BAPVC Annual Project Report

Project Title: Grain Boundary Engineering in Solution-Processed CdTe Solar Cells
PI: A. Paul Alivisatos
E-mail: alivis@berkeley.edu

Summary:
The Alivisatos group has developed a new method for systematically controlling the grain structure in thin film CdTe solar cells. By printing successive layers of nanocrystal inks, we are able to make films in which a single grain spans the thickness of the device. First, the group synthesized a CdTe-Cl nanocrystal building block. By controlling the concentration of the nanocrystal solution and the number of layers in a layer-by-layer sintering method, they have shown that the resulting film morphology can be tuned from a grainy, porous structure, to a dense film with columnar grains. Solar cells incorporating the columnar film exhibit nearly a 10-fold improvement in efficiency improved over devices incorporating grainy films.

Key Accomplishments:
Cadmium telluride (CdTe) solar cell performance relies on the CdTe film microstructure. The most efficient devices require exposure to chloride in a multistep process making grain structure control difficult. The Alivisatos group is seeking to engineer a CdTe nanocrystal (NC) building block that can be deposited from solution and subsequently sintered as a method to control film microstructure for device optimization.

The Alivisatos group has successfully synthesized a solution stable building block. This carefully designed material is a CdTe NC decorated with surface chloride, seen in the far left of **Fig 1**. The nanocrystal is colloidally stabilized with octylamine, a labile ligand that is removed upon heating above 300°C. The group has shown that the CdTe-Cl building block solution can be deposited and subsequently sintered into a film with grain size range 50-150 nm at a low temperature and quick time of 350C and 30s, also shown in **Fig 1**.

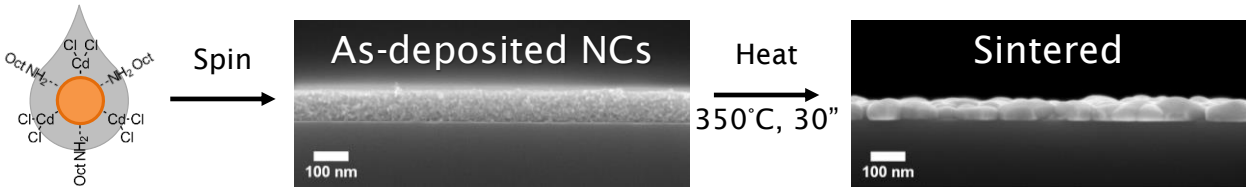


Figure 1: Sintering scheme of a single layer of deposited CdTe-Cl NCs; center and right images: SEM

The Alivisatos group has demonstrated film morphology control by controlling the NC concentration ([NC]). CdTe films were sintered into thick films by a layer-by-layer process as illustrated in the first row of **Fig 3**. First, a NC layer is deposited from solution and sintered. The consecutive NC layer fills the voids and upon sintering and increases the film thickness. Grain morphology in these films was manipulated by changing the [NC] as shown in Fig 2. Solutions with high [NC] produced porous and grainy films while low [NC] yielded continuous films with a columnar grain structure.

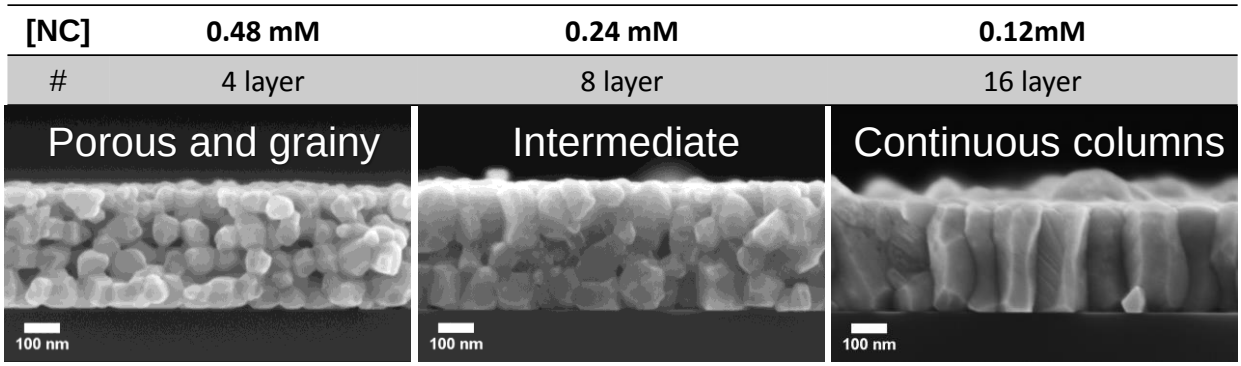


Figure 2: Cross sectional SEM images showing grain morphology as a function of [NC].

