JOHN G. EKERDT

RESEARCH FOCUS

We study the surface, growth and materials chemistry of metal, dielectric, ferroelectric, and polymer thin films. We seek to understand and describe nucleation and growth of films and nanostructures, their structure-property relationships, and site-specific reactions that lead to their formation. The programs are motivated by applications in electronic materials, energy and sensors.

www.che.utexas.edu/ekerdt-group

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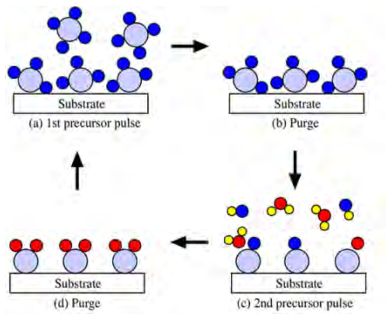
Projects 2 Positions	Subject Areas	Fundamental Aspects	Technology Applications
•Nucleation and Growth of Ultra Thin Metal Films •Selective Growth of Metal and Dielectric Films •Epitaxial Growth and Properties of Crystalline Oxides and Perovskites •Limits of Nanoshape Control	•Surface Science •Materials Science •Nanotechnology •Materials Chemistry •Reaction Kinetics •Atomic Layer Deposition •Chemical Vapor Deposition •Molecular Beam Epitaxy •Reactive and Atomic Layer Etching	•Chemical nature of surface sites that serve as activation sites and nucleation sites •Enabling chemistry for film growth or nanoparticle growth •Nature of bonding across interfaces •Approaches to stabilizing metastable structures •Relations between bonding, structure and properties •Selective activation of surfaces with ions and radicals	•Advanced memory devices •Sensors •Diffusion barriers for advanced microelectronic devices •Low power devices •Integration of functional crystalline oxides on Si(001), Ge(001) and GaN

Low Temperature ALD of Crystalline Oxides

Shen Hu; Ed Lin; Bryce Edmonson

Alternating delivery affords digital control

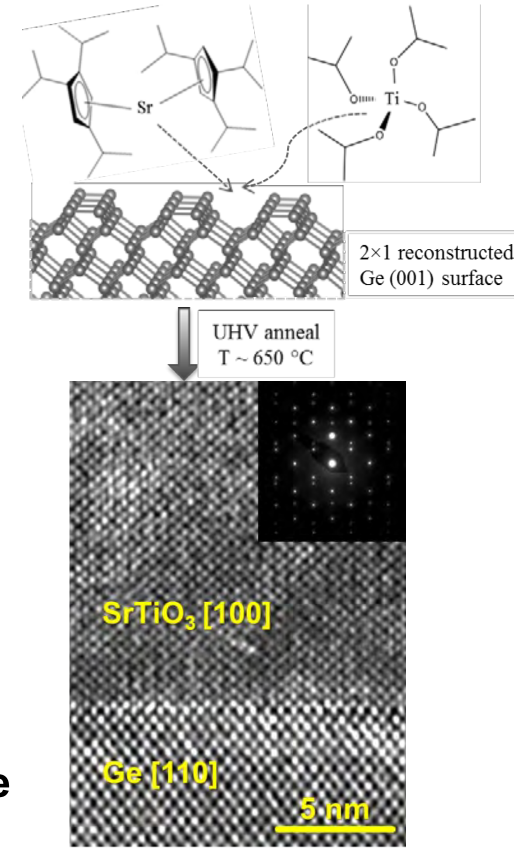


Atomic Layer Deposition

- Commercial metalorganic precursors
- Oxidant = water
- T = 200-250 °C, P ≈ 1 torr

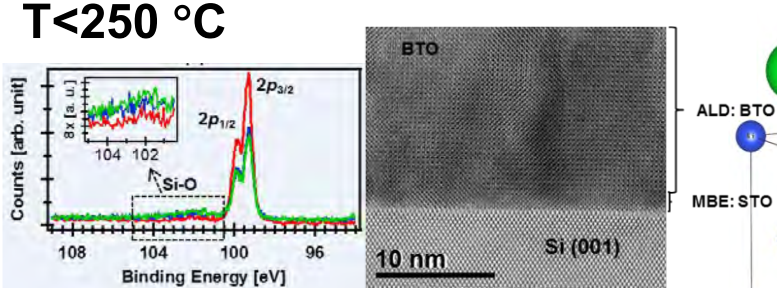
1.6-nm $SrTiO_3$ buffer by MBE needed on Si(001)

ALD directly on Ge(001) – $SrTiO_3$, $(Al,Sr)TiO_3$, $SrHfO_3$

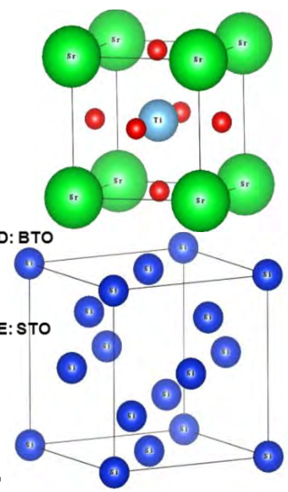


McDaniel, Adv. Mater. Interf. (2014).

