JOHN G. EKERDT

RESEARCH FOCUS

We study surface and materials chemistry as it relates to the growth and properties of ultrathin metal, dielectric and ferroelectric films for optical and electronic applications, and we study the catalytic conversion of lignin to chemicals. We seek to understand and describe nucleation and growth of films and nanostructures, structure-property relationships, and site-specific reactions.

Current Group/Collaborators

Topical Area	Students	Collaborators
Thin Films (Metals, Dielectrics, Polymers, Ferroelectrics)	Dan Bost, Tyler Elko-Hansen, Brad Leonhardt, Martin McDaniel, Tuo Wang	A. Demkov (Physics), Dina Triyoso (Global Foundries)
Nanostructures (Si, Ge, Metal, Polymer, Ferroelectrics)	Brad Leonhardt, Joe McCrate	B. A. Korgel, D. P. Neikirk (ECE)
Biomass Conversion (Lignin)	Blair Cox, Thong Ngo	

Funding: AEC, Intel Corp., NSF, ONR, Welch

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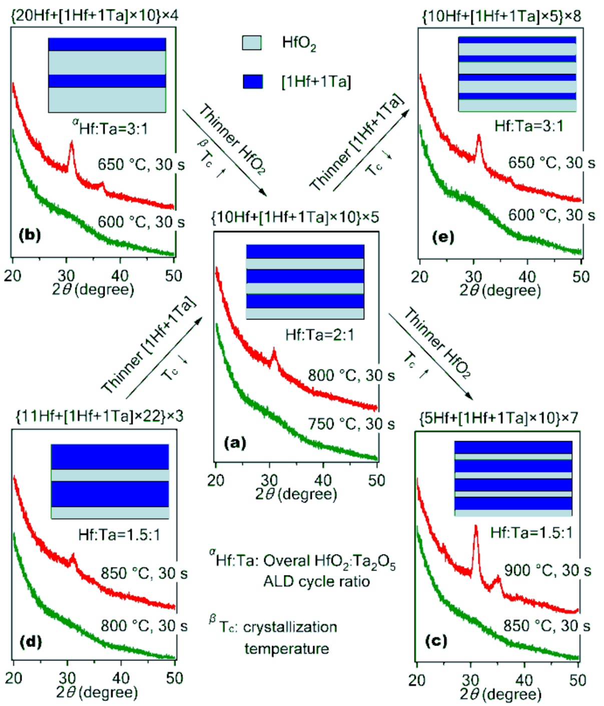
Projects	Subject Areas	Fundamental Aspects	Technology Applications
•Ultra Thin Metal and Metal Alloy Films •Si/Ge Nanostructures •Chemistry of Dielectric Surfaces •Epitaxial Growth of Ferroelectrics •CVD Polymer Films •Biomass Catalysis	•Surface Science •Materials Science •Nanotechnology •Materials Chemistry •Reaction Kinetics •Catalytic Chemistry •Atomic Layer Deposition •Chemical Vapor Deposition •Molecular Beam Epitaxy •Self-Assembly	•Chemical nature of surface defects that serve as activation sites and nucleation sites •Enabling chemistry for film growth or nanoparticle growth •Nature of bonding across interfaces •Role of alloying and doping in phase stability •Relations between bonding, structure and properties •Catalysis in ionic liquids	•Advanced Memory Devices •Sensors •Diffusion Barriers for 45 and 32 nm Technology Nodes •Dielectrics for Nanowire Devices •Monolithic Integration of Ferroelectrics/Si/ Compound Semiconductors •Efficient Biomass Conversion Processes

