

# Modeling Cu Migration in CdTe Solar Cells Under Device-Processing and Long-Term Stability Conditions

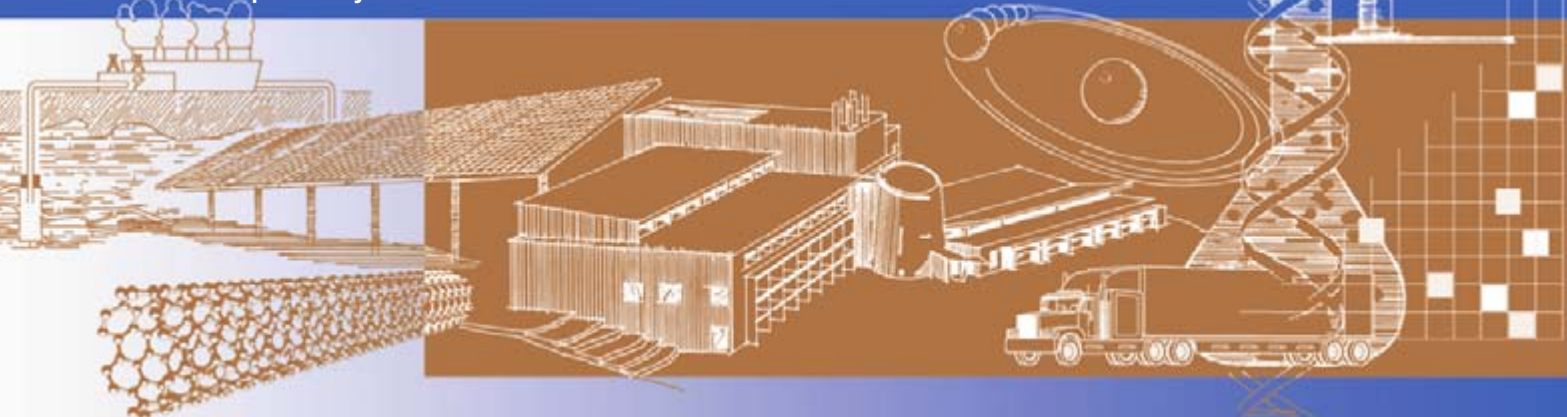
## Preprint

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# MODELING Cu MIGRATION IN CdTe SOLAR CELLS UNDER DEVICE-PROCESSING AND LONG-TERM STABILITY CONDITIONS

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## ABSTRACT

An impurity migration model for systems with material interfaces is applied to Cu migration in CdTe solar cells. In the model, diffusion fluxes are calculated from the Cu chemical potential gradient. Inputs to the model include Cu diffusivities, solubilities, and segregation enthalpies in CdTe, CdS and contact materials. The model yields transient and equilibrium Cu distributions in CdTe devices during device processing and under field-deployed conditions. Preliminary results for Cu migration in CdTe photovoltaic devices using available diffusivity and solubility data from the literature show that Cu segregates in the CdS, a phenomenon that is commonly observed in devices after back-contact processing and/or stress conditions.

## INTRODUCTION

It is well known that Cu plays an important role in CdTe-based solar cells by helping to form an Ohmic back contact (BC). (See, e.g., references in Ref. [1].) Also, Cu migration in CdTe solar cells has been implicated in device degradation [2-6]. However, the role of Cu in degradation remains unclear, in part because the kinetics and equilibria of Cu migration phenomena in CdTe photovoltaic (PV) devices are not well understood. Cu incorporation in CdTe devices is generally controlled through time-consuming empirical optimization procedures. Similarly, device degradation issues related to Cu migration have typically relied on empirical approaches [7]. The present work provides a simple physical model for Cu migration in CdTe devices that can be used to understand and potentially optimize Cu incorporation processes.

