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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 PV 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.

Diffusion-Segregation Model: Pseudo-Binary Diffusion Couple Formulation

Free Energy

$$A = \sum_i \left[\left(n_i X^i_{Cu}\right)\mu^i_{Cu} + \left(n_i X^i_p\right)\mu^i_p \right]$$

Chemical Potential

$$\mu^i_{\text{Cu-}p} = \frac{1}{n_i}\frac{\partial A}{\partial X^i_{\text{Cu}}} = \Delta H^i_{\text{Cu-}p} + kT \ln \frac{X^i_{\text{Cu}}}{1 - X^i_{\text{Cu}}}$$

Migration Potential

$$\Delta H^i_{\text{Cu-}p} = -\left(E^i_D + \phi^i_{\text{Cu-}p}\right)$$

Segregation Enthalpy

$$H_{\text{seg}} = \Delta H_{\text{Cu-}p} - \Delta H_{\text{Cu-}p'}$$

POhenomenological Flux Eq.

$$J_{\text{Cu}} = -M C_{\text{Cu}} \frac{\partial \mu_{\text{Cu-}p}}{\partial x}$$

Mobility

$$M = \frac{D}{kT}\frac{C_p}{C_0}$$

Migration Flux

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

Continuity Equation

$$\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x}$$

Fick's 1st Law

$$J = -D\left(\partial C / \partial x\right)$$

Migration Potential Near a Pseudo-Binary Diffusion Couple Interface

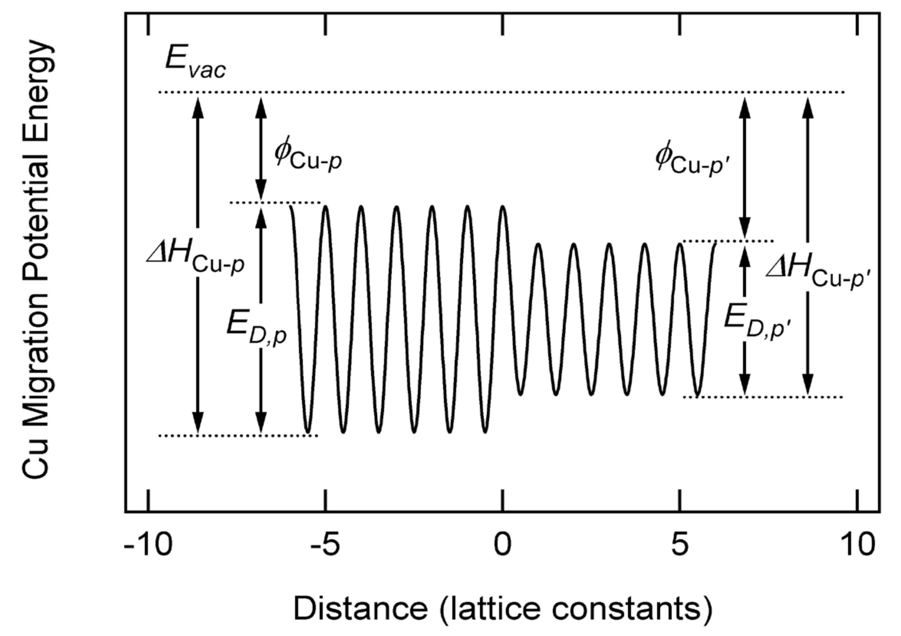

Figure 1. Schematic illustration of the ideal-solution Cu migration potential near a hypothetical material interface.

Device-Processing Simulation Results: High-Diffusivity Case

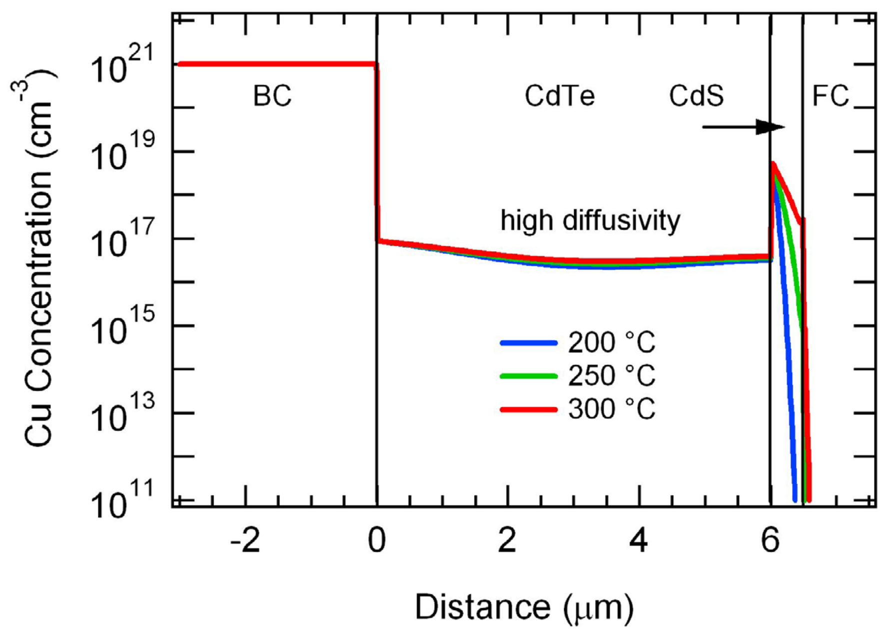

Figure 2. Device-processing simulation of Cu migration in CdTe PV device for the high-diffusivity case.