ALD growth of high-*k* dielectric and expitaxial oxides

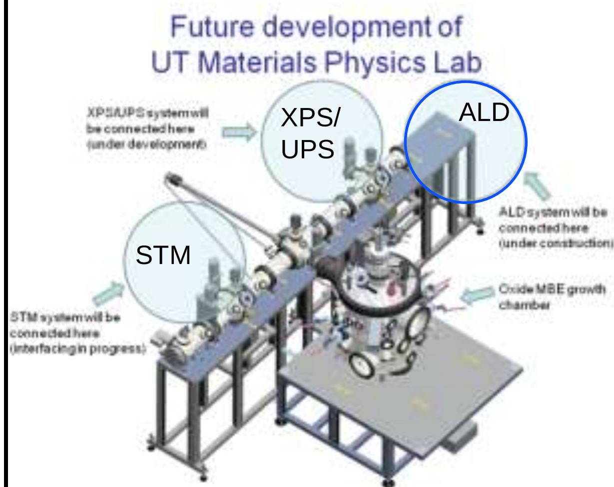
Primary Goal: Stabilize the amorphous phase of HfO_2;
Grow expitaxial oxides on epi-surfaces prepared by MBE

Atomic Layer Deposition (ALD) of amorphous high-*k* dielectric

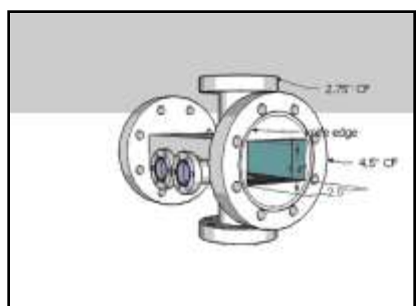
- Amorphizing elements (La, Al, Ta, *etc*.) can be incorporated into HfO_2 to increase the film crystallization temperature
- The distribution of the amorphizer also affects film crystallization temperature



Molecular Beam Epitaxy (MBE) system

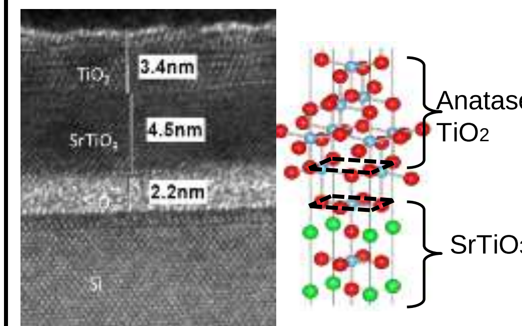


ALD system (to be connected with the MBE)



Customized ALD chamber, ensuring *in situ* sample transfer and high efficiency deposition

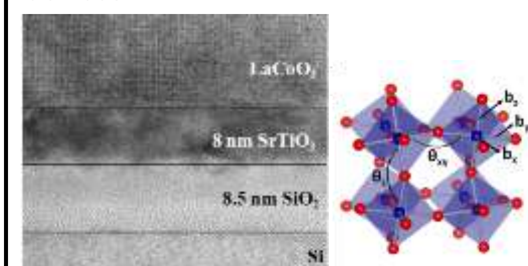
Photocatalyst TiO_2 on $SrTiO_3$-buffered Si



Cross-sectional TEM of TiO_2 on $SrTiO_3$

$LaCoO_3$ on $SrTiO_3$-buffered Si grown using MBE with atomic oxygen

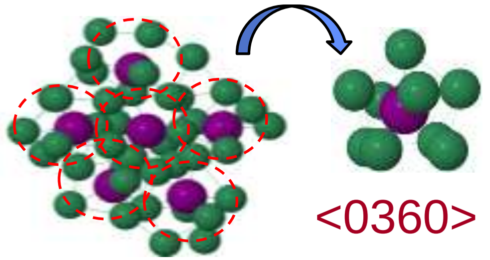
Strain from $SrTiO_3$ induces a ferromagnetic state in $LaCoO_3$ that can possibly be exploited for novel devices



