PARADIM
AN NSF MATERIALS INNOVATION PLATFORM

MBE Lab #1

Oxide MBE of Binary Oxides (SnO, MgO, Dy_2O_3 depending on your group)

Darrell G. Schlom

Questions for MBE Lab #1

- Substrate to use (material and orientation)?
- Source material(s) to use?
- Temperature(s) of source material(s)?
- Crucible(s) to contain them?
- Deposition strategy (codeposition, shuttered growth, etc.)?
- Substrate temperature during growth?
- Oxidant and its pressure during growth?
- How to calibrate growth rate?

PARADIM

NSF

Substrate to Use (material and orientation)

- "Substrate Picker" from Materials Project

  https://www.materialsproject.org

H. Ding, S.S. Dwaraknath, L. Garten, P. Ndione, D. Ginley, and K.A. Persson, "Computational Approach for Epitaxial Polymorph Stabilization through Substrate Selection," *ACS Applied Materials and Interfaces* **8** (2016) 13086–13093.

PARADIM

NSF

Source Material(s) to Use

- Vapor Pressure of the Elements

  R.E. Honig and D.A. Kramer, “Vapor Pressure Data for the Solid and Liquid Elements,” *RCA Review* **30** (1969) 285–305.

- Vapor Pressures of Oxides

  R.H. Lamoreaux, D.L. Hildenbrand, and L. Brewer, “High-Temperature Vaporization Behavior of Oxides II. Oxides of Be, Mg, Ca, Sr, Ba, B, Al, Ga, In, Tl, Si, Ge, Sn, Pb, Zn, Cd, and Hg,” *Journal of Physical and Chemical Reference Data* **16** (1987) 419–443.

- “Material Deposition Chart” from Kurt J. Lesker Co.

  https://www.lesker.com/newweb/deposition_materials/materialdepositionchart.cfm?pgid=0

PARADIM

NSF

Source Temperature(s)

- Vapor Pressure of the Elements

  R.E. Honig and D.A. Kramer, "Vapor Pressure Data for the Solid and Liquid Elements," *RCA Review* **30** (1969) 285–305.

- Vapor Pressures of Oxides

  R.H. Lamoreaux, D.L. Hildenbrand, and L. Brewer, "High-Temperature Vaporization Behavior of Oxides II. Oxides of Be, Mg, Ca, Sr, Ba, B, Al, Ga, In, Tl, Si, Ge, Sn, Pb, Zn, Cd, and Hg," *Journal of Physical and Chemical Reference Data* **16** (1987) 419–443.

- "Material Deposition Chart" from Kurt J. Lesker Co.

  https://www.lesker.com/newweb/deposition_materials/materialdepositionchart.cfm?pgid=0

Crucible(s)

- “Material Deposition Chart” from Kurt J. Lesker Co.
  https://www.lesker.com/newweb/deposition_materials/materialdepositionchart.cfm?pgid=0

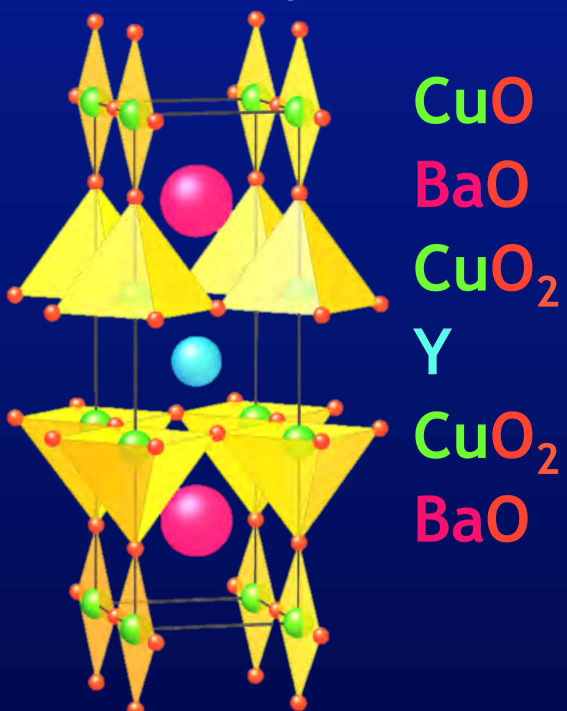
- Phase Diagrams
  Desk Handbook: Phase Diagrams for Binary Alloys, edited by H. Okamoto (ASM International, 2000).

