Modeling Copper Diffusion in Polycrystalline CdTe Solar Cells

R. Akis[1], D. Brinkman[2], I. Sankin[3], T. Fang[3], D. Guo[1], D. Vasileska[1], and C. Ringhofer[2]

[1]*School of ECEE, Arizona State University, Tempe, AZ, USA*

[2]*School of Mathematical & Statistical Sciences, Arizona State University, Tempe, AZ, USA*

[3]*First Solar, Perrysburg, OH, USA*

e-mail: richard.akis@asu.edu

Polycrystalline thin-film CdTe solar cells are considered to be one of the most promising candidates for photovoltaic technologies due to their similar efficiency and low costs when compared to traditional Si-based solar cells. In these devices, Cu is the key dopant, defining major performance parameters such as the open-circuit voltage, short-circuit current, and filling factor by affecting the built-in potential of the junction, collection efficiency, and resistivity of the back contact [1].

In polycrystalline devices, the penetration of Cu into CdTe is dominated by grain boundary (GB) diffusion. In this work, we present two dimensional (2D) finite-difference simulations of Cu diffusion in CdTe with GBs, fitting the results to experiments.

In dealing with GBs, the Fisher model [2] is typically employed. The basic situation is shown schematically in Fig. 1, where a GB of thickness δ centered at $x=0$ is shown extending into a CdTe layer. The diffusion process is governed by two coupled diffusion equations:

$$\frac{\partial C_g}{\partial t} = D_g \left[\frac{\partial^2 C_g}{\partial x^2} + \frac{\partial^2 C_g}{\partial y^2} \right], \quad |x| > \frac{\delta}{2} \tag{1}$$

$$\frac{\partial C_g}{\partial t} = \frac{2D_g}{s\delta} \frac{\partial C_g}{\partial x} + D_{gb} \frac{\partial^2 C_g}{\partial y^2}, \quad |x| < \frac{\delta}{2} \tag{2}$$

where D_g and D_{gb} are the diffusion coefficients of the grains and GBs respectively. C_g is the grain concentration. The GB concentration, C_{gb} has been eliminated by making the substitution $C_{gb} = s\, C_g$, where s is the segregation factor, which in general can be much larger than one. One significant problem with the Fisher model is that δ generally cannot be independently determined and is a source of ambiguity. In mapping the problem onto a rectangular finite difference lattice, we have found that δ can be eliminated. In terms of the lowest order finite difference approximations, the above differential equations can be replaced by:

$$\left(C_g\right)_t = D_x \left(C_g\right)_{xx} + D_y \left(C_g\right)_{yy} \tag{3}$$

$$\begin{aligned} D_x = D_g / s, \, D_y = D_{gb}, & \quad x = 0 \\ D_x = D_y = D_g, & \quad x \neq 0 \end{aligned} \tag{4}$$

Fig. 2 shows the results of a 2D simulation. The domain represents one unit cell which is approximately the average size of the grains in the direction parallel to the interfaces. Fig. 3 shows the average Cu concentration over the cell, which is used to directly compare with experimental results. There are three important regions: the bulk region, from which D_g can be determined; a GB dominated "tail" from which information about D_{gb} and s is usually extracted via fitting to approximate analytical formulas [3]; and a fast surface diffusion region, which can be treated in a similar manner to the GBs[4]. Fig. 4 shows diffusion coefficients obtained by fitting to experiments done at different temperatures. To conclude, we note that our numerical approach not only eliminates the ambiguous "GB thickness" parameter, but can also be used to determine diffusion coefficients more accurately than the usual analytical models.

ACKNOWLEDGMENT

REFERENCES

[1] B. Tetali, V. Viswanathan, D. L. Morel and C. **S.** Ferekides, *Effects of thermal stressing on CdTe/CdS solar cells*, Proceedings of 30th IEEE Photovoltaic Specialist Conference,600 (2002).

[2] J. C. Fisher, *Calculation of Diffusion Penetration Curves for Surface and Grain Boundary Diffusion*, J. Appl. Phys. **22**, 74 (1951).

[3] I. Kaur, Y. Mishin and W. Gust, *Fundamentals of Grain and Interphase Boundary Diffusion (Wiley, Chichester, 1995)*.