Large changes in bond lengths and angles due to strain

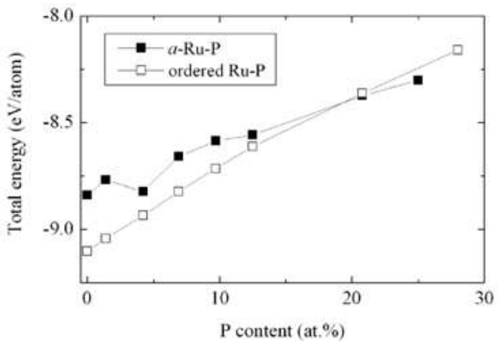
Ultrathin Continuous Metal Films

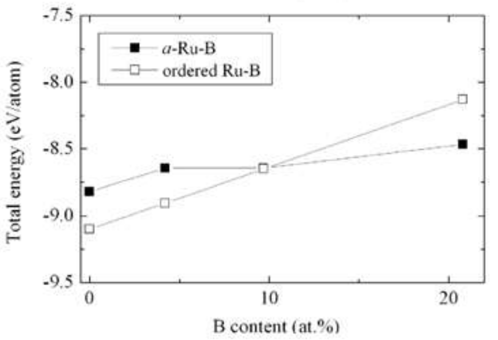
Primary Goal: Examine the nucleation, deposition, and material properties of thin metal films, with a focus on the control of composition and nucleation.



Amorphous Ru(P) Model

Validate the predictions for Ru and Co films using P and B grown from the hydrides PH_3 and B_2H_6, and determine how properties scale with thickness

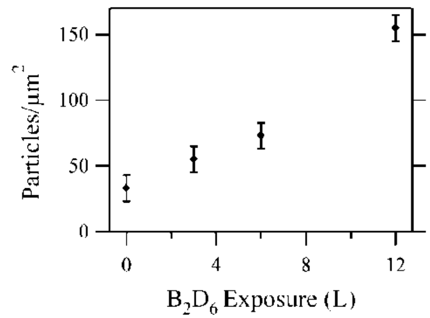


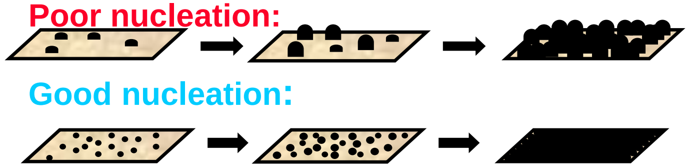


Increased B_2D_6 exposure leads to trap sites that increases the number of particles forming on HOPG

Nucleation Promotion:

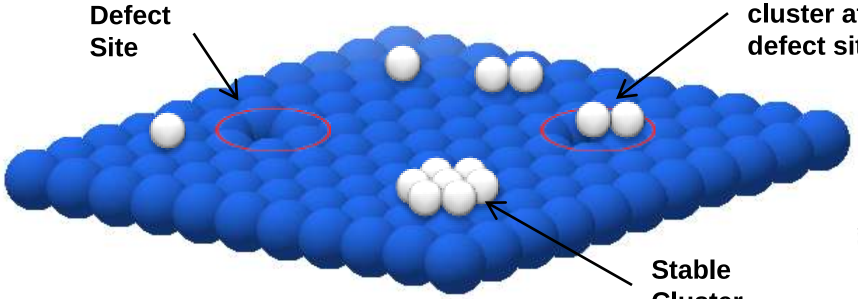
Control of the nucleation behavior of Pt on HOPG is achieved through the use of Boron implantation to create defect sites, altering the number of nuclei formed and the final structure of the material.



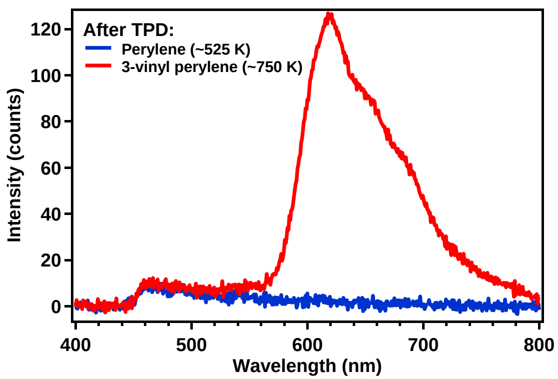


Nanoparticle nucleation on oxides

Primary Goal: Determine the chemical nature of native and synthesized defects on oxides and use this knowledge to control particle nucleation on these materials.