Insignificant oxidation of substrate because T<250 °C



Ngo, et al., Appl. Phys. Lett. 104, 082910 (2014).

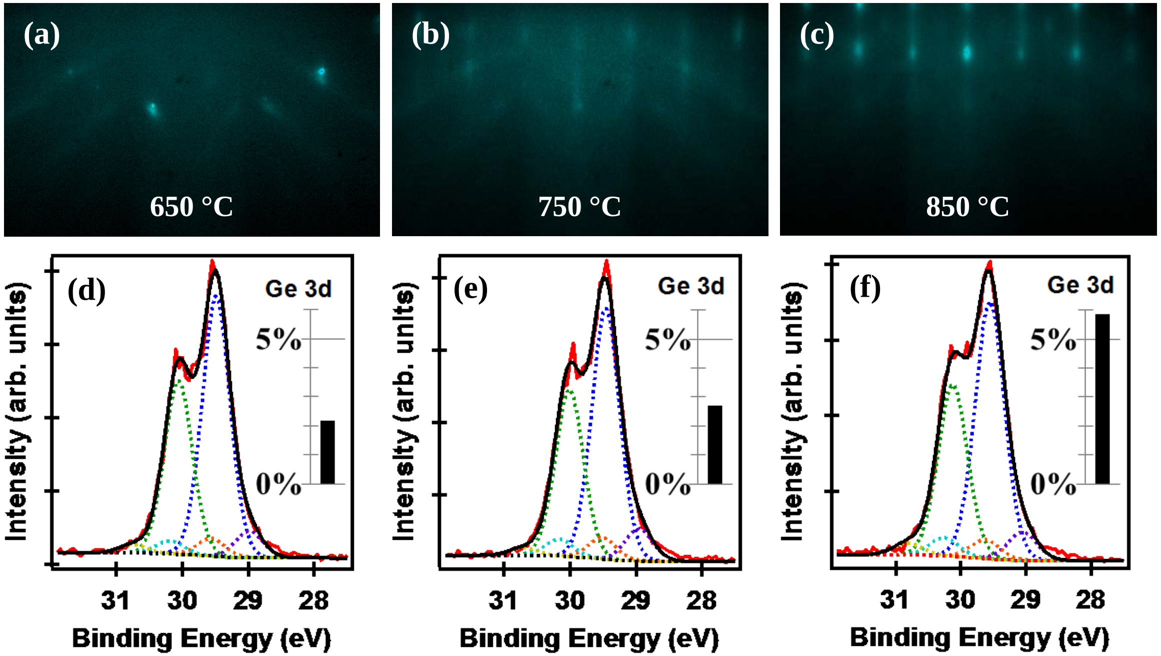


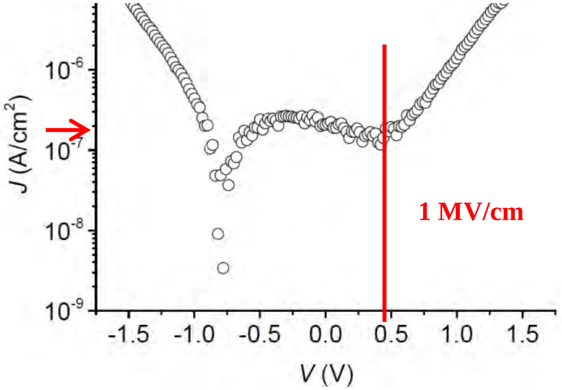
$SrTiO_3$ template

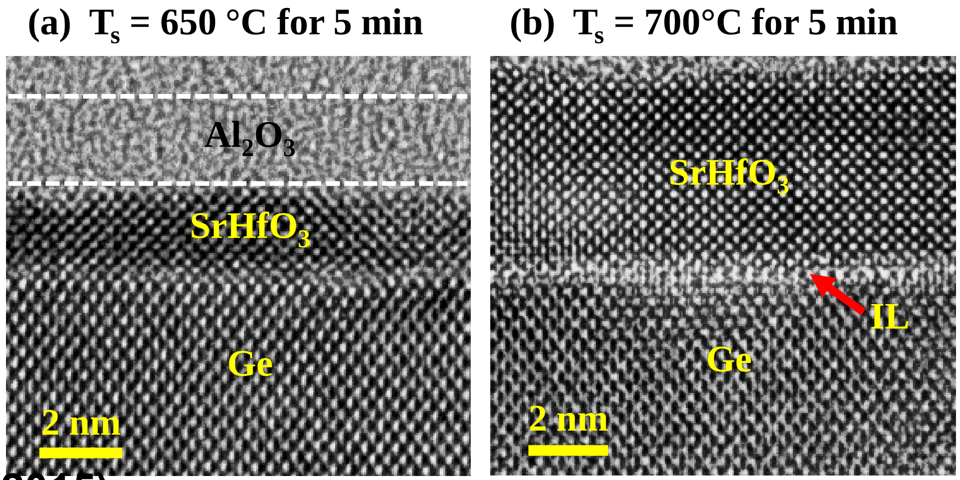
Si substrate

A scaleable, low cost of ownership approach with potential for 3D structures. Enables coupling of function directly to the substrate.