[4] G. H. Gilmer and H.H. Ferrell, *Grain Boundary Diffusion in Thin Films. II. Multiple grain boundaries and surface diffusion*, J. Appl. Phys. **47**, 4373 (1976).
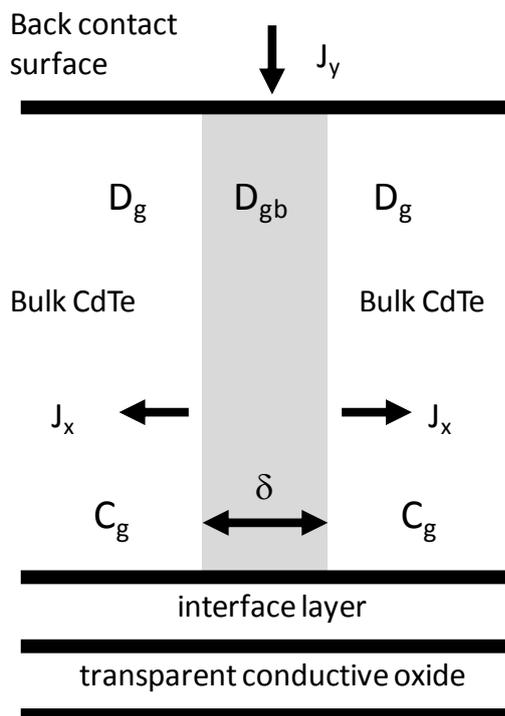
Fig. 1. Geometry illustrating bulk CdTe grains separated by a grain boundary. A flux of Cu dopants, J_y comes in from the back contact. Since $D_{gb} \gg D_g$ in most instances of interest, diffusion along the grain boundary is much faster than in the grain. Here J_x represents the leakage flux of Cu dopants from the grain boundary back into the grains.
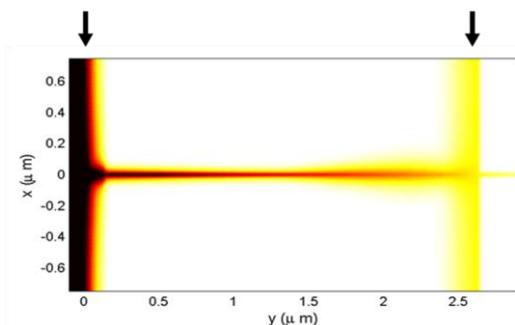

Fig. 2. The results of a two dimensional simulation with the darker shading corresponding to higher Cu concentration. The diffusion parameters were chosen to fit an experiment where a CdTe device was annealed at 260 C for 6 minutes. Beyond the basic grain boundary model, the effect of rapid surface diffusion is taken into account at the CdTe end. In essence it acts as a perpendicular grain boundary. In order to compare with experiments, which typically give an *average* Cu profile, one must average these results along the *x* direction (the vertical direction in this plot). Arrows indicate locations of absorber interfaces (back contact/CdTe on the left and CdTe/interface layer on the right).
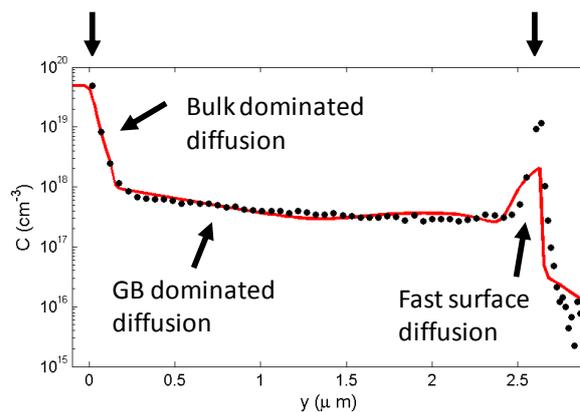

Fig. 3. Overlaid simulated data (taken from averaging the results in Fig. 2) and measured profiles of the *average* Cu concentration in the CdTe absorber as a function of depth. Arrows indicate locations of absorber interfaces (back contact/CdTe on the left and CdTe/interface layer on the right).
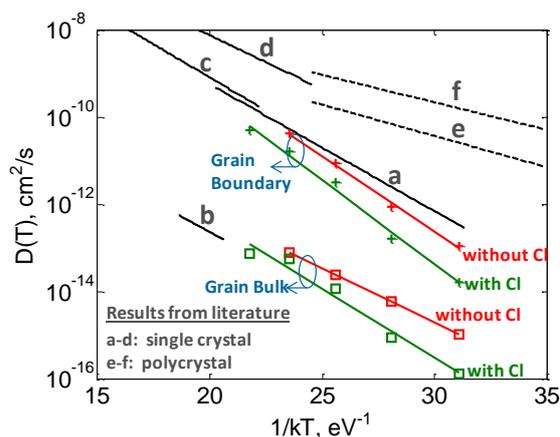

Fig. 4. Diffusion coefficients are plotted as a function of 1/kT. Simulations were performed to extract Cu diffusion parameters for the CdTe bulk and GBs from two sets of experiments with and without Cl treatment. The results are plotted as indicated. For comparison, several sets of data for single crystal and polycrystalline CdTe obtained by other groups are also given.