The Alivisatos group has established the relationship between grain structure and solar cell performance. Since grain boundaries disrupt charge transport in crystalline materials, the group hypothesized that devices incorporating columnar films will have better performance than those with a grainy texture. The group fabricated simple devices in which the CdTe layer was deposited on an ITO substrate, paired with n-ZnO and capped with aluminum (see **Fig 3** for scheme.) Solar cells with a columnar film performed up to 10x better than devices with a grainy structure, as shown in **Fig 4**. To increase hole transport, solar cells with columnar films sintered in air (oxygen source, facilities p-type doping) provided an addition boost to performance and double the device efficiency.

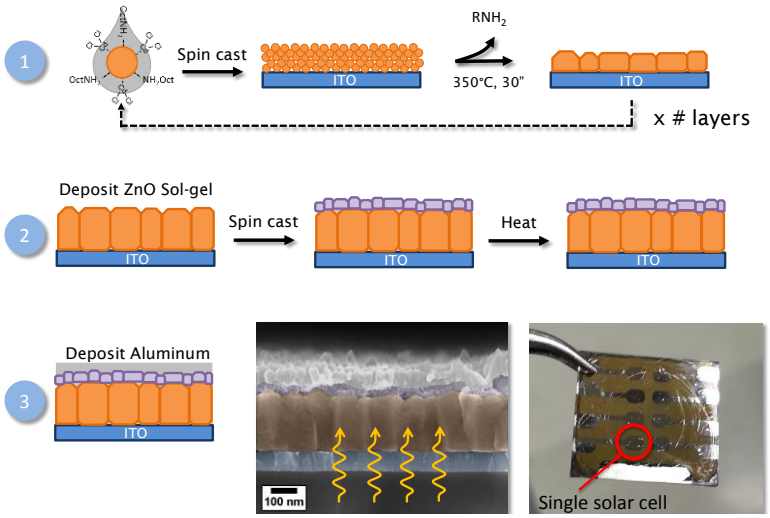
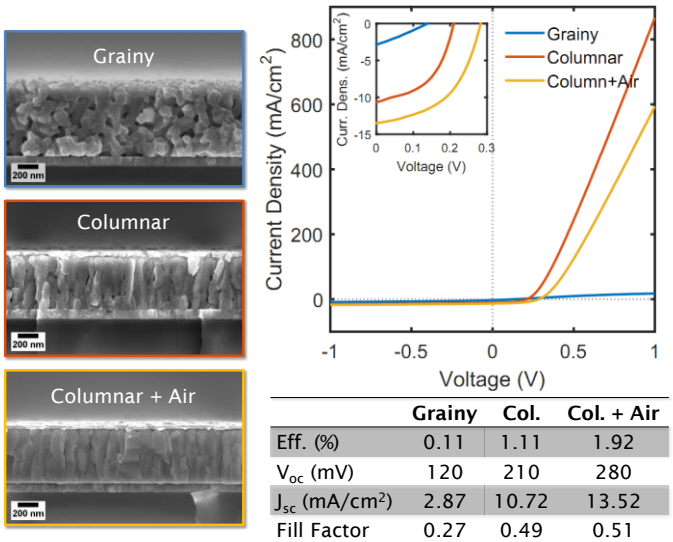


Figure 3: Solar cell fabrication scheme



	Grainy	Col.	Col. + Air
Eff. (%)	0.11	1.11	1.92
V_{oc} (mV)	120	210	280
J_{sc} (mA/cm²)	2.87	10.72	13.52
Fill Factor	0.27	0.49	0.51

Figure 4: Solar cell device performance

Future Work:

The next steps in this project is to optimize the sintered CdTe films for solar cells. We have a CdTe-Cl building block that can be sintered layer-by-layer into continuous, columnar films. Devices will be optimized using column width and doping profiles. We will modulate column width using sintering temperature. For doping, we will look to oxidation regents that can be added to the solution instead of air such as pyridine oxide. Film structure and composition will be characterized by EDS and XRD while performance will be characterized by scanning probe techniques such as kelvin probe and c-AFM.