UCI center for solar energy | SCHOOL OF PHYSICAL SCIENCES

Growth and Characterization Update

March 2011 Pyrite Meeting

Meeting schedule

1:00	Growth & Char. Update	Matt
	Growth Modeling	Arvind
	Growth Modeling II	Solmaz
	Surface DFT	Yanning
	Bulk DFT	Jun
	X-ray Characterization	Ming

Thin Film Growth Activities

CVD

- good ~1 cm^2 pyrite films on glass (test substrate) and molybdenum-coated glass (device substrate)
- not yet successful in scaling up to larger substrate sizes
- conclusive evidence that sodium favors pyrite growth
- strong evidence for homoepitaxial growth of pyrite on thin pyrite layers, even with conditions that normally give marcasite → avoids the need for sulfur annealing

Thin Film Growth Activities

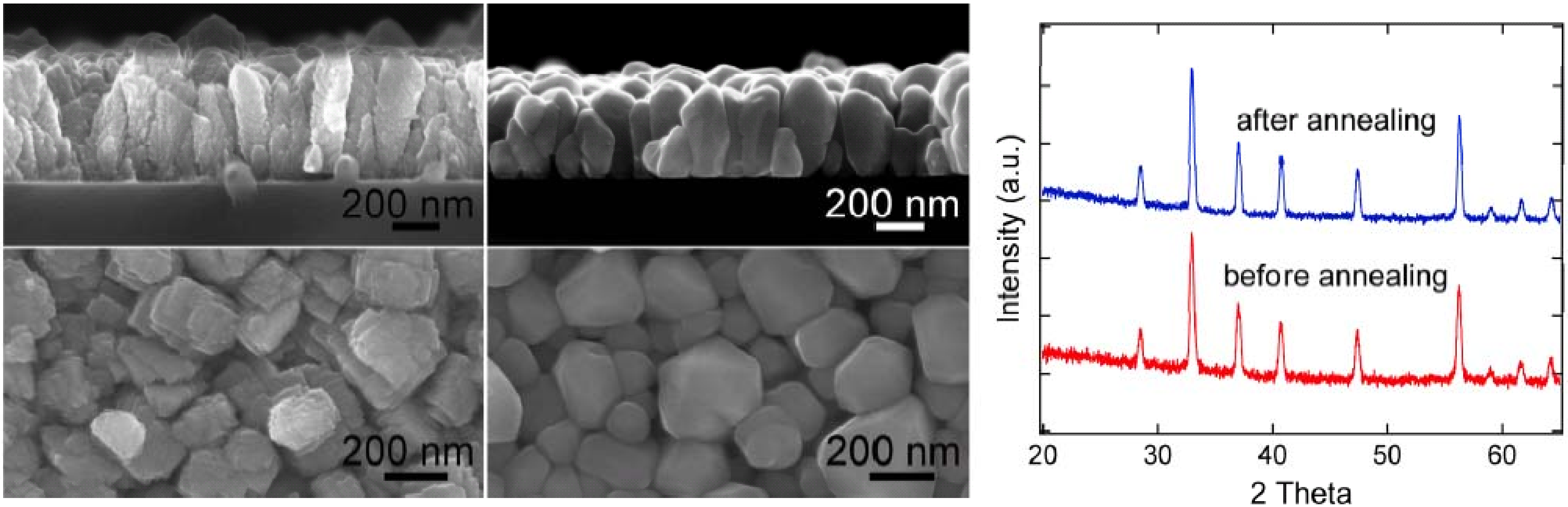


Figure 7. Preliminary data. SEM images of a pyrite thin film grown by CVD on glass before (*left*) and after (*middle*) sintering at 500°C in S_2 vapor. XRDs (*right*) show the film remains pure pyrite.