## IMPURITY MIGRATION MODEL

A general impurity migration model has been developed recently at the National Renewable Energy Laboratory (NREL) [8]. The model applies to systems with material interfaces (e.g., CdTe/CdS) that lead to discontinuities in the properties that control impurity segregation; diffusivity, solubility, and segregation enthalpy. The impurity migration model derived in Ref. [8] is reviewed here briefly. Consider a system where individual atomic planes perpendicular to the diffusion coordinate  $x$  are indexed by subscript  $i$ . The free energy is calculated by summing the product of particle number and chemical potential over all species and planes:

$$A = \sum_i \left[ (n_i X_{Cu}^i) \mu_{Cu}^i + (n_i X_p^i) \mu_p^i \right]. \quad (1)$$

Subscript  $p$  denotes the local matrix (CdTe, CdS, etc.) in which Cu is diffusing. Species are labeled by  $s = Cu, p$ , and the number of sites per plane is  $n_i$ . The species- $s$  mole fraction in plane  $i$  is  $X_s^i$ . For simplicity, the ideal-solution model is used for  $\mu_{Cu}^i$  and  $\mu_p^i$ . Now a chemical potential,  $\mu_{Cu-p}^i$ , is defined for plane  $i$  that accounts for both species, subject to the complementarity condition  $X_{Cu}^i + X_p^i = 1$ . Differentiating Eq. (1) with respect to the amount of Cu in plane  $i$  leads to

$$\mu_{Cu-p}^i = \frac{1}{n_i} \frac{\partial A}{\partial X_{Cu}^i} = \Delta H_{Cu-p}^i + kT \ln \frac{X_{Cu}^i}{1 - X_{Cu}^i}. \quad (2)$$

Physically,  $\Delta H_{Cu-p}^i$  is the energy difference that accompanies the exchange of a matrix atom  $p$  with a Cu atom in plane  $i$ . The relationship between  $\Delta H_{Cu-p}^i$  and the Cu migration potential is illustrated in Fig. 1, and is summarized by the parameterization

$$\Delta H_{Cu-p}^i = -(E_D^i + \phi_{Cu-p}^i). \quad (3)$$

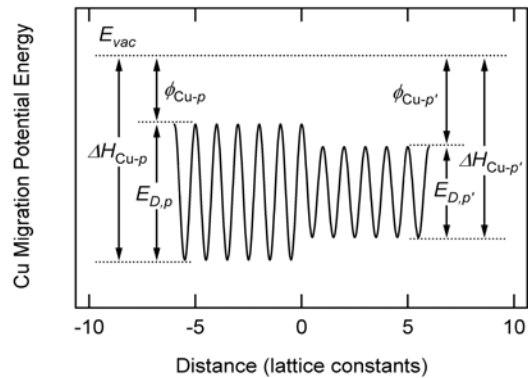


Figure 1. Schematic illustration of the ideal-solution Cu migration potential near a hypothetical material interface.

Equation (3) permits the diffusion activation energy,  $E_D^i$ , and the local potential energy offset,  $\phi_{\text{Cu-p}}^i$ , to be written as functions of position rather than concentration.

From Fig. 1, the Cu segregation enthalpy between adjacent layers in the thin-film stack is given by the Cu migration potential difference across the interface:

$$H_{\text{seg}} = \Delta H_{\text{Cu-p}} - \Delta H_{\text{Cu-p}'} . \quad (4)$$

The layer- $i$  chemical potential, Eq. (2), describes a discretized system of atomic planes. Dropping the  $i$  subscripts yields a continuum description. The Cu flux is given by the standard phenomenological relation:

$$J_{\text{Cu}} = -MC_{\text{Cu}} \frac{\partial \mu_{\text{Cu-p}}}{\partial x} , \quad (5)$$

where  $C_{\text{Cu}}$  is the Cu concentration. The Cu flux acts to minimize the free energy with respect to the Cu concentration profile, and it vanishes at equilibrium. Requiring equal and opposite Cu and matrix fluxes leads to a generalization of the Einstein relation [9] to non-dilute systems [8], in which mobility ( $M$ ) is related to diffusivity ( $D$ ) through

$$M = \frac{D}{kT} \frac{C_p}{C_0} . \quad (6)$$

$C_0$  is the Cu solubility, and  $C_p$  is the matrix concentration in the Cu-available sites, defined by  $C_0 = C_{\text{Cu}} + C_p$ . Dropping the unnecessary 'Cu' subscripts and assuming an Arrhenius form for  $D$  leads to

