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 cm² 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
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 S₂ vapor. XRDs (right) show the film remains pure pyrite.
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

B field

FIB contacts and measure

http://cfse.uci.ps.edu
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)
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°C 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 H₂S or S₈ annealing
**Molecular inks**

- large grain, rough, often porous films with sulfur annealing at relatively high temperatures (>500°C)

- denser, more uniform pyrite films with H₂S 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.*
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$_2$S to the ink favors pyrite growth.

- initial results show that adding zinc to the ink may be making Fe$_{1-x}$Zn$_x$S$_2$ (as hoped), but more data needed.

- paper on initial aspects of this work in the spring.