Thin Film Growth Activities

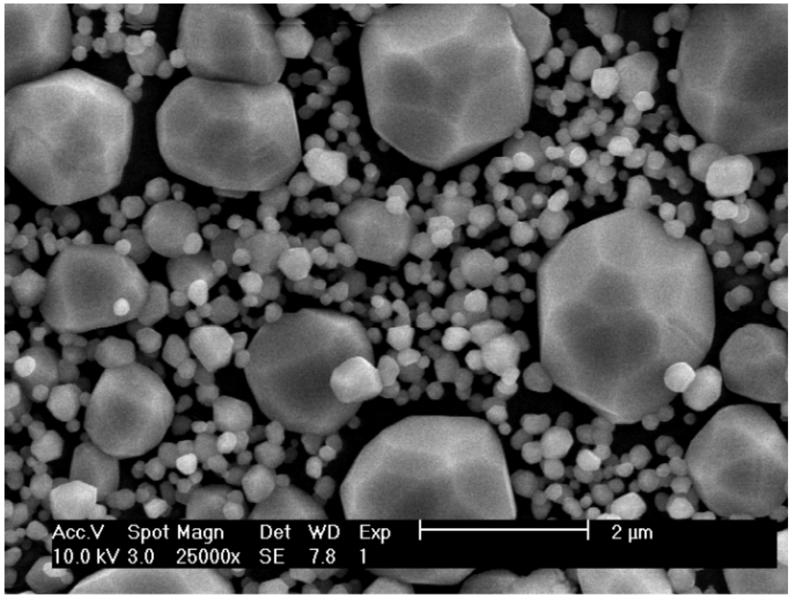
CVD cont.

- proceeding with optical (UV-Vis, PDS, SE) and electrical (Seebeck, conductivity) characterization of optimized films

- Hall effect experiments are unsuccessful (in-plane mobility too low) → attempting Hall measurements on individual grains

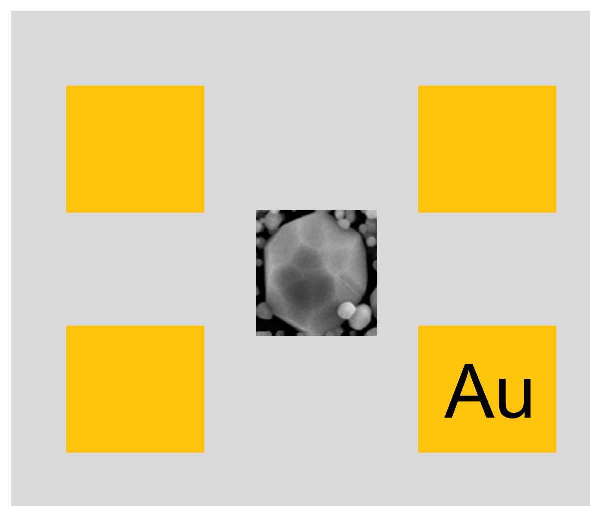
- starting to make solar cells based on FeS_2/ZnS and FeS_2/CdS junctions