Device-Processing Simulation Results: Low-Diffusivity Case

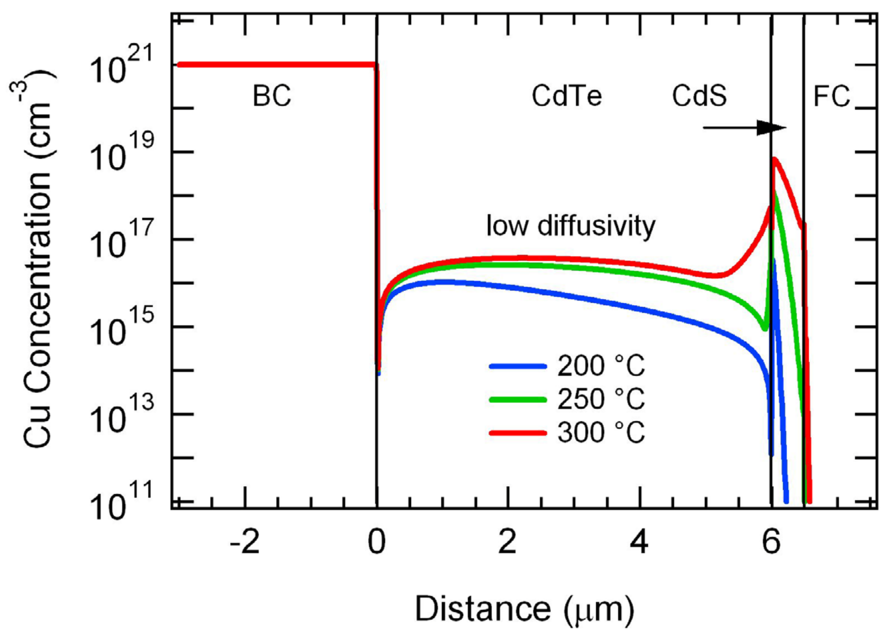

Figure 3. Device-processing simulation of Cu migration in CdTe PV device for the low-diffusivity case.

Survey of Cu Diffusivities and Solubilities in CdTe and CdS

CdTe:Cu diffusivity data				
D_0 (cm^2 s^{-1})	E_D (eV)	Ref.	SC or PX	Diffusion mode
1.70E-06	0.24	[1]		
6.65E-05	**0.57**	**[2]**	SC	low
7.30E-07	0.33	[3]		
1.30E-06	**0.29**	**[4]**	PX	high
8.20E-08	0.64	[5]		
3.70E-04	0.67	[6]		
9.57E-04	0.7	[7]		
CdTe:Cu solubility data				
C_0 (cm^{-3})	E_a (eV)	Ref.		
1.56E+23	**0.55**	**[2]**	SC	low
~2E+17	**~0**	**[4]**	PX	high
3.73E+24	0.68	[8]		
CdS:Cu diffusivity data				
D_0 (cm^2 s^{-1})	E_D (eV)	Ref.		
1.20E-02	1.05	[9]	SC	
2.10E-03	0.96	[10]	SC	
1.60E-03	0.77	[11]	SC	
—	0.95	[12]	SC	
6.00E-09	**0.5**	**[13]**	PX	
—	1.0	[14]	SC	
CdS:Cu solubility data				
C_0 (cm^{-3})	E_a (eV)	Ref.		
8.00E+21	**0.27**	**[13]**	PX	
6.60E+22	0.505	[10]	SC	