$$J = \frac{C_p}{C_0} \left( \frac{DC}{kT} \frac{\partial \phi_{\text{Cu-p}}}{\partial x} - C \frac{\partial D}{\partial x} \right) - D \left( \frac{\partial C}{\partial x} - \frac{C}{C_0} \frac{\partial C_0}{\partial x} \right) , \quad (7)$$

and the continuity equation is

$$\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x} . \quad (8)$$

In any uniform layer, Eq. (7) reduces to  $J = -D(\partial C/\partial x)$ , Fick's first law of diffusion. Equations (7) and (8) can be solved numerically for the Cu concentration profile in the device for any initial conditions. Required inputs include the Cu diffusivities, solubilities, and segregation enthalpies for each layer. The device model consists of a BC, CdTe, CdS, and a front contact (FC). A thicker-than-typical CdS layer (0.5  $\mu\text{m}$ ) is chosen to make this layer more visible in the simulation plots.

## SURVEY OF DIFFUSIVITY AND SOLUBILITY DATA

Solubility and diffusivity data for Cu in CdTe and CdS are summarized in Table I. Cu solubility and diffusivity

data are not available for ZnTe. However, SIMS measurements indicate that high levels of Cu can be incorporated in sputtered ZnTe:Cu BCs [10-12]. Therefore, for preliminary modeling purposes, a low solubility activation energy was chosen (0.11 eV) for the BC, such that  $[\text{Cu}]_{\text{BC}}^{\text{max}} > 10^{21} \text{cm}^{-3}$  for  $T > 20$  °C. Despite the lack of solubility and diffusivity data for ZnTe:Cu, this allows the BC layer to act as Cu reservoir in the simulation, and is consistent with SIMS measurements of sputtered ZnTe:Cu BCs [10-12]. The CdTe:Cu diffusivity parameters were also used for the BC, again due to the lack of data. Arbitrary low values were chosen for the solubility and diffusivity in the FC layer. This leads to low Cu segregation levels in the FC layer in the simulations, but has little effect on the Cu profile in other layers of the device.

Table I. Diffusivity and solubility data for Cu in CdTe and in CdS. Values used in simulations are in bold type. Single-crystal based measurements are denoted by SC; measurements from polycrystalline films are indicated by PX. Diffusion mode refers to cases described in the text.

CdTe:Cu diffusivity data				
$D_0$ ( $\text{cm}^2 \text{s}^{-1}$ )	$E_D$ (eV)	Ref.	SC or PX	Diffusion mode
1.70E-06	0.24	[13]		
<b>6.65E-05</b>	<b>0.57</b>	<b>[14]</b>	SC	low
7.30E-07	0.33	[15]		
<b>1.30E-06</b>	<b>0.29</b>	<b>[16]</b>	PX	high
8.20E-08	0.64	[17]		
3.70E-04	0.67	[18]		
9.57E-04	0.7	[19]		
CdTe:Cu solubility data				
$C_0$ ( $\text{cm}^{-3}$ )	$E_a$ (eV)	Ref.	SC or PX	Diffusion mode
<b>1.56E+23</b>	<b>0.55</b>	<b>[14]</b>	SC	low
<b>~2E+17</b>	<b>~0</b>	<b>[16]</b>	PX	high
3.73E+24	0.68	[20]		
CdS:Cu diffusivity data				
$D_0$ ( $\text{cm}^2 \text{s}^{-1}$ )	$E_D$ (eV)	Ref.	SC or PX	Diffusion mode
1.20E-02	1.05	[21]	SC	
2.10E-03	0.96	[22]	SC	
1.60E-03	0.77	[23]	SC	
—	0.95	[24]	SC	
<b>6.00E-09</b>	<b>0.5</b>	<b>[25]</b>	PX	
—	1.0	[26]	SC	
CdS:Cu solubility data				
$C_0$ ( $\text{cm}^{-3}$ )	$E_a$ (eV)	Ref.	SC or PX	Diffusion mode
<b>8.00E+21</b>	<b>0.27</b>	<b>[25]</b>	PX	
6.60E+22	0.505	[22]	SC	