Interfacial Layer observed for SHO

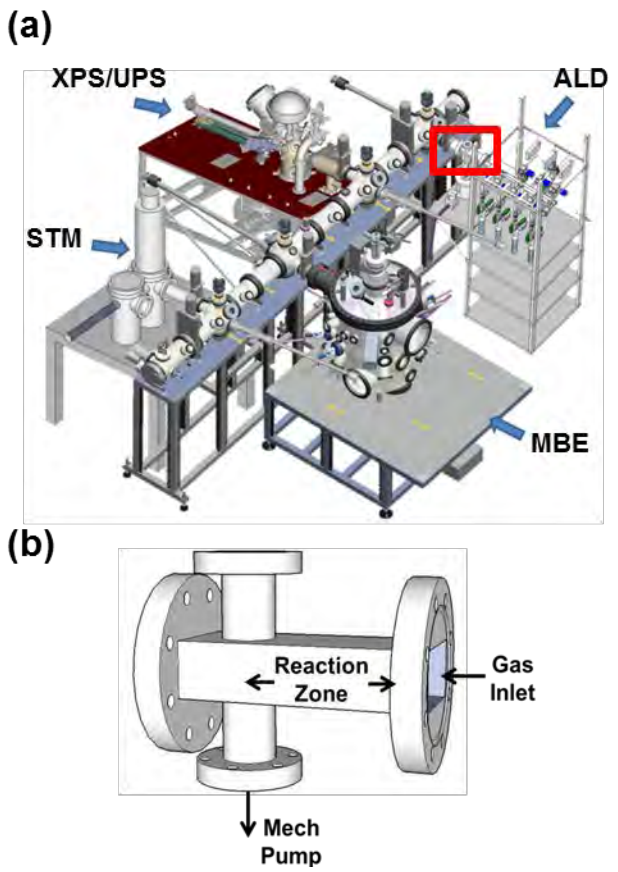






McDaniel et al., JAP 117, 05410 (2015).

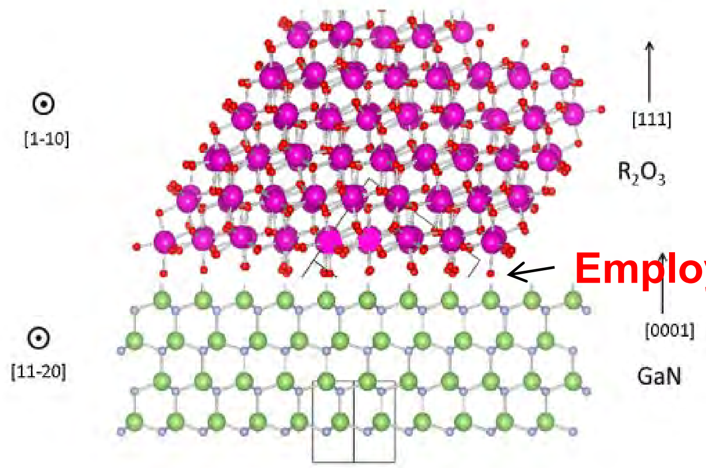
The Materials Physics Laboratory



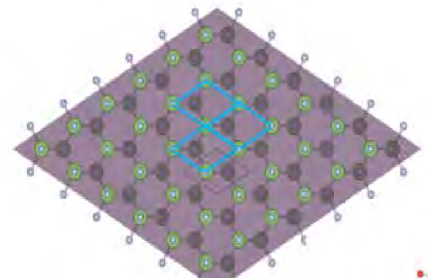
A shared facility located in RLM and managed by a Senior Scientist, Agham Posadas

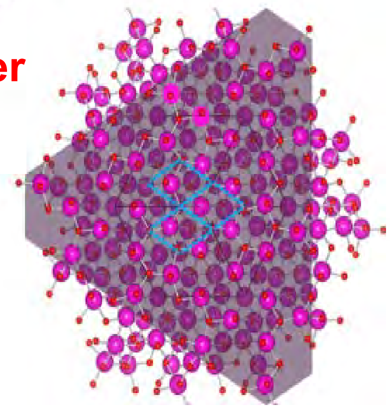
Allows for co-location of students from the A. A. Demkov and J. G. Ekerdt groups working on common projects

How to Grow Crystalline Rare Earth Oxides on Nitrides?