Single Grain Hall Measurements

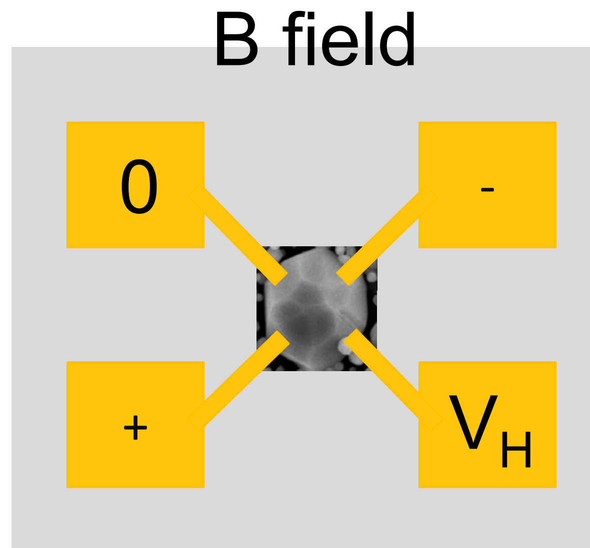


sonicate
into solution

drop cast
onto pre-patterned
electrode set



FIB contacts
and measure



Initial Solar Cell Design

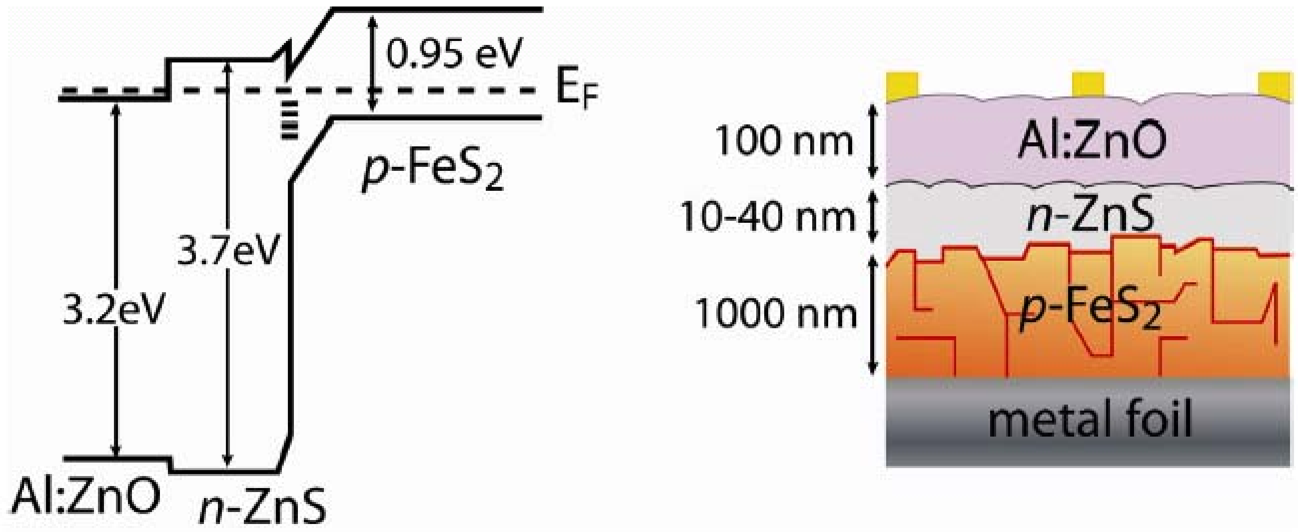
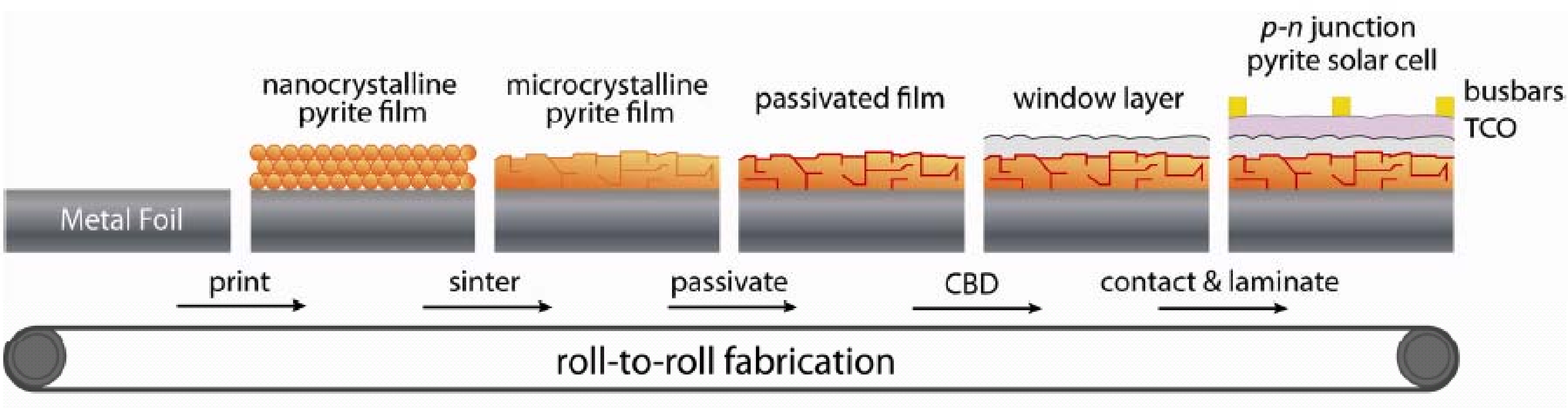


