CdTe Solar Cells: The Role of Copper

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There is a wide variety of renewable energy sources: solar, wind, geo–thermal, biomass and hydro. Among these renewable energy sources, however, only solar energy has a large enough potential to meet the major fraction of the world's energy needs. Of course, the other renewable sources can also generate a significant fraction of a TW of energy.

Thin-film *CdTe* based solar cells are one of the leading contenders for providing low cost and pollution-free energy. The formation of a stable, low resistance, non-rectifying contact to *p-CdTe* thin-film is one of the major and critical challenges associated with this technology in the fabrication of efficient and stable solar cells. The effect of *Cu* inclusion is not limited to the back–contact layer where it is deposited. *Cu* is a known fast diffuser in *p-CdTe*, and therefore, a significant amount of *Cu* reaches both the *CdTe* and *CdS* layers. Hence, the effect of the presence of *Cu* on the individual layers: back-contact, the absorber (*CdTe*), and the window (*CdS*) layers is discussed, respectively.

Small amount of *Cu* partially diffused into the *CdTe* absorber layer results in increased hole density, and improved *Voc*. However, excess *Cu* creates recombination centers that significantly reduce the fill factor (*FF*) and open-circuit voltage (*Voc*). The presence of *Cu* in the *CdS* window layer has minimal effect on device performance. It was found, however, to be responsible for anomalies such as dark/light crossover and distortions in apparent quantum efficiency, neither of which has a direct impact on the device performance.

The basic computational problem here consists of solving a complex system of reaction diffusion equations for the densities u_n of various species of charged particles, specifically *Cu* and *Cd* interstitials and *Cu* at *Cd* site in this work, coupled to Poisson's equation in a mean field theory. The general system can be written as:

$$\partial_t u_n = \nabla_x \cdot [D_n \nabla_x u_n - \mu_n q_n u_n \nabla_x V_n] \\ + R_n(u_1,...,u_N), n = 1 : N \tag{1}$$

$$\nabla_x(\varepsilon \nabla_x V) = \sum_{n=1}^{N} q_n u_n + d + C \tag{2}$$

Here, q_n denotes the charge of a particle of species n (either ions or free carriers) and R_n are the reaction terms (for ions) or the generation – recombination rates (for electrons and holes). The reaction terms are calculated as bi-molecular reaction rates using the following equation [4]:

$$Cu_i + Cd_{Cd} \Leftrightarrow Cu_{Cd} + Cd_i \tag{3}$$
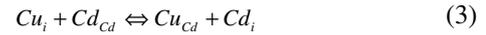
$$\begin{cases} R_f = K_f \left(u_{Cu_i} u_{Cu_{Cd}} - u^*_{Cu_i} u^*_{Cu_{Cd}} \right) \\ R_b = K_b (u_{Cu_{Cd}} u_{Cu_{Cd}} - u^*_{Cu_i} u^*_{Cu_{cd}}) \end{cases} \tag{4}$$

In Eq. (4), subscripts f and b indicate the forward and the backward reactions from Eq. (3). $K_{f,b}$ is the reaction constant, u_n^*, the equilibrium concentration of defect n, is determined by their formation energies [5], as illustrated in Fig. 1, and total *Cu* concentration [6]. To get a convergent solution of this multi-scale problem, continuity equations for the defects and free carriers are discretized using Scharfetter-Gummel discretization scheme and are self-consistently coupled to the linearized and discretized Poisson equation. Crank-Nicholson algorithm is used for the time-domain discretization and the resultant system of algebraic equations, each of the form *Ax=f*, is solved using the Gummel's iterative scheme, where each individual matrix equation is solved using the *LU*-decomposition method.

