Improving the accuracy of novel materials screening: growing defect-tolerant photovoltaic absorbers

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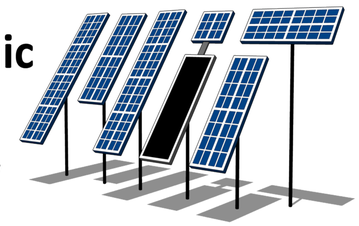
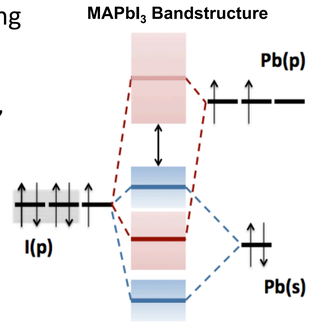
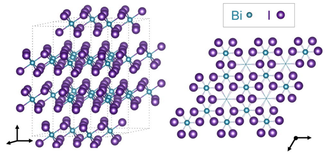
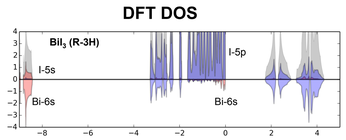


Background: Materials Search and BiI_3

- We have proposed a materials screening methodology focusing on transport in addition to optical properties [1]
- We computationally screen for "proxy" properties that enable high lifetime including antibonding VBM
- As a first test case, we synthesized BiI_3 [2] in two different vapor transport systems







- In an effort to develop best practices for rapid experimental screening that avoids false negatives, we investigate the effects of different growth conditions on film structure and properties

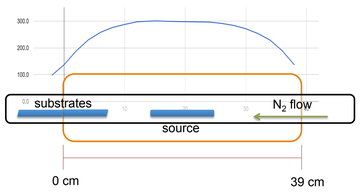
1. R. E. Brandt, *et al.*, MRS Communications, 1-12 (2015). DOI: 10.1557/mrc.2015.26
2. R. E. Brandt, R. C. Kurchin, *et al.*, J. Phys. Chem. Lett., 4297-4302 (2015). DOI: 10.1021/acs.jpclett.5b02022

Vapor Transport Growth Systems

Process parameters: temperature set point(s), substrate material, substrate position(s), N_2 flow rate, background pressure

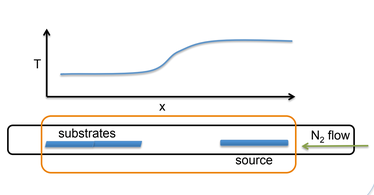
[grey text = parameter was not varied in this study]

One-Zone Furnace



- Allows "combinatorial" deposition across range of substrate temperatures
- Properties highly dependent on precise positioning of substrate

Two-Zone Furnace

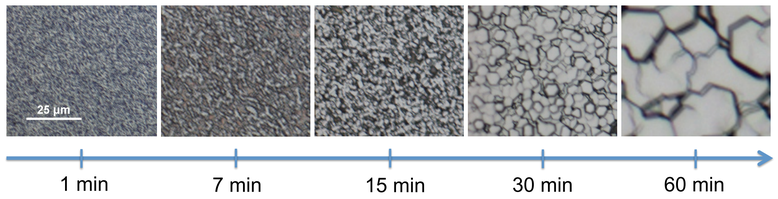


- Larger uniform temperature region
- Allows more precise control and greater uniformity/ reproducibility

In both systems, high-temperature growth is limited by reevaporation. However, the reproducibility afforded by the two-zone apparatus makes it preferable overall.

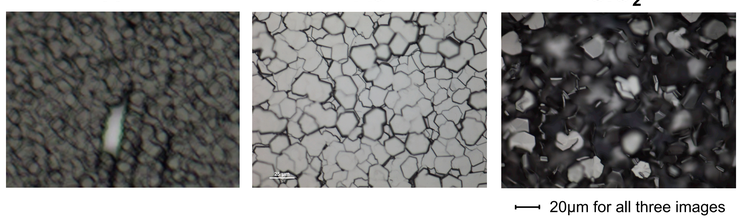
Effects of Process Parameters on Growth Kinetics

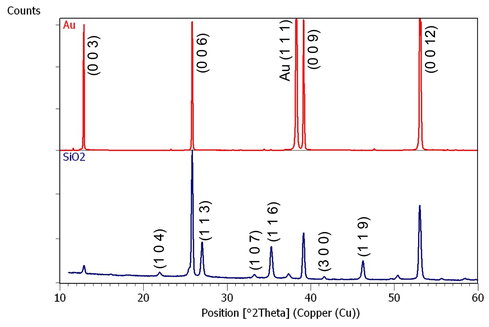
Growth Time



On gold substrates (shown above), there seems to be dense nucleation followed by competitive growth such that grain size on the surface gets larger as the film thickens.

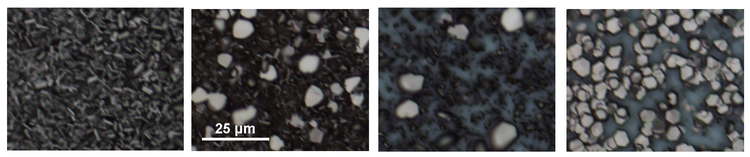
Substrate Choice





Substrate effects include CTE mismatch, nucleation density, and preferred orientation

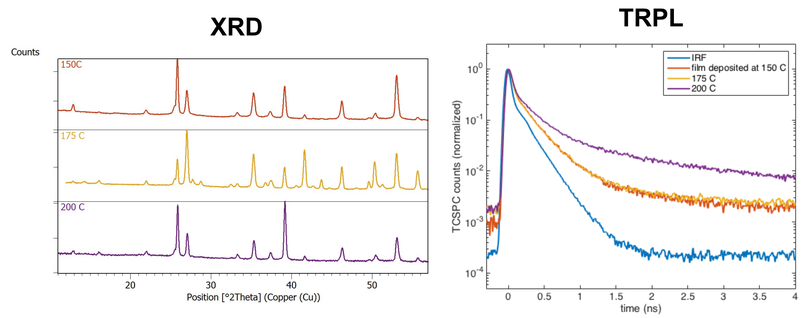
Position within Furnace Tube (Two-Zone)



A vapor transport setup in this geometry inherently samples different source partial pressures – and in the one-zone scheme, this is convoluted with growth temperature as well.

Optoelectronic Properties

Effect of Growth Temperature



Higher growth temperature leads to longer carrier lifetimes.

Next Steps

- We hypothesize that higher lifetimes are due to lower intragranular structural defect density – but we need a way to quantify this!
- Further experimentation with growth conditions and substrate choice are desirable to grow compact, continuous films that would be appropriate for devices
- Measure band offsets and perform device modeling to determine optimum device architecture
- Make devices to measure I-V characteristics, QE, etc.

Conclusions & Acknowledgements

- We designed a growth system and explored the effects of various process parameters on properties of interest in the resulting thin films
- Best practices (primarily, to grow at highest achievable deposition temperature) will be incorporated into future materials screening efforts

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