Employ Crystalline Zintl Layer





Surface unit cell of GaN overlaid on
(111) surface of bixbyite
(Ga-O bonding assumed)

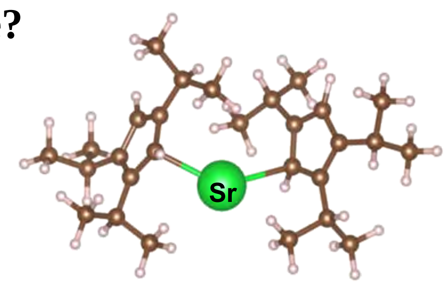
La_2O_3, Gd_2O_3 and Er_2O_3

Ionic oxides on a highly covalent semiconductor

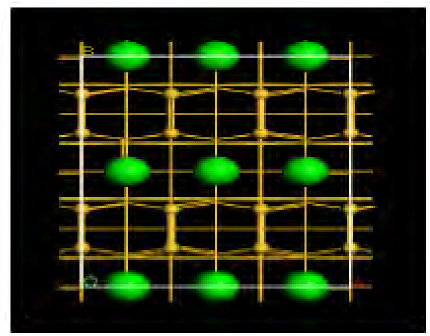
Lattices align – surface energy (wetting) needs to be resolved

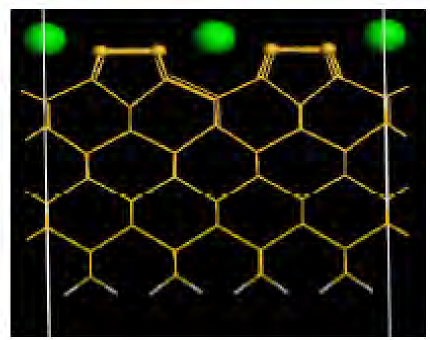
Understanding interface structure: Zintl phase and passivation

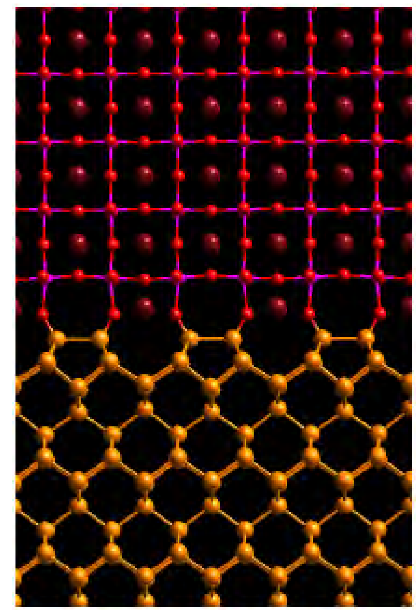
- **MBE growth of STO on Si**
  - **Utilize ½-monolayer of Sr to passivate Si surface**
  - **Creates strontium silicide layer (Zintl phase)**
- **ALD growth of STO on Ge**
  - **Sr precursor has affinity for Ge dangling bonds**
  - **Does the Sr precursor order on the surface? What is the interface structure?**



½-ML Sr (2×1)



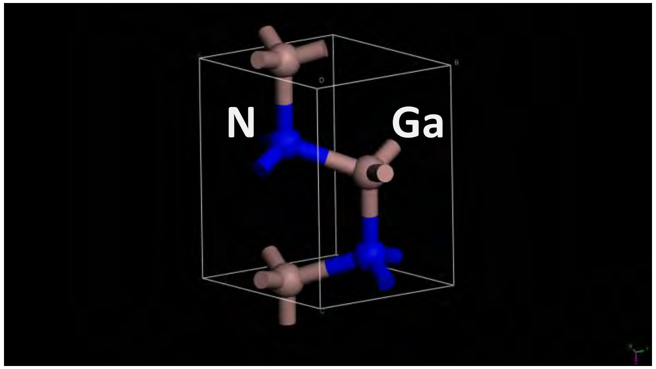




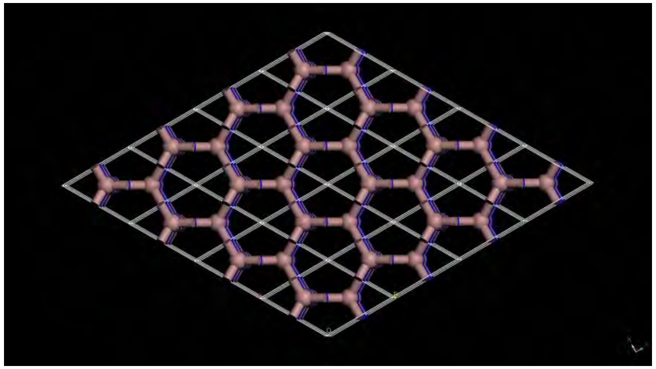
A.A. Demkov, X. Zhang, JAP 103 (**2008**) 103710.

