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DESIGN OF A CHEMICAL REACTOR FOR INVESTIGATING THE DEPOSITION OF NOVEL SULFIDE SEMICONDUCTOR COATINGS

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Copper Bismuth Sulfide (CBS) is a semiconductor that shows promise as a photovoltaic material. It is formed from inexpensive and relatively abundant elements, is non-toxic and can be made in atmosphere at a low temperature. In order to make a solar cell, one needs a dense and even layer of the photovoltaic material. We have been successful in making CBS in a simple solvothermal process and we are now evaluating how to grow a dense layer of CBS directly from solution on fluorine-doped tin oxide (FTO) coated glass. To perform this evaluation we designed a small benchtop reactor having a linear temperature gradient across the flow/deposition zone. COMSOL Multiphysics was used to simultaneously model mass and heat transfer within the reactor design.

One important aspect of this flow through reactor is the implementation of a well-defined temperature gradient. Since this reactor was meant to help determine the best conditions for CBS deposition to occur, a known, linear temperature gradient would allow us to test many conditions at once. Utilizing COMSOL simulations, we designed a flow chamber and coupled heating arrangement to achieve both uniform flow and a linear temperature gradient of the desired temperature range within the chemical reactor. An image demonstrating this is seen in Figure 1. Flow uniformity was enhanced by small channels of high flow resistance feeding into the deposition area of the reactor. The temperature gradient was provided by placing the reactor in contact with an aluminum bar, which was heated at one end and cooled at the other.

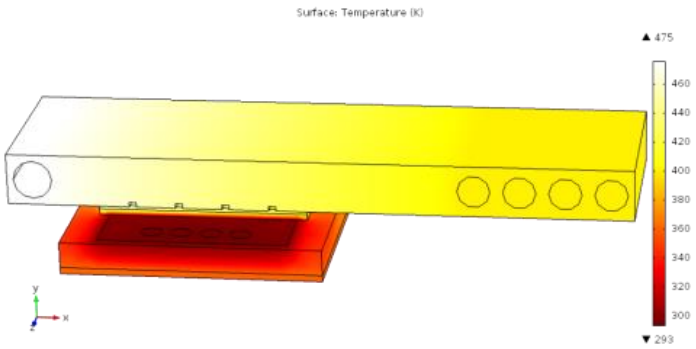

Figure 1. COMSOL simulated image of the temperature of the reactor. White is hottest, dark red is coolest.

This reactor design relied on the liquid passing through it being able to heat up to its reaction temperature in the time it takes for the liquid to pass the FTO. COMSOL was used to simulate the velocity of the liquid, as well as the temperature profile at the surface of the FTO, taking into account the properties of the solvent and all materials used in the construction of the reactor. The simulations showed that the design enabled the liquid to reach the required temperature within the flow/deposition zone for certain heating and cooling rates. The simulated results of the temperature gradient can be seen in Figure 2.

This reactor has been constructed and operated under different deposition conditions, and yielded improved CBS microstructure in the deposited samples. We will present a combination of the computational work on reactor design, experimental validation of the simulations, and a rundown of the experimental observations on coating growth in the new flow-through reactor.

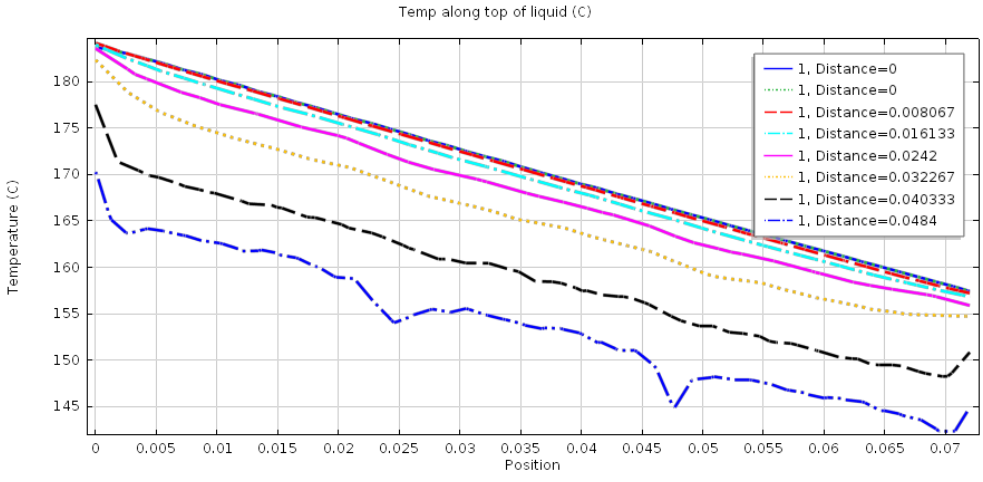

Figure 2. COMSOL simulation of the temperature gradient present in the liquid as it is passed under the heating element.