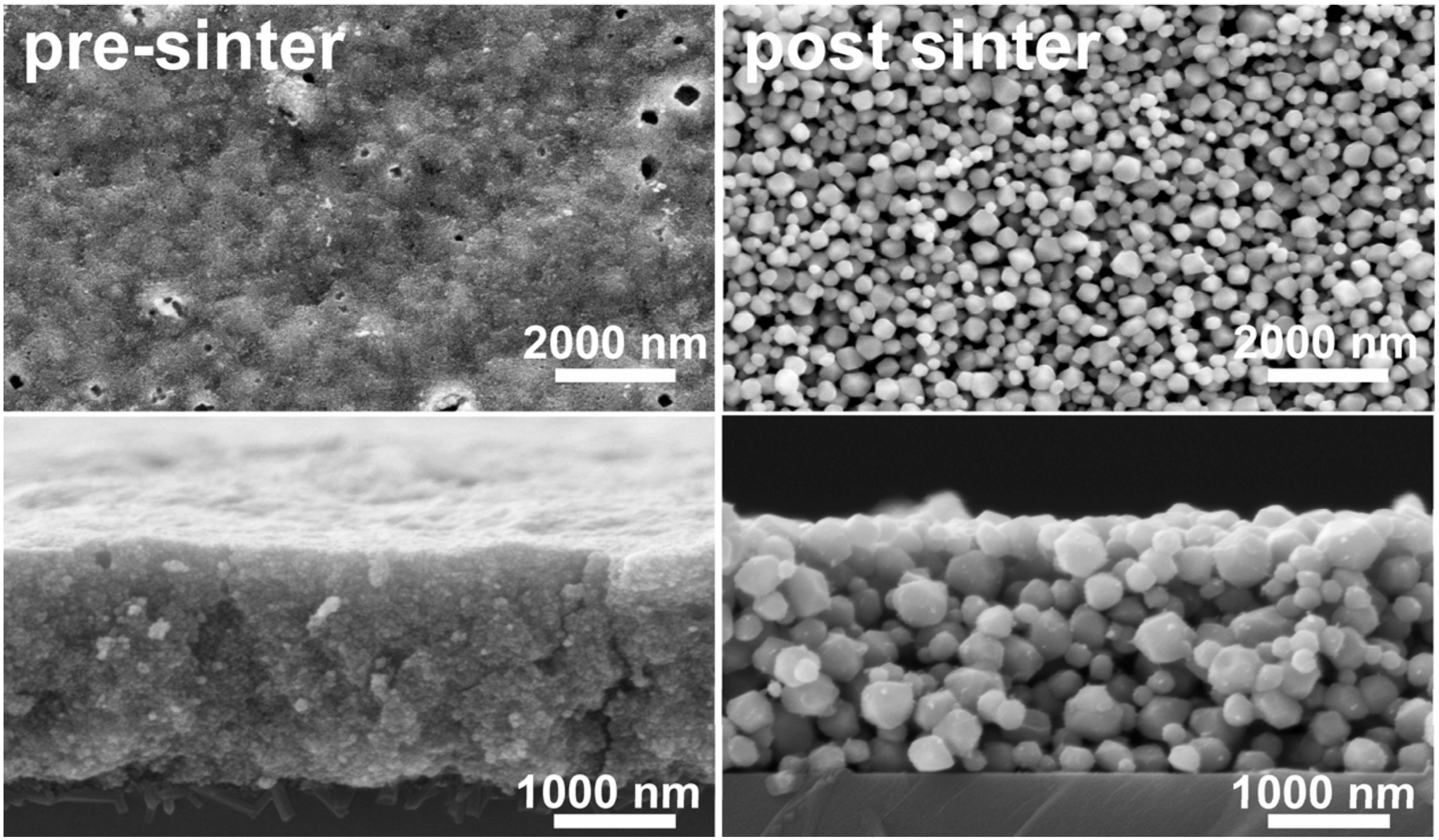
Figure 2.7. (*left*) Band diagram of the heterojunction cell. (*right*) The device structure.