Intermetallic Zintl Compounds to Grow Crystalline Oxides on GaN(0001)

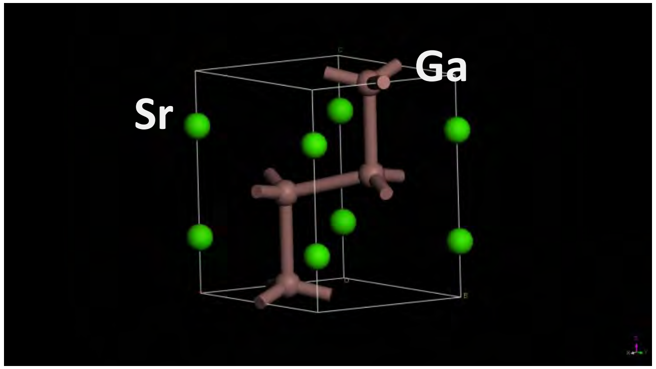
GaN (wurtzite, Space group $P6_3mc$)



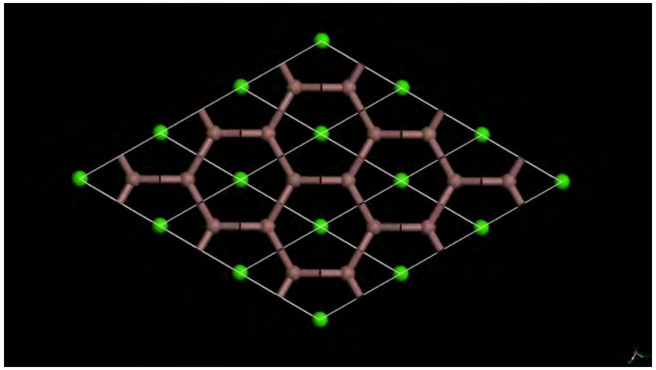
GaN (0001) surface



$SrGa_2$ ($CaIn_2$-type, Space group $P6_3/mmc$)



(0001) surface



Zintl compounds A_aX_x (A = Group 1, 2; X = Group 3, 4, 5), such as $SrGa_2$, $SrAl_2$, and $EuGa_2$ support/bridge ionic and covalent bonding

Selective Growth of Metal and Dielectric Films

Sonali Chopra
Zizhuo Zhang
Himmi Nallan

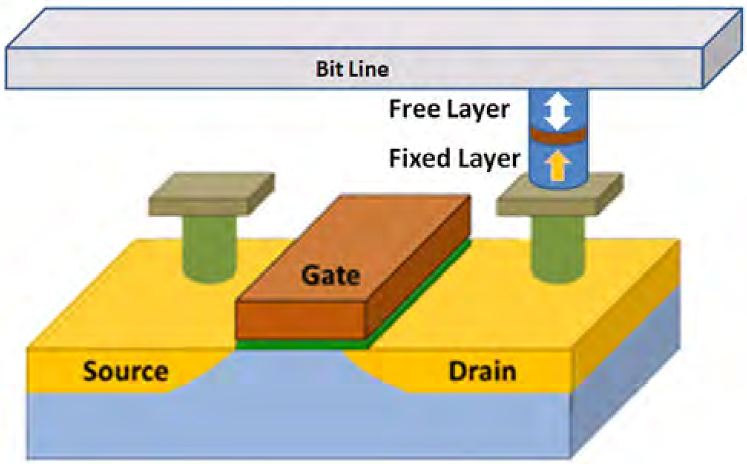


Figure: A schematic presentation of a STT-RAM cell

We seek selective chemical routes to form the metallic word line and the magnetic bit line for the STT-RAM structure using self-assembly and ALD.