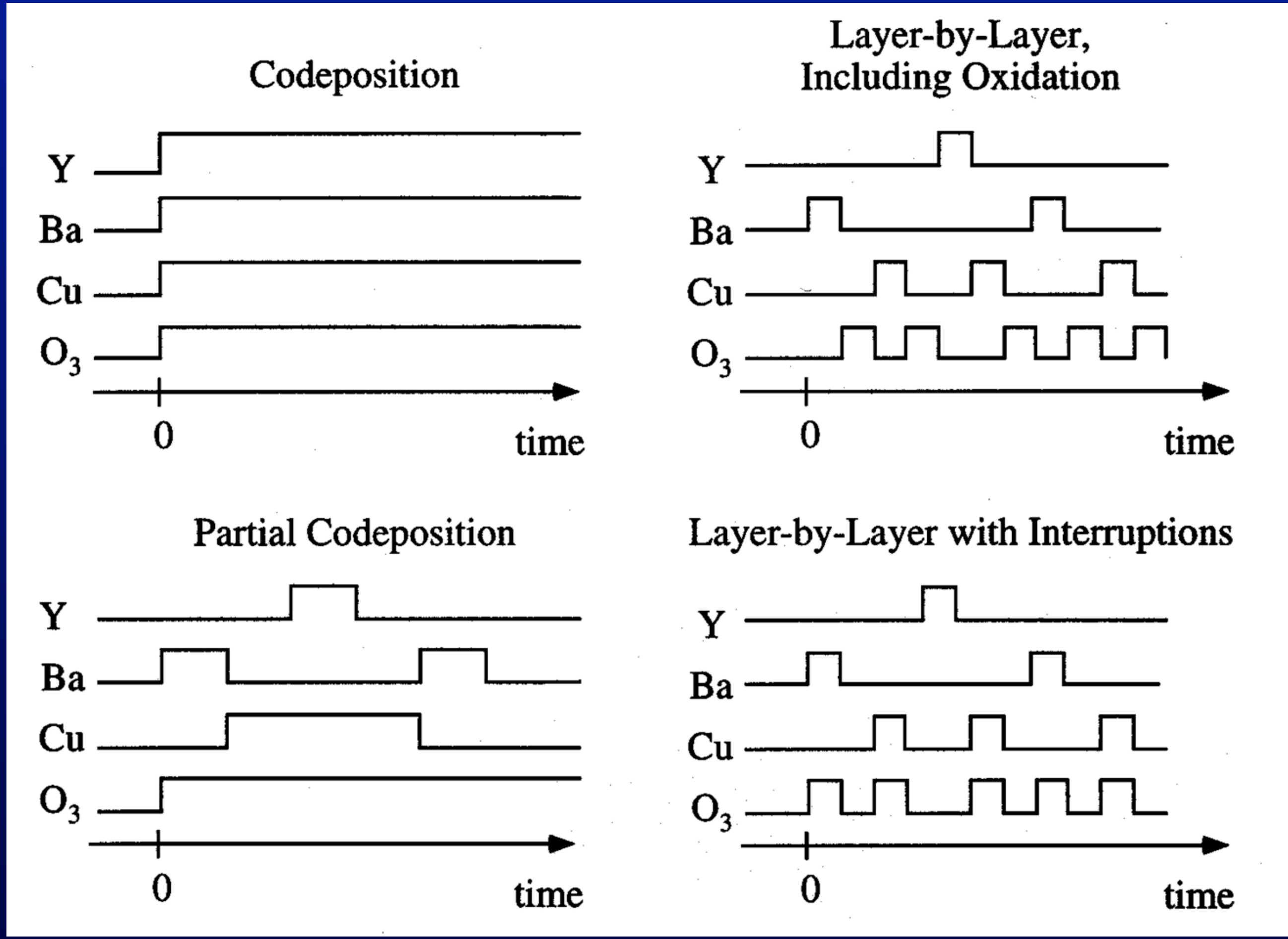
  ACerS—NIST Phase Equilibria Diagrams On-Line

Deposition Strategy
(codeposition, shuttered growth, etc.)