Thin Film Growth Activities

Nanocrystal ink

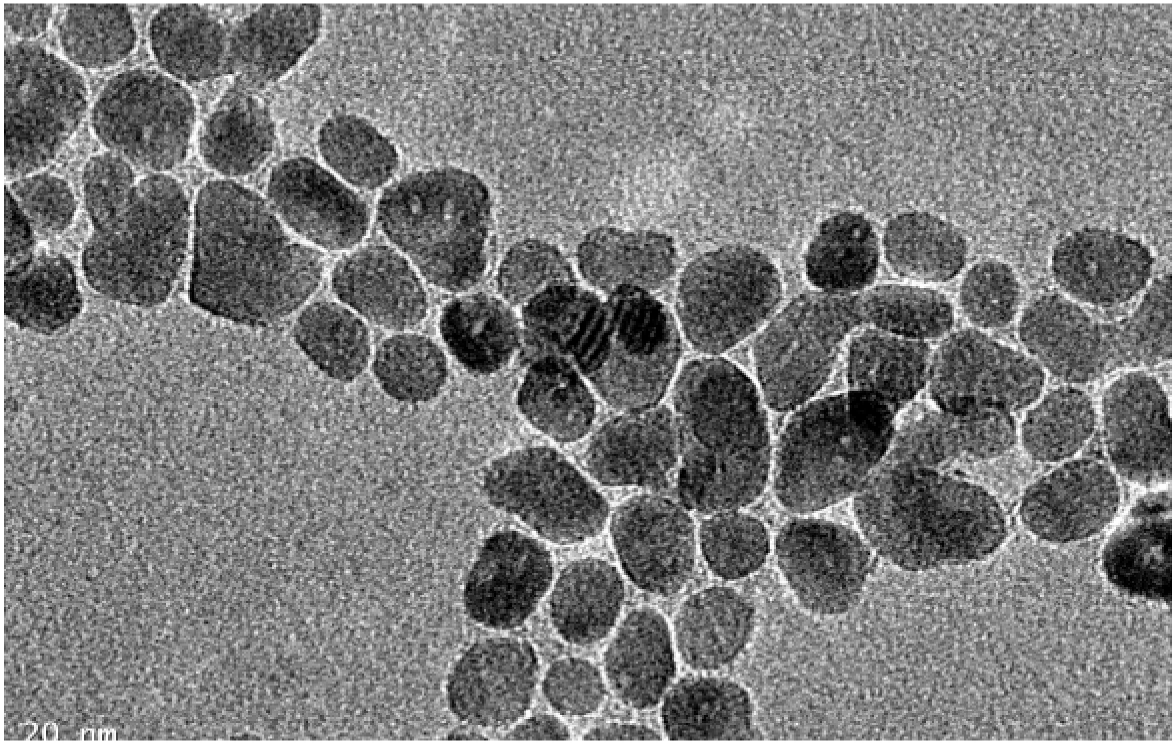
- little progress since first paper (January)



Thin Film Growth Activities

Nanocrystal ink cont.

- Solmaz and Sean will study the sintering of pairs of nanocrystals by SEM to assist the modeling effort



Thin Film Growth Activities

Molecular inks

Fe-S ink

Form mixture of DMSO and ethanolamine (6.5:1)

↓

Dissolve S (1 M) in solution and stir for >6 hours (at room temp)

↓

Add Fe (0.33 M) and stir for >24 hrs.