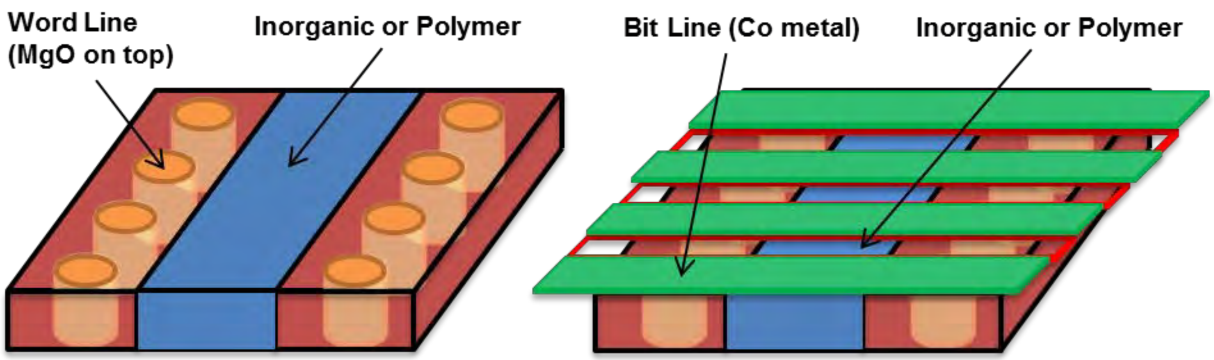


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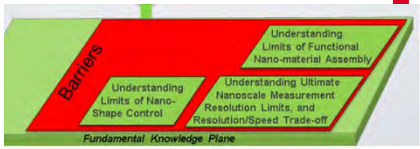
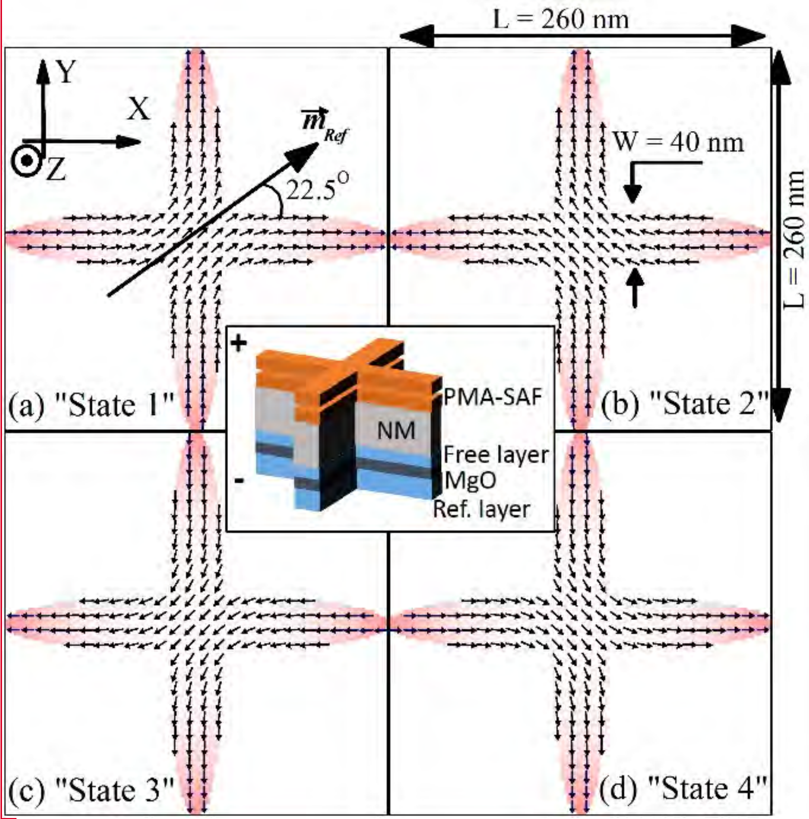
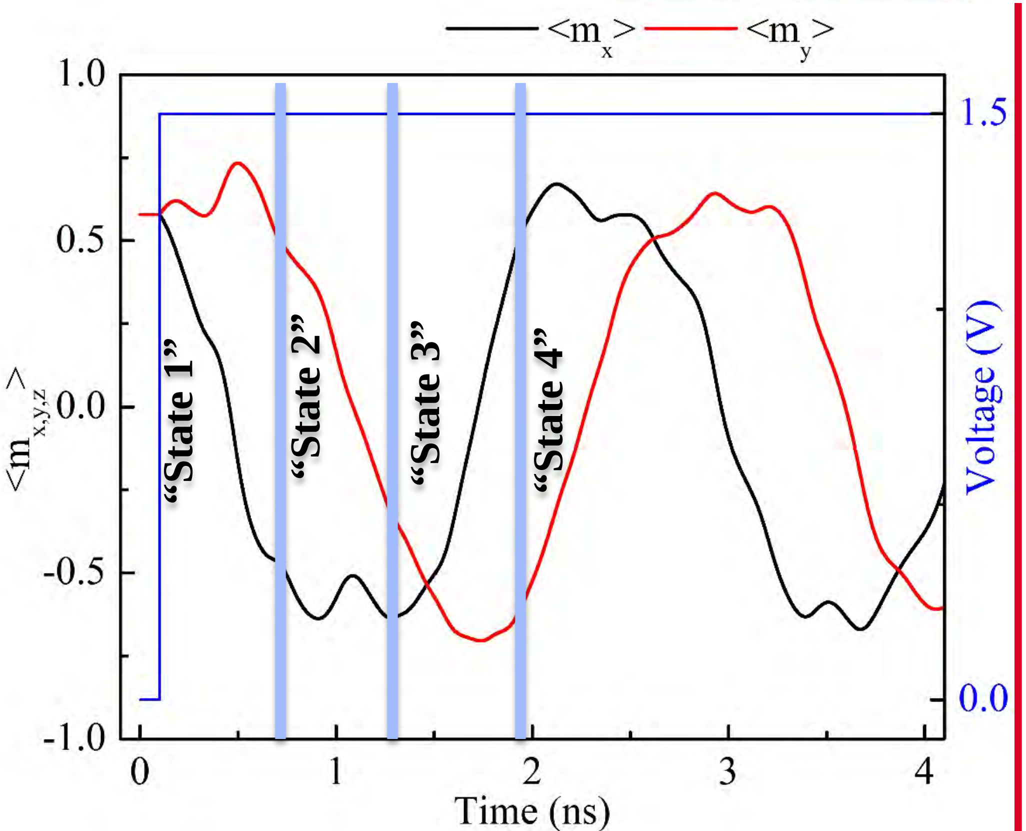
Figure: Schematic presentation of word and bit lines in STT-RAM structure

Voltage controlled switching of cross-shaped nanomagnet

- **Proposed a switching method based on Voltage Controlled Magnetic Anisotropy (VCMA)**