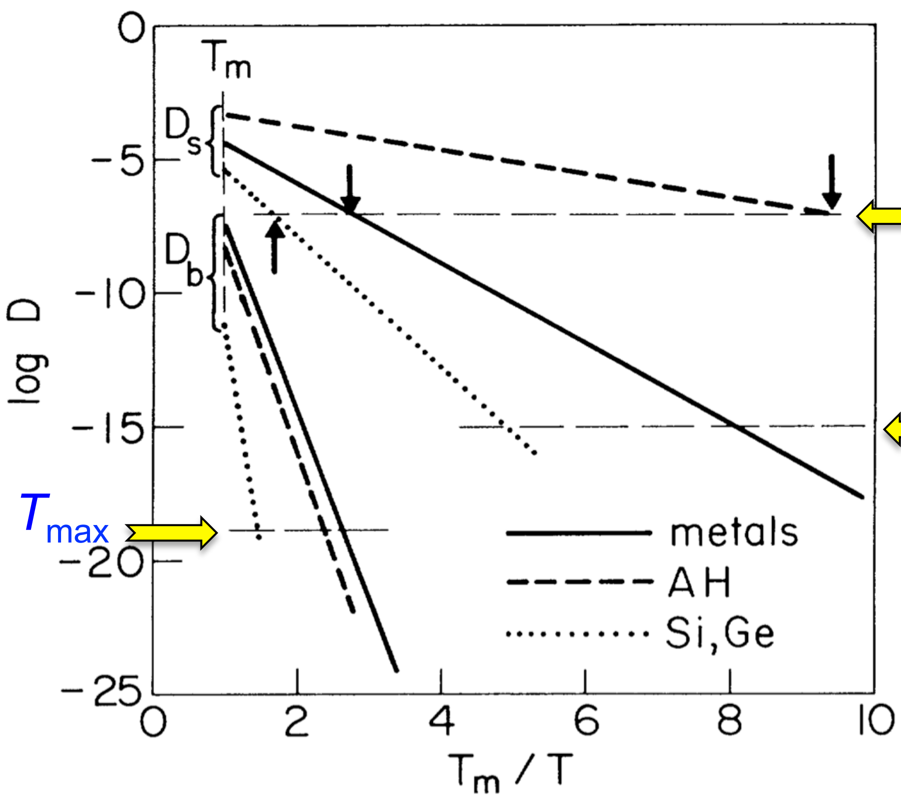
- This is the fun and freedom of MBE!

$YBa_2Cu_3O_7$





Substrate Temperature



Assuming growth rate of 0.1 monolayer/sec

T_{min} for smooth epitaxial films (growth by step propagation)

T_{min} for epitaxy

Optimal Growth Temperatures

$$0.55 < \frac{T_{sub}}{T_{melt}} < 0.7 \text{ for semiconductors}$$

$$0.35 < \frac{T_{sub}}{T_{melt}} < 0.4 \text{ for metals}$$

$$0.1 < \frac{T_{sub}}{T_{melt}} < 0.4 \text{ for simple ceramics}$$

M.H. Yang and C.P. Flynn
"Growth of Alkali Halides from Molecular Beams: Global Growth Characteristics"
Physical Review Letters **62** (1989) 2476-2479.

PARADIM

NSF

Oxidant and its Pressure

- Ellingham Diagram

  I. Barin, Thermochemical Data of Pure Substances, 3rd Ed., Vol. I and Vol. II (VCH, Weinheim, 1995).

- Thermodynamics of MBE (TOMBE) Diagram

  H.P. Nair, Y. Liu, J.P. Ruf, N.J. Schreiber, S-L. Shang, D.J. Baek, B.H. Goodge, L.F. Kourkoutis, Z.K. Liu, K.M. Shen, and D.G. Schlom, "Synthesis Science of $SrRuO_3$ and $CaRuO_3$ Epitaxial Films with High Residual Resistivity Ratios," *APL Materials* **6** (2018) 046101.

- If Desire Highest Oxidation State of all cations, then higher activity is better

  (within the limits of MBE, the equipment, and stable fluxes)

PARADIM

NSF

How to Calibrate Growth Rate

- Shadow Mask and Surface Profilometer
- Quartz Crystal Microbalance
- Ion Gauge
- RHEED Oscillations
- Shuttered RHEED Oscillations
- Rutherford Backscattering Spectrometry
- Mass Spectrometer
- Atomic Absorption Spectroscopy
- Atomic Emission Spectroscopy
- X-Ray Reflectivity, Ellipsometry, ⋯

PARADIM

NSF

If your desired flux of Sr is 30% higher than your measured flux or Sr, by how many °C do you need to increase the temperature of the Sr effusion cell to get the desired flux?

PARADIM

MBE ≈ Atomic Spray Painting