↓

Spin coat at 1500 rpm for 60s

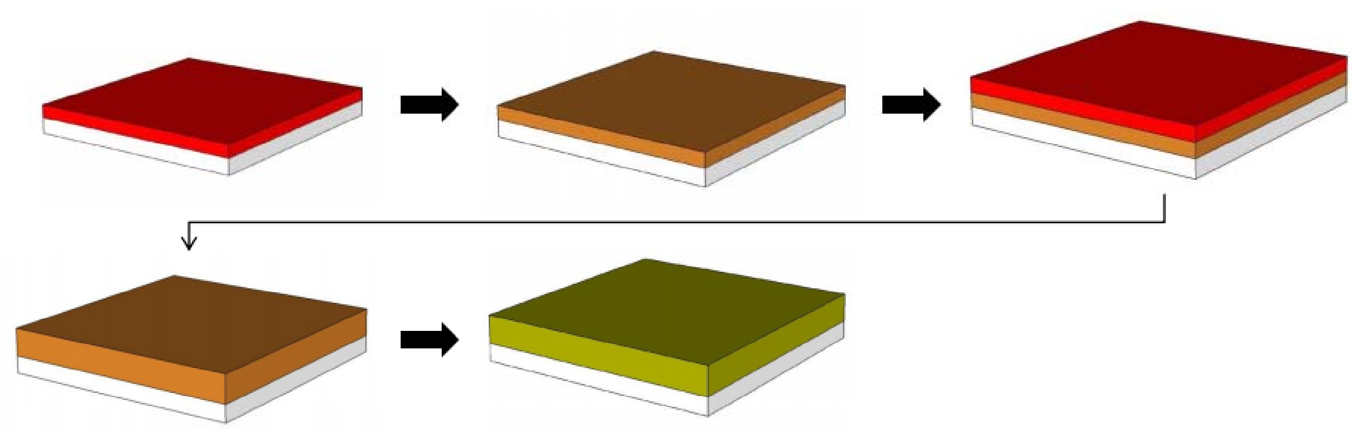
↓

Pre-bake on hotplate at 200 ℃ for 5 min.

↓

Anneal in S (25 mg) at 550 ° C for 6 hours

$Fe(acac)_3$ ink



- Iron (III) Acetylacetonate molecular ink is coated onto a glass slide
- The layer is then baked in air at 350 C for 30 minutes to form an amorphous iron oxide layer
- This process can be repeated to build varying thicknesses of films
- The final film is then converted to pyrite with either H_2S or S_8 annealing

