SAND2007-6462P

Synthesis and Characterization of Gallium Alkoxides

James Griego, Timothy J. Boyle, Timothy N. Lambert, Leigh Anna M. Ottley, Harry D. Pratt

Advanced Materials Laboratory

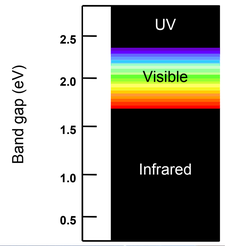
Sandia National Laboratories

Introduction:

Gallium based materials are used in many different systems of semiconductors and thin film photovoltaics. This project has been focused on the development of novel Ga precursors in the form of alkoxides and chalcogenides for these types of systems. Nanoparticle synthesis will also be discussed, concerning the synthesis, processing, and the various effects on the final nanoparticles morphologies.

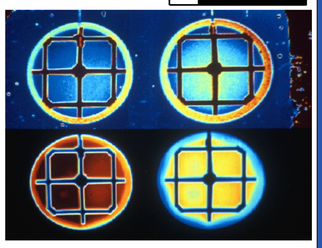
Solar Cells being utilized:

- Most solar cells are made using silicon
- The problem at hand:
  - silicon is highly inefficient
  - collects light at a narrow spectrum (1.1 eV)



Solar Cells of interest to Sandia:

- Those which utilize a large spectrum of light
- Good semi conducting capabilities with good band gaps
- Those of thin film nanoparticles: high surface area is achieved



CdS/CuInSe2 thin film solar cells
Sawvas Damaskinos, Alfonso Ribes
University of Waterloo

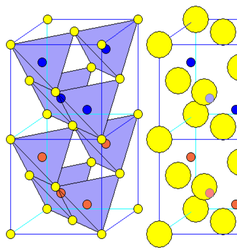
Sandia's Approach to Better Solar Cells:

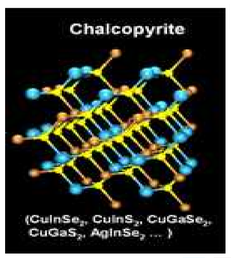
Chalcopyrite:

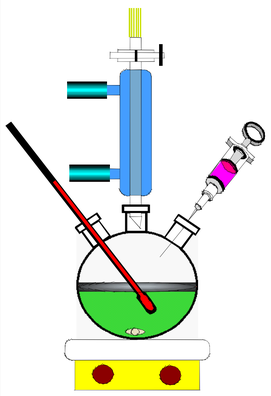
- Cu based chalcopyrites
  - chalcopyrite is a system that contains: Cu, Ga, and a chalcogenide
- Some of the common chalcopyrite systems:

$CuGaSe_2$, $CuGaS_2$, $CuFeS_2$, $CuAlS_2$, $CuInGaS_2$

- Pros of Chalcopyrite:
  - Very efficient material (13% ~ 20%)
  - Band gap of ~ 1.04 -2.7 eV







Nano Prep:

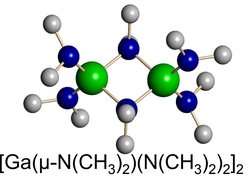
- Solution Precipitation Route
  - Take a solution and heat to reflux temperature, then inject a cold solution
- Prep is considerably effective due to the temperature shock
- This kind of system allows more control over the different morphologies

Building Up To Our Nanopaticles:

- In choosing gallium we will first begin by making an amide compound
- Next we will take that amide and react our metal with an alcohol in a metathesis reaction
- This will give us new materials to try and obtain new nanoparticle systems

General Synthesis of $Ga(OR)_3$:

$$Ga(N(CH_3)_2)_3 + 3\ HOR \rightarrow Ga(OR)_3 + 3\ HN(CH_3)_2$$

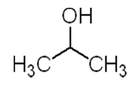


$[Ga(\mu\text{-}N(CH_3)_2)(N(CH_3)_2)_2]_2$

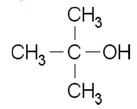
Increasing steric bulk

Increasing steric bulk

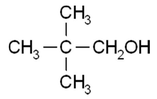
Alkyl Alcohols:



iso-Propanol (H-OPr^i)

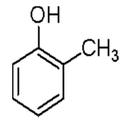


tert-Butanol (H-OBu^t)

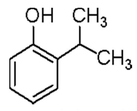


neo-Pentanol (H-ONep)

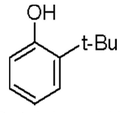
Mono-substituted phenols:



2-Methylphenol (H-*o*MP)