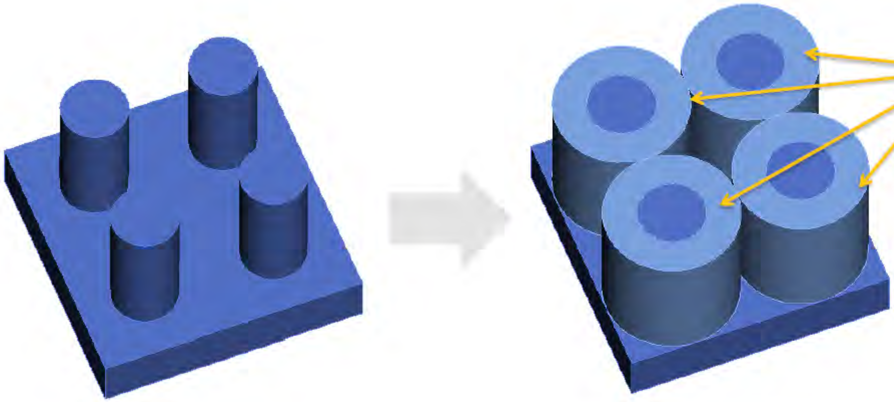




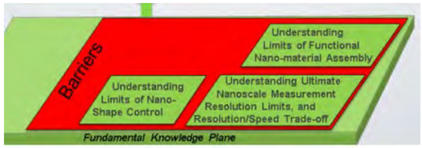


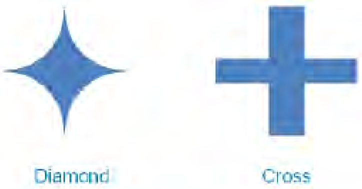
- **No STT required for switching**
- **Low power alternative to STT (write energy ~ fJ)**

Limits of Nanoshape Printing



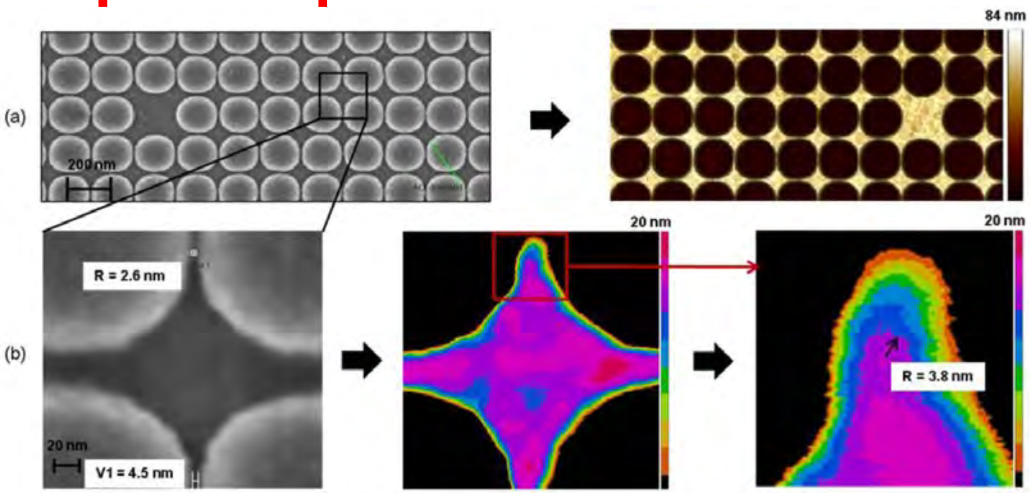
ALD Deposition of TiN & SiO_2 to create diamond shaped holes from a pillar pattern



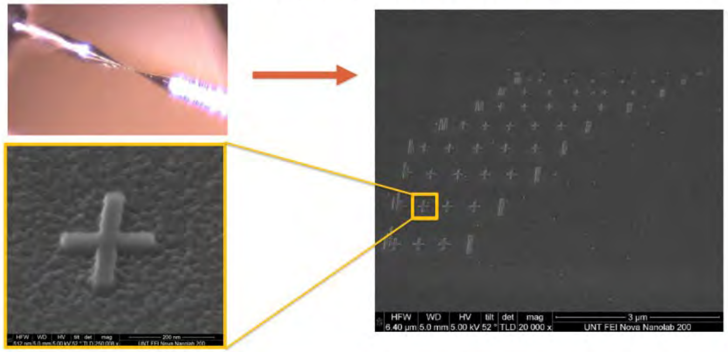


Nanoshapes being investigated with imprint lithography

Master template fabrication and imprint replication demonstrated



Methods and Results



STM tip based fabrication of cross structures by Zyvex

Collaboration with Zyvex Labs

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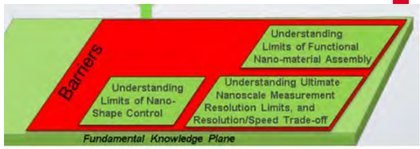
Modeling of Image Fidelity and Anisotropic Etch Transfer