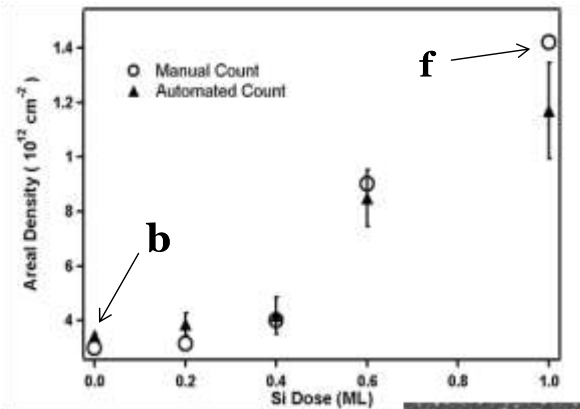
Schematic of nucleation processes on surfaces with defect sites that are capable of trapping adatoms. Smaller clusters are stable at trap sites, increasing the total nuclei density.



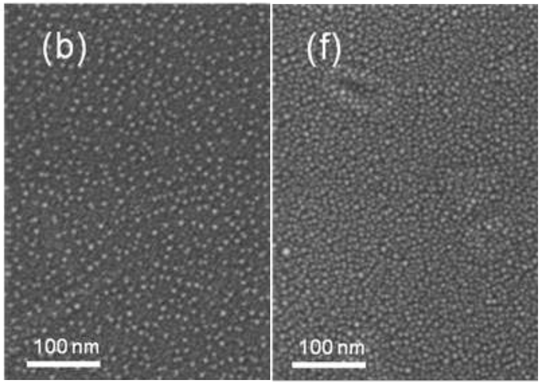
PL spectra from compounds deposited on silica after heating to ~525 K for the perylene dosed sample and ~ 750 K for the 3-vinyl perylene dosed sample.

Defect mediated nucleation:

Particle density can be controlled by creating surface defects that can act as traps for adatoms. Defect concentration is controlled on SiO_2 by etching with Si. Ge particle density can be enhanced by an order of magnitude with this method.



Left: Plot of areal density versus Si dose showing influence of etching on density.
Below: SEM images of Ge particles on SiO_2 exposed to no (b) and 1.0 ML (f) Si etching.



Defect chemistry and structure:

Fluorescent molecules with specific functional groups (vectors) bind to defect sites on these materials. Photoluminescence (PL) spectra can then provide direct information about the types and density of defects.

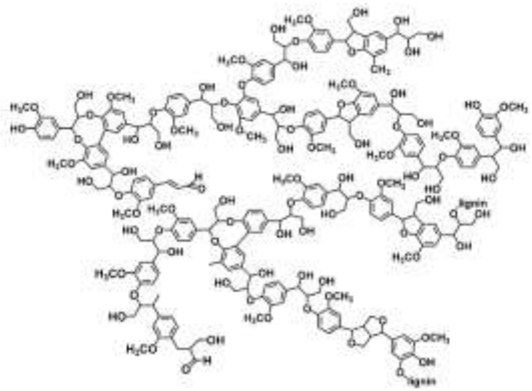
Biomass Processing in Ionic Liquids

Primary Goal: Develop methods for separation, depolymerization, and hydro-deoxygenation of lignin for use as a fuel or aromatic feedstock in ionic liquids