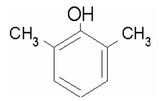


2-Isopropylphenol H-*o*PP

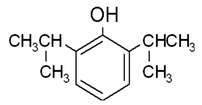


2-*tert*-Butylphenol H-*o*BP

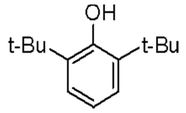
Di-substituted phenols:



2,6-di-Methyl Phenol (H-DMP)

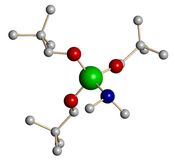


2,6-di-*iso*-Propyl Phenol (H-DIP)

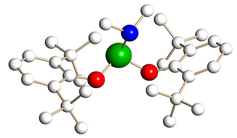


2,6-di-*tert*-Butyl Phenol (H-DBP)

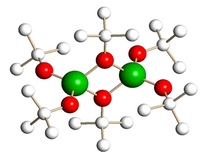
Novel Gallium Alkoxides:



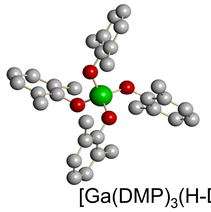
$[Ga(ONep)_3(HNR_2)]$



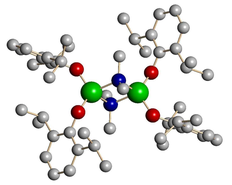
$[Ga(N(CH_3)_2)(DBP)_2]$



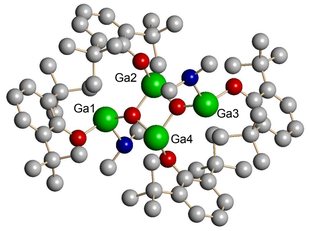
$[Ga(\mu\text{-}OBu^t)(OBu^t)_2]_2$



$[Ga(DMP)_3(H\text{-}DMP)]$

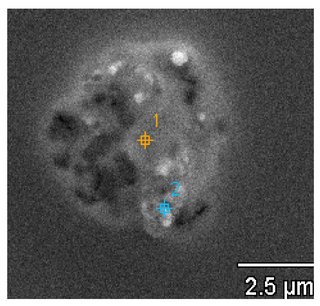


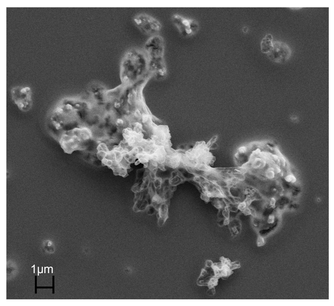
$[Ga(\mu\text{-}N(CH_3)_2)(DIP)_2]_2$



$Ga_4(DBP)_4(N(CH_3)_2)_2(\mu_3\text{-}O)_2 \bullet$ tol

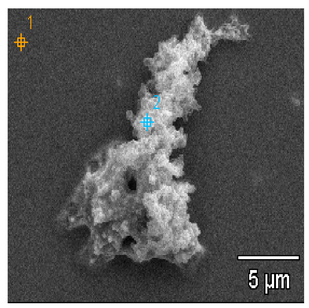
GaAs Thin Films

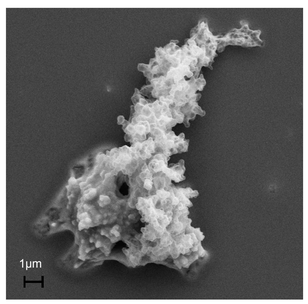




Thin Films: thin material layers ranging from a nanometer to several micrometers in thickness

- commonly used in electronic semi conducting and optical devices

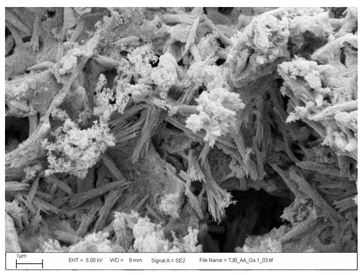




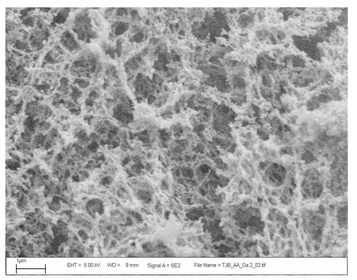
Aerogels

Aerogel – a solid state material that has low density
- nearly transparent and very lightweight
- effective insulator

Ga MeOH



Ga EtOH



Summary and Conclusion

- Have successfully been able to synthesize novel gallium alkoxides
- Began initial nano synthesis routes
- Applied gallium precursors to thin film and aerogel synthesis
- We can now see if what we've obtained will be useful to apply to hopefully more efficient materials for light absorption