It has been pointed out that there appear to be two mechanisms for Cu diffusion in CdTe: via Cu atoms on Cd lattice sites ( $\text{Cu}_{\text{Cd}}$ ), and via interstitial Cu ions ( $\text{Cu}_i^+$ ) [16, 18]. Other workers have suggested that the dominant diffusion mechanism is a neutral Cu interstitial Cd vacancy ( $\text{Cu}_i\text{-V}_{\text{Cd}}$ ) complex [14, 27]. Single-crystal measurements indicate that the  $\text{Cu}_{\text{Cd}}$  (or  $\text{Cu}_i\text{-V}_{\text{Cd}}$ ) solubility is significantly higher than that of  $\text{Cu}_i^+$ , and that  $\text{Cu}_{\text{Cd}}$  has the lower diffusivity [14, 18]. The  $\text{Cu}_i^+$  solubility is apparently nearly

constant with temperature [14]. Data for both mechanisms are used in this study for comparative purposes: the diffusivity from Ref. [14] is the 'low-diffusivity' case, and that from Ref. [16] is 'high-diffusivity' case. The corresponding solubilities are also used.

It is very likely that grain-boundaries in polycrystalline films significantly enhance the diffusivity and solubility of Cu compared to in single-crystal samples. Currently, there is not sufficient data available in the literature to definitively quantify these effects in CdTe PV devices. Nevertheless, it should be noted that the high-diffusivity case referred to in this work is based on measurements of polycrystalline films, whereas the low-diffusivity case is based on single-crystal measurements. Therefore, the high-diffusivity case is probably more relevant to Cu migration in thin-film based CdTe solar cells. For CdS, there is only one set of diffusivity and solubility measurements available for polycrystalline thin films [25]. Therefore, solubility and diffusivity data for the simulations were chosen from this study.

The segregation enthalpy, Eq. (4), depends on the diffusivities and local potential-energy offsets for Cu in each material layer, and therefore must be measured independently for each pseudo-binary diffusion couple. These data are not presently available, so the simulations assume that the corresponding term in Eq. (7) is zero.

### Cu MIGRATION SIMULATION RESULTS

For all simulations, the initial Cu concentration was set to  $10^{21} \text{ cm}^{-3}$  in the BC layer, and zero elsewhere. For the device-processing simulation, the temperature was ramped from room temperature to the indicated temperatures at  $20 \text{ }^\circ\text{C min}^{-1}$ , held at temperature for a time equal to the duration of the temperature ramp, then ramped back to room temperature. These preliminary simulation results are shown in Figs. 2 and 3.

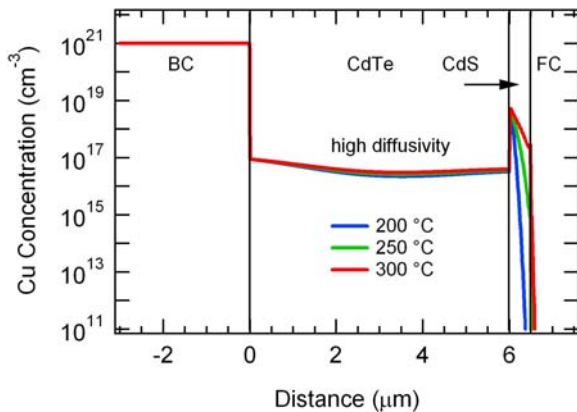


Figure 2. Device-processing simulation of Cu migration in CdTe PV device for the high-diffusivity case.

The extent of Cu segregation increases with annealing temperature, due to increased CdTe:Cu diffusivity and CdS:Cu solubility. There are also Cu-depleted regions near the BC interface for the low-diffusivity case. This results from Cu re-segregation to the BC during the ramp back to room temperature, caused by the corresponding decrease of Cu solubility in CdTe. In

spite of this phenomenon, the simulations show that a metastable Cu concentration in excess of the Cu solubility can be established during BC processing: the  $\text{Cu}_{\text{Cd}}$  solubility is  $5 \times 10^{13} \text{ cm}^{-3}$  at  $20 \text{ }^\circ\text{C}$  [14].