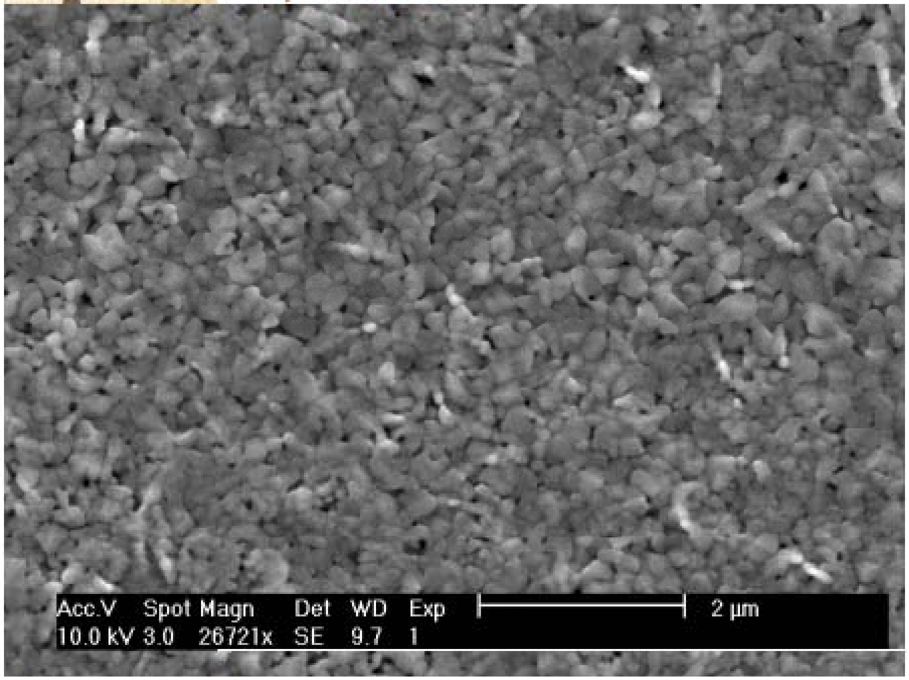
Thin Film Growth Activities

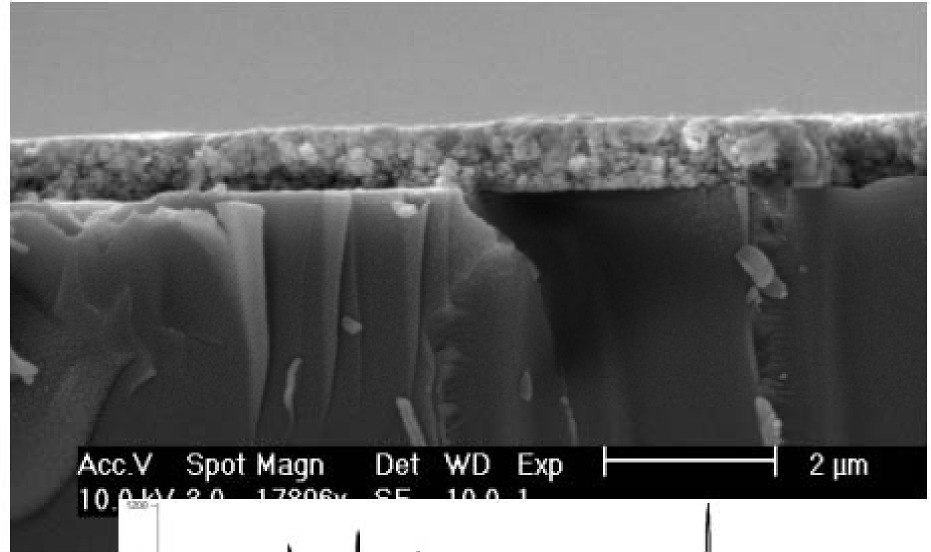
Molecular inks

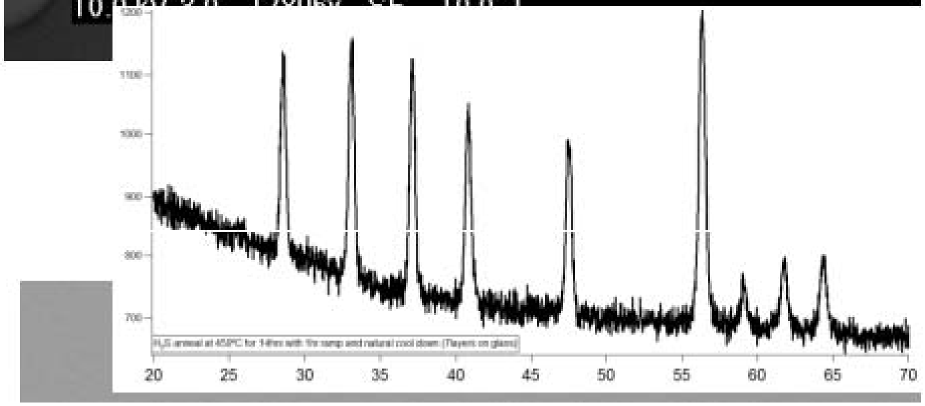
- large grain, rough, often porous films with sulfur annealing at relatively high temperatures (>500°C)
- denser, more uniform pyrite films with H_2S annealing at lower temperatures (350-450°C)
- annealing on glass gives pure pyrite (sodium effect)
- conditions for Mo-coated glass now being worked out

*Initial goal is to dial-in conditions for good films of any thickness on either substrate, then characterize them fully and start making junctions.