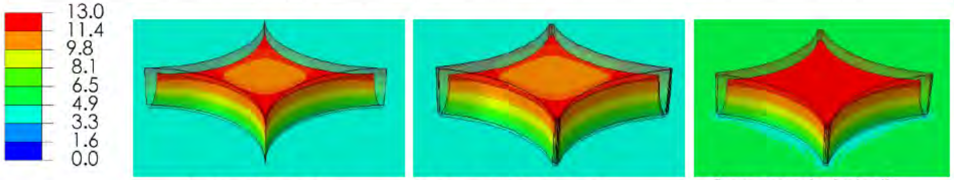


Modeling and Simulation Methods

Governing Equations

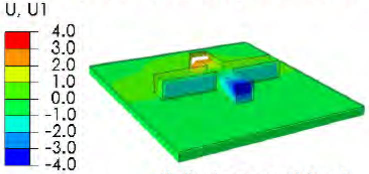
$$(\lambda + G)\frac{\partial e}{\partial x} + G\nabla^2 u = 0 \quad (\lambda + G)\frac{\partial e}{\partial y} + G\nabla^2 v = 0 \quad (\lambda + G)\frac{\partial e}{\partial z} + G\nabla^2 w = 0$$

where $e = \partial u/\partial x + \partial v/\partial y + \partial w/\partial z$, $\lambda = vE/((1+v)(1-2v))$, and $G = E/(2(1+v))$.

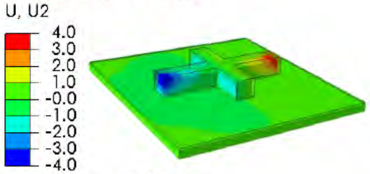


Sharp diamond | 2 nm rounded elastic diamond | 2 nm rounded plastic diamond

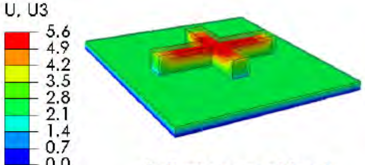
Sharp diamond stays sharp while both rounded diamonds get sharper. Plasticity does not impact on shape distortion.



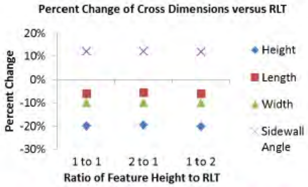
X displacement (nm)



y displacement (nm)

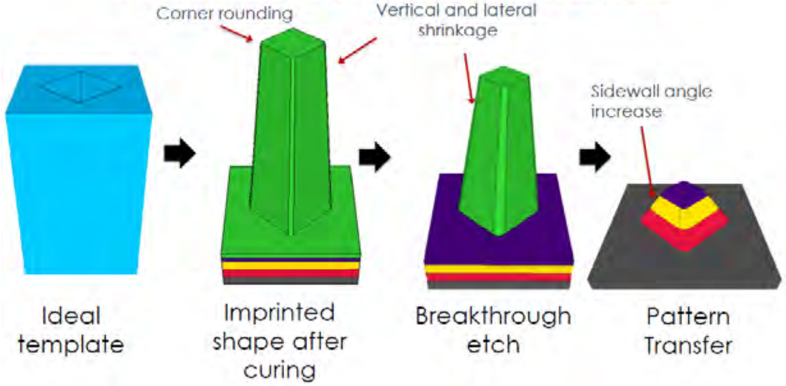


Z displacement (nm)



Lateral shrinkage is concentrated along the corners of the cross. Vertical shrinkage dominates at the center of the feature RLT does not impact distortion

Fundamental Research Barriers



Stresses are large at corners of nanoshapes and multi-tiered structures

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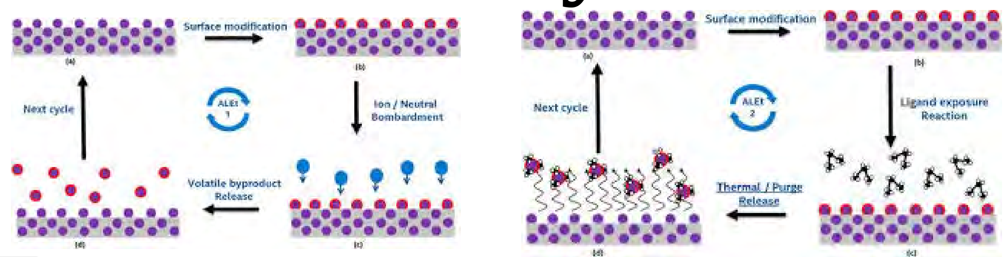
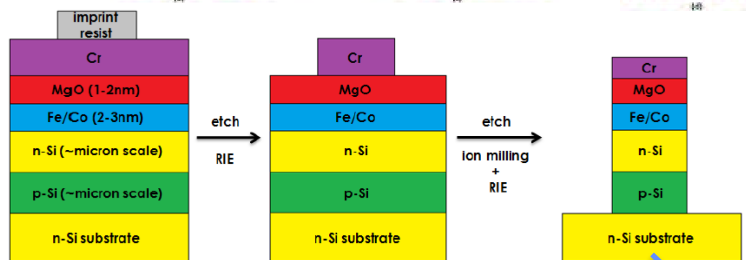
Exploring Etch Transfer of Shapes for Heterostacked Layers

NEED for Atomic Layer Etching





Schematic of the methods