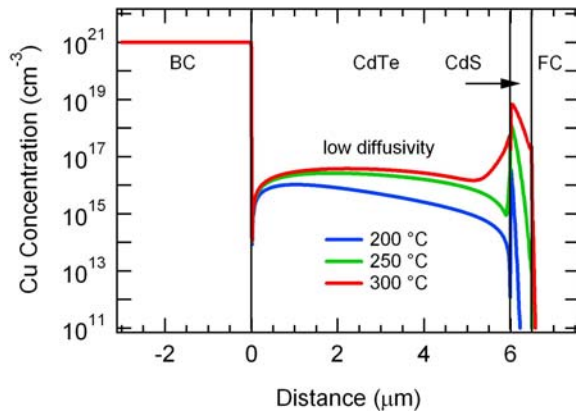


Figure 3. Device-processing simulation of Cu migration in CdTe PV device for the low-diffusivity case.

Figures 4 and 5 show the results from the preliminary long-term stability simulations, for  $T = 65 \text{ }^\circ\text{C}$ .

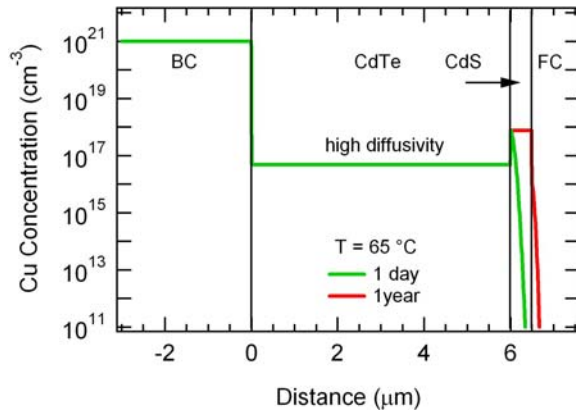


Figure 4. Long-term stability simulation of Cu migration in CdTe PV device for the high-diffusivity case.

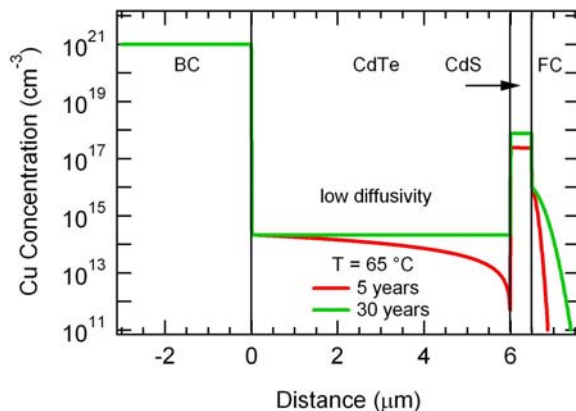


Figure 5. Long-term stability simulation of Cu migration in CdTe PV device for the low-diffusivity case.

For these results, it is noteworthy that high levels of Cu in the CdS layer are established relatively quickly. For

the high-diffusivity case, the detailed temporal evolution of the Cu profile (not shown for lack of space) show that equilibrium in the CdTe and CdS layers is established within about 20 weeks at 65 °C. Similarly, for the low-diffusivity case, a large Cu concentration develops in the CdS after about 5 years, and equilibrium is established in 10-15 years.

As was observed for the CdTe layer, the Cu levels in the CdS layer in the device-processing simulation again exceed the solubility (*cf.* Figs. 2 and 4 and Figs. 3 and 5). Therefore, in actual devices, it is possible under some conditions that a gradual *decrease* in Cu concentration in the CdS layer could be observed following BC processing.

Cu accumulation in the CdS layer is observed in all of the simulations, consistent with observations of real devices [4]. It is apparent from the model that both enhanced solubility and decreased diffusivity of Cu in CdS compared to CdTe contribute to this phenomenon. Without more systematic diffusion, solubility and migration measurements on thin-film materials (and diffusion couples) used in CdTe devices, it will be difficult to address this issue definitively. Nevertheless, in the simulations reported here it appears that solubility is the primary driving force for Cu accumulation in the CdS layer. This observation is consistent with the interpretation of enhanced grain-boundary segregation in CdS films, which typically have smaller grains and therefore more grain-boundary surface area per unit volume than CdTe films, is responsible for Cu accumulation in this layer.