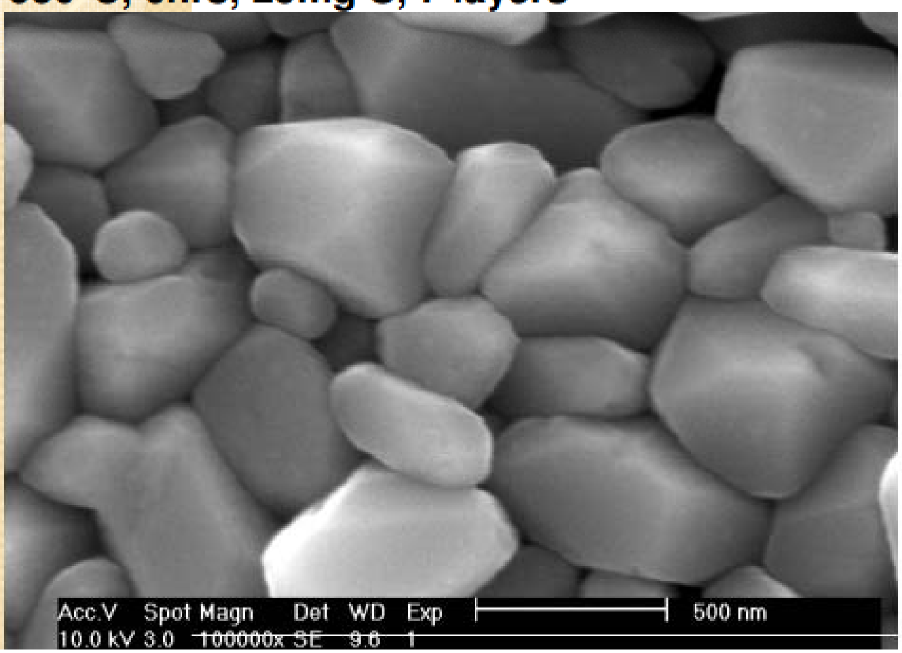
H_2S 450°C, 15hrs

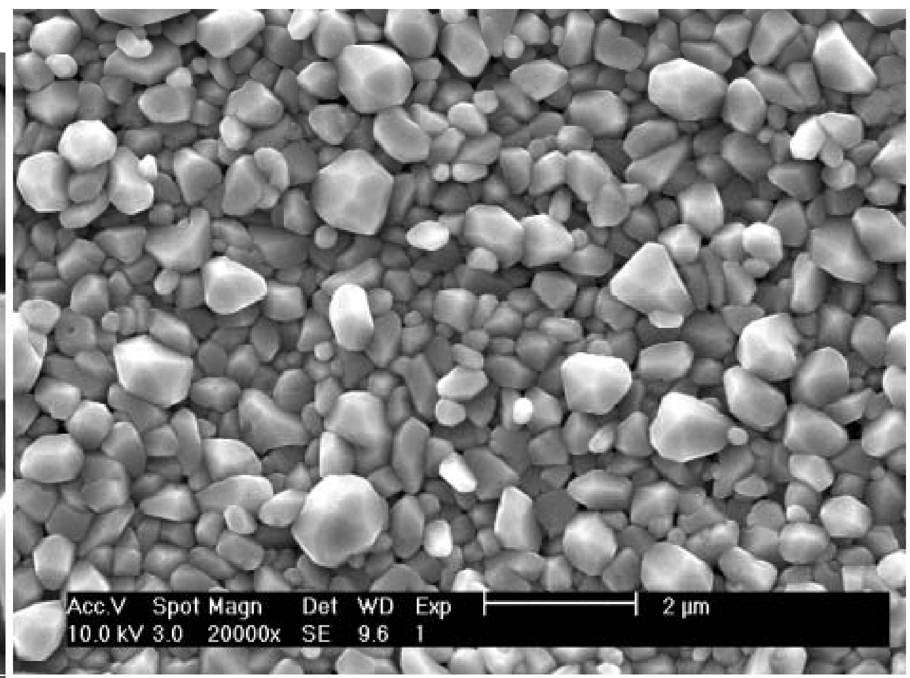






550°C, 6hrs, 25mg S, 7 layers





Thin Film Growth Activities

Molecular inks cont.

- Fe-S ink is our best shot at making very pure pyrite films (no C, O, halogens). We will determine Fe:S with RBS and impurity concentrations with SIMS and ICP-MS (Evans Analytical)

- adding Na_2S to the ink favors pyrite growth

- initial results show that adding zinc to the ink may be making $Fe_{1-x}Zn_xS_2$ (as hoped), but more data needed

- paper on initial aspects of this work in the spring