In summary, the reaction-diffusion model has been applied to *Cu* in *CdTe* PV devices. The simulation results from this study give us a deeper understanding of the role of *Cu* in *CdTe* solar cells.
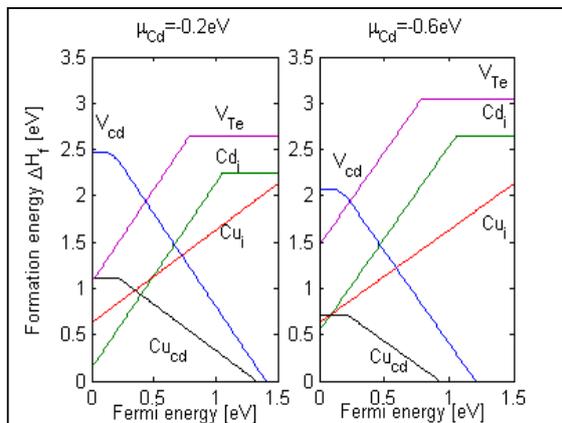
Fig. 1. The formation energy of involved defects as a function of the Fermi energy at both *Cd*-rich and *Cd*-poor cases. The slope of the energy line gives the charge state of the defect. The transition energy level corresponds to the Fermi energy at which the slope changes. The line intersects at positions where Fermi energy might be pinned for equilibrium.
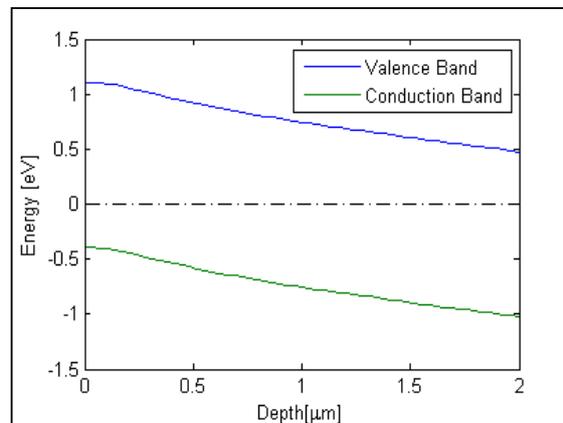

Fig. 3. The band diagram of the *CdTe* layer in one particular moment in the 415K stress simulation. Due to the accumulation of Cu_{Cd} and its ionized acceptor state, it behaves as *p*-type near the back contact. As the byproduct of Cu_{Cd}, the fast *Cd* interstitials diffused deep into the bulk, became donors, and made the *CdTe* n-type in the bulk.
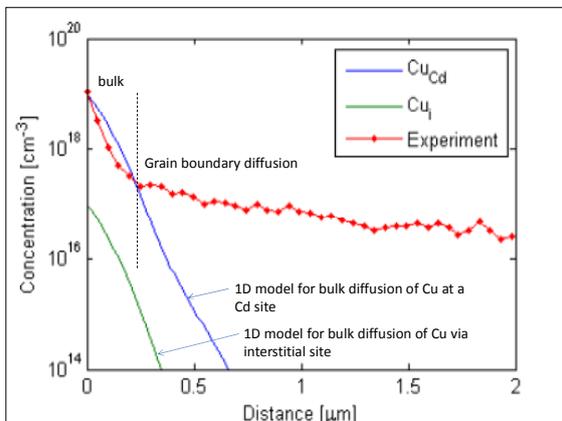

Fig. 2. Comparison between simulated *Cu* profile and experiments in poly-*CdTe* layer after 415K and 100 minutes stress. The reaction diffusion simulation reproduced the accumulation of Cu_{Cd} near the back contact, which can be seen as forming a low resistance Cu_2Te contact layer. The long tail of the experimental data is caused by *Cu* migration in grain boundaries, which cannot be simulated in a one-dimensional solver.
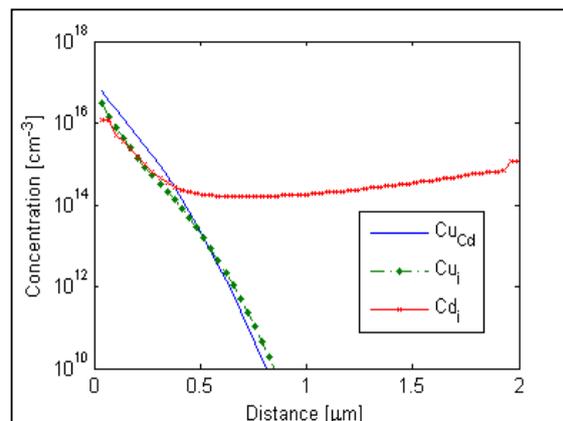

Fig. 4. The corresponding defect concentration profiles in the stress simulation that produced the band diagram shown in Fig. 3. The ionized Cd_i in the CdTe layer could be responsible for the dark/light crossover and distortions in apparent quantum efficiency, since the photo generated holes became minority carriers in the CdTe layer and could not be collected by the back contact.