For comparison to the simulation results, a SIMS depth profile of Cu obtained from a CdTe solar cell is shown in Fig. 6. The cell was fabricated on Tec 15 glass with vapor-transport-deposited CdTe/CdS absorber and vapor-CdCl<sub>2</sub> processed. The back contact was a sputter-deposited bi-layer of ZnTe:Cu followed by Ti, deposited at temperatures of ~325 °C and ~185°C, respectively. The Ti was removed prior to SIMS analysis.

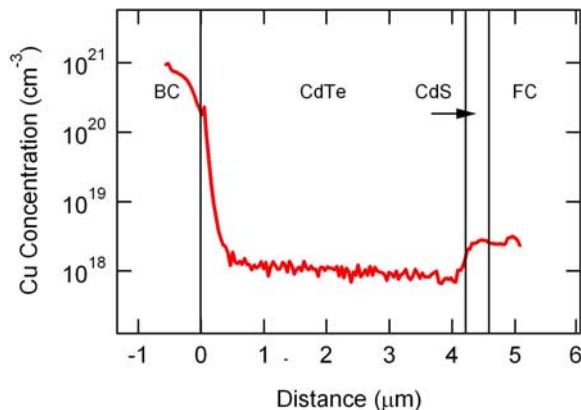


Figure 6. Typical SIMS profile of a ZnTe:Cu back-contacted device after back-contact processing.

The Cu distribution measured by SIMS is similar to the simulated high-diffusivity case. The Cu concentration in the simulation is roughly one order of magnitude lower, and the concentration in the CdS is somewhat higher, than in the SIMS profile, indicating that the parameters used in the model are not quite correct for these particular thin-films. For example, the effective solubilities in these layers

are highly dependent on grain size. Additionally, the kinetic and thermodynamic parameters controlling diffusivity and segregation in these thin-film layers might be influenced by the particular growth parameters, or other processing steps such as the CdCl<sub>2</sub> treatment. It is also important to note that artifacts in SIMS data, such as sputter-induced roughening or other morphological effects, are not accounted for in the migration model. These types of artifacts in SIMS data tend to broaden profiled, whereas the model assumes abrupt interfaces. Nevertheless, there is sufficient qualitative (or semi-quantitative) agreement between the simulations and SIMS profiles of actual devices to suggest that the segregation model captures all relevant thermodynamic driving forces for Cu migration. Further experimental data and simulations will allow the model and material parameters to be refined.

## SUMMARY AND CONCLUSIONS

An impurity migration model has been applied to Cu in CdTe PV devices using available diffusivity and solubility data. The device-processing simulations agree qualitatively with observations of Cu segregation in the CdS layer [4, 10-12], an effect attributed primarily to enhanced grain-boundary segregation in fine-grained CdS films. For the diffusivity measured in single-crystal CdTe [14], long-term stability simulations show that Cu segregation to the CdS layer equilibrates within about 15 years. The much faster diffusivity measured in polycrystalline CdTe leads to a Cu profile in the device equilibrates within weeks. These timescales are clearly relevant to discussions of device degradation in the field. However, more experiments are needed to definitively identify the dominant Cu diffusion mechanism in CdTe thin-films used for PV applications.

In order to verify and refine the Cu migration model, it would be extremely useful to measure (or re-measure) Cu diffusivities, solubilities, and segregation enthalpies for relevant thin-film PV materials. Grain boundaries are known to affect both the diffusivity and solubility of Cu in CdTe [2], and similar behavior is expected in CdS, ZnTe, etc. Therefore these properties must be measured in actual thin-film PV materials.

## ACKNOWLEDGMENTS

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<b>14. ABSTRACT (Maximum 200 Words)</b> An impurity migration model for systems with material interfaces is applied to Cu migration in CdTe solar cells. In the model, diffusion fluxes are calculated from the Cu chemical potential gradient. Inputs to the model include Cu diffusivities, solubilities, and segregation enthalpies in CdTe, CdS and contact materials. The model yields transient and equilibrium Cu distributions in CdTe devices during device processing and under field-deployed conditions. Preliminary results for Cu migration in CdTe photovoltaic devices using available diffusivity and solubility data from the literature show that Cu segregates in the CdS, a phenomenon that is commonly observed in devices after back-contact processing and/or stress conditions.						
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