Biomass

Lignin

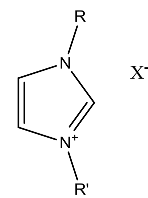
Cellulose/
hemicellulose



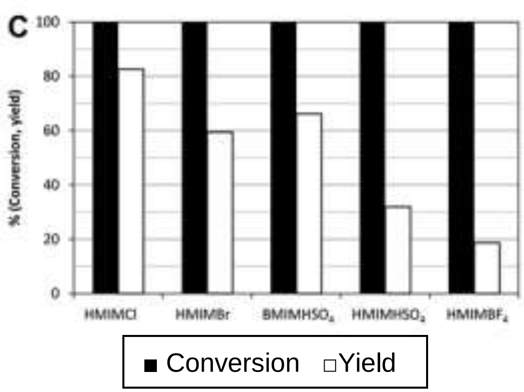
→ **Fuel, Chemicals**

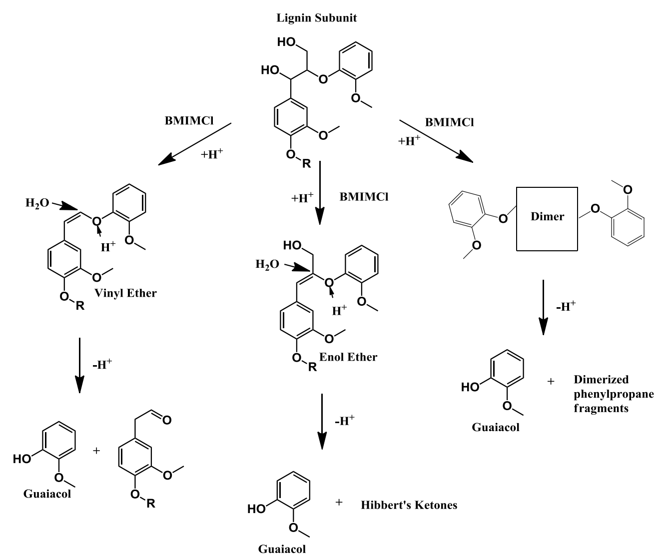
Ionic liquids

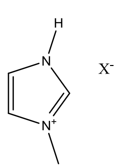
- Can dissolve biomass
- Tuneable properties
- No vapor pressure
- Can act as solvent/catalysts



Acid catalyzed depolymerization

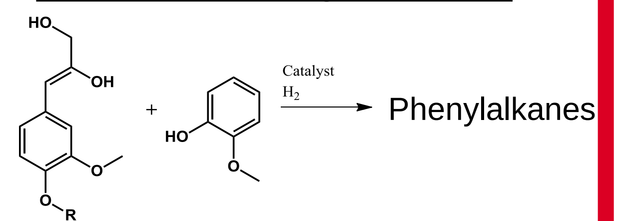






- Up to 82.5% yield
- Anion influences reaction mechanism
- Acidity of ionic liquids measured

Hydrodeoxygenation



Lignin fragments

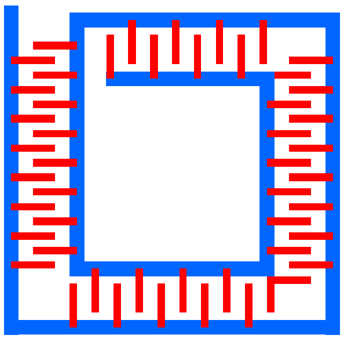
Remove heteroatomes while maintaining aromatic character

Testing various catalysts and conditions is the next step in the project

iCVD Deposition of Conformal Polymer

Primary Goal: Utilize iCVD deposition techniques to create a nanoscale, conformal polymer coating as a responsive surface layer in a small RFID sensor

Interdigitated Circuit
(from collaborator: Neikirk, UT)



Interdigitated pattern allows very high capacitance sensors

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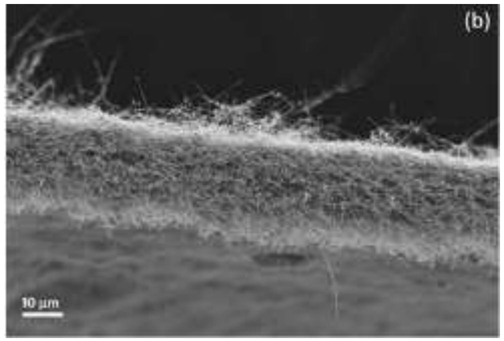
Ge Nanowire Paper
(from collaborator: Korgel, UT)



Nanowire mats have very high surface area to volume ratios, ideal for a sensor substrate

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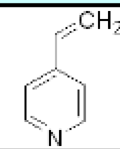
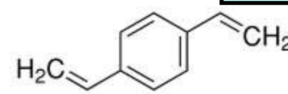
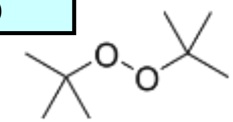
Initiated Vapor Phase Polymerization



Monomer
(Vinyl Pyridine)



Crosslinker
(Divinylbenzene)



Initiator
(di-tert-butyl peroxide)

iCVD deposition allows conformal coating even in deep wells and sub-micron gaps

The iCVD Reactor

The coating type will determine sensitivity of the sensor:

Aromatic:	polystyrene
Straight-chain oil:	polyethylene
Salinity:	polyacrylate
pH:	polymethacrylic acid

Complete Sensor
(coated nanowires atop circuit)