Long-Term Stability Simulation Results: High-Diffusivity Case

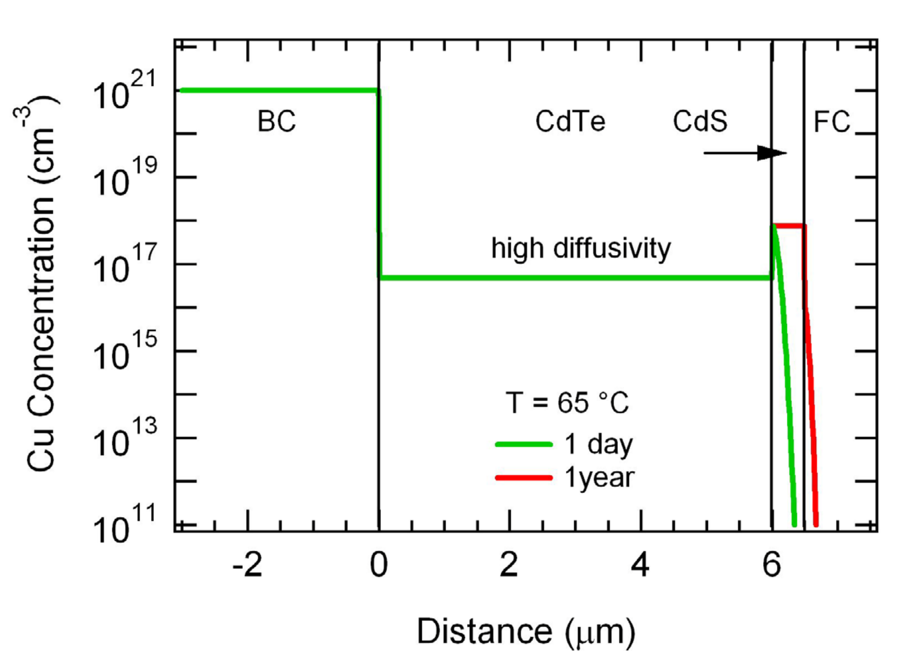

Figure 4. Long-term stability simulation of Cu migration in CdTe PV device for the high-diffusivity case.

Long-Term Stability Simulation Results: Low-Diffusivity Case

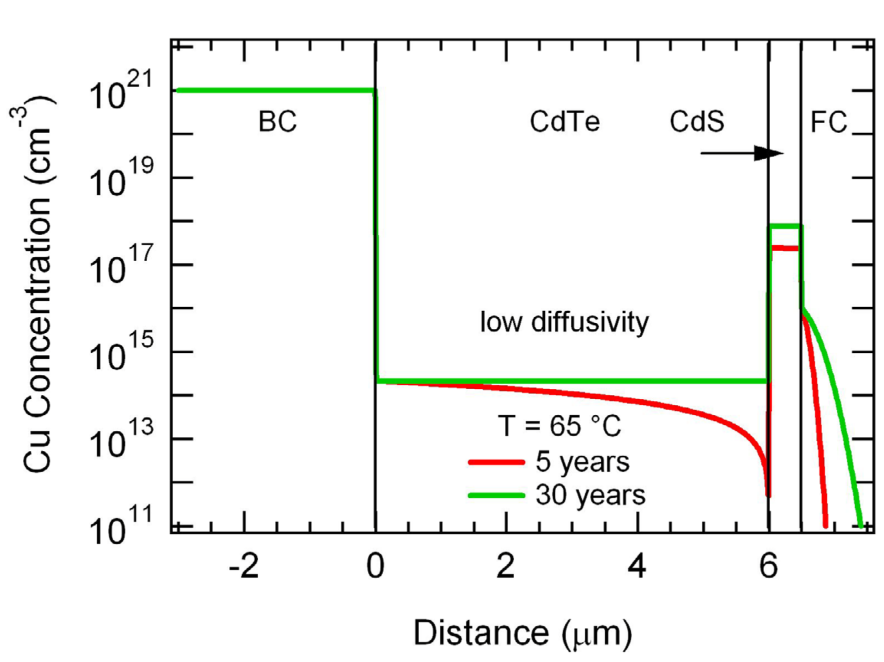

Figure 5. Long-term stability simulation of Cu migration in CdTe PV device for the low-diffusivity case.

SIMS Depth Profile

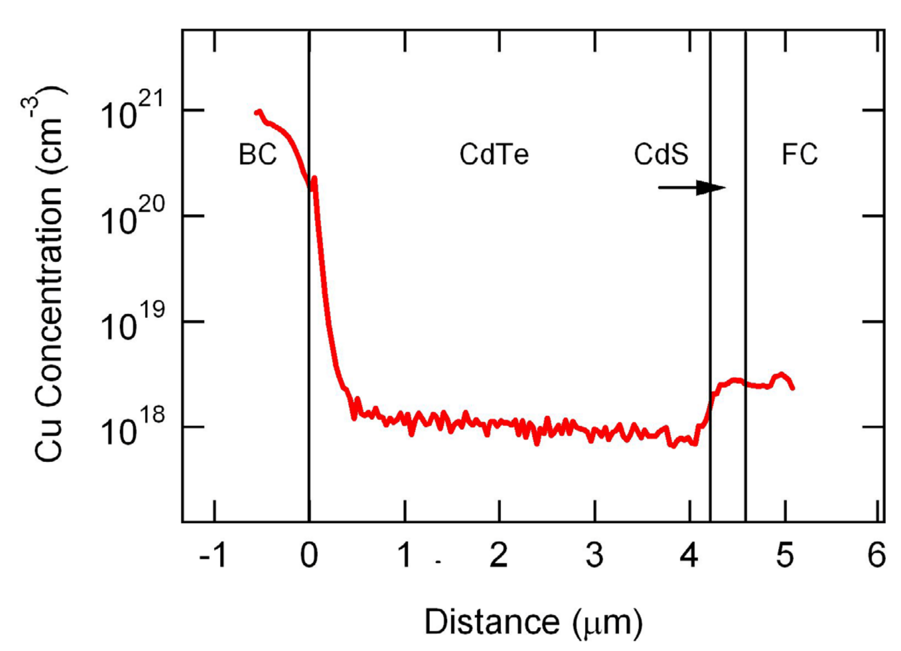

Figure 6. Typical SIMS profile of a ZnTe:Cu back-contacted device after back-contact processing.

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