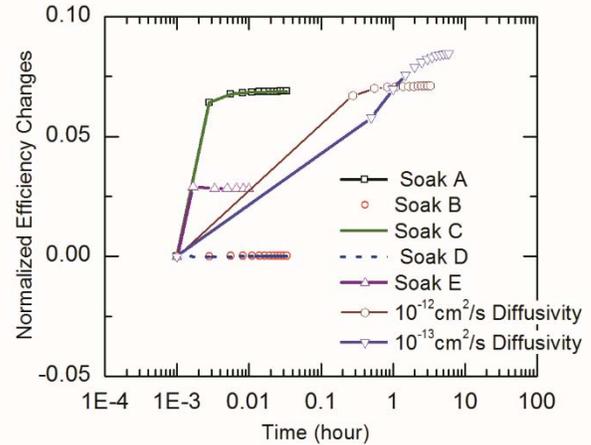


Figure 3 Device performance changes as a function of soaking time with various conditions.

simulated with much smaller diffusivities of the $Cu_i(+)$ donors in order to achieve longer transient behavior [5]. As plotted in Figure 3, $Cu_i(+)$ diffusion coefficient around $10^{-13} \text{ cm}^2/\text{s}$ at 65°C could be the cause of the 10-hour long device metastable behaviors under normal light soak conditions.

Conclusion:

At present, we have only studied simplified Cu compensation but inclusion of other complicated defects (such as $Cl_{Te}-Cu_{Cd}(0)$ and $Cl_{Te}(+)$), defect-defect interactions, interface traps, advanced life time modeling and grain boundary in 2D simulator will allow us to investigate light soaking effect from a more comprehensive viewpoint.

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