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Diffusion study of metal precursor layers for CZTS solar cell

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The core of a CZTS solar cell is the p-type absorber layer that gives this type of solar cell its name. It consists of copper, tin, zinc and sulfur in a single crystal structure: $\text{Cu}_2\text{ZnSnS}_4$. In this study two methods are investigated to deposit the copper, zinc and tin as precursor layers for the formation of the $\text{Cu}_2\text{ZnSnS}_4$ layer, namely electroplating and electron beam evaporation. One of the advantages of CZTS solar cells is that the constituent elements are a lot more common and less toxic than what are usually used in other types of solar cells. The elements used in the solar cell itself is only one half of the picture, one also needs careful consideration of the methods and chemicals used during the manufacturing. This is why reline, an environmentally friendly deep eutectic solvent, is used as the electrolyte during electroplating. The 3 metals were deposited in the correct stoichiometric ratio in different sequences on Mo coated glass, and then annealed in vacuum. To estimate annealing times and temperatures, Fick's diffusion equation was solved [1] for a finite diffusion region with finite diffusion source:

$$C(x,t) = \frac{1}{2} C_0 \left[\text{erf} \left(\frac{h+2nL-x}{2\sqrt{Dt}} \right) + \text{erf} \left(\frac{h-2nL+x}{2\sqrt{Dt}} \right) \right]$$

From the calculated depth profiles the annealing times and temperatures were chosen 500 K, 550 K, 650 K and 725 K, all for 1 hour. The annealed samples were characterised using Auger Electron Spectroscopy depth profiling, and from these depth profiles the inter-diffusions were calculated. .

[1] J Crank, The Mathematics of Diffusion, 2nd edition, (1975)

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