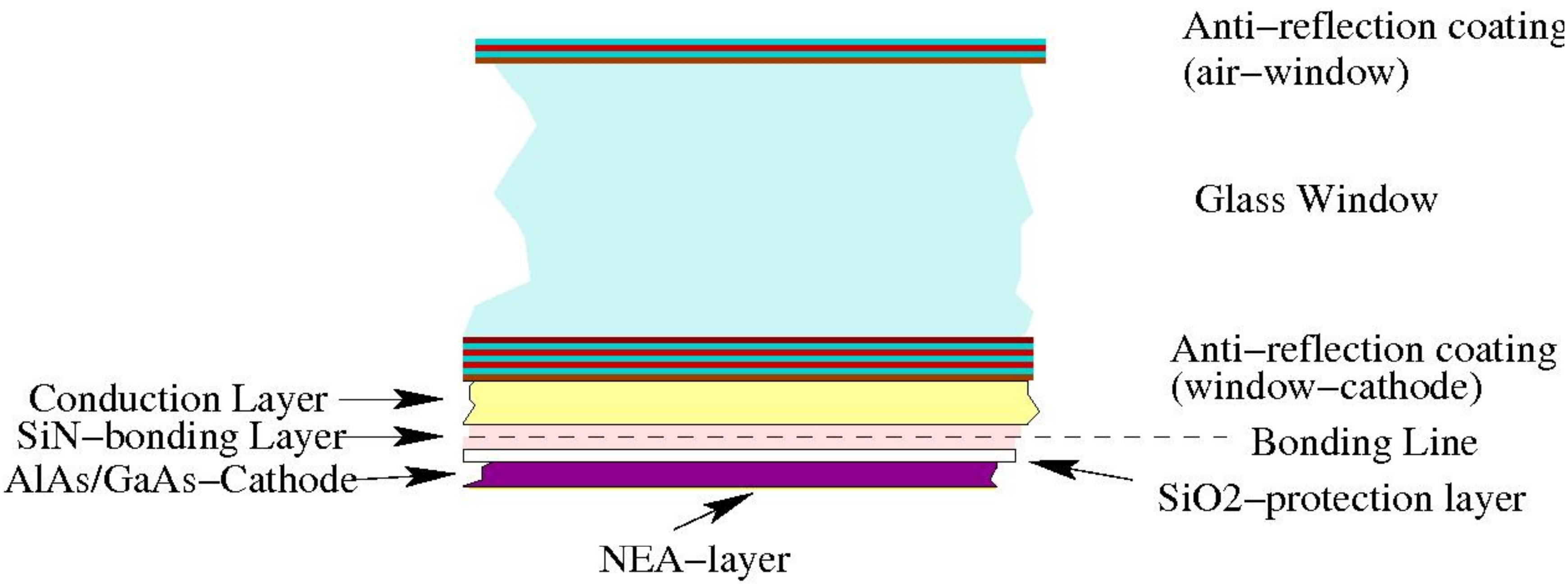
Progress And Scientific Goals at ANL and UIUC

Klaus Attenkofer	50%	growth; characterization; facility	XSD
Zikri Yusof	30%	growth; facility	HEP
Bernhard Adams	~10%	characterization	XSD
Igor Veryovkin	~10%	characterization	MSD
Zeke Insepov	~20%	Theory	MCS
Junqi Xie	100%	growth; characterization; facility	HEP
Seon Wu Lee	20%-100%	growth; characterization;	HEP
Alexander Paramonov	30%	growth; facility	HEP
Slade Jokela	30%	characterization	HEP
Matth Wetstein	20%	timing characterization (in future)	HEP
Ryan Dowdy	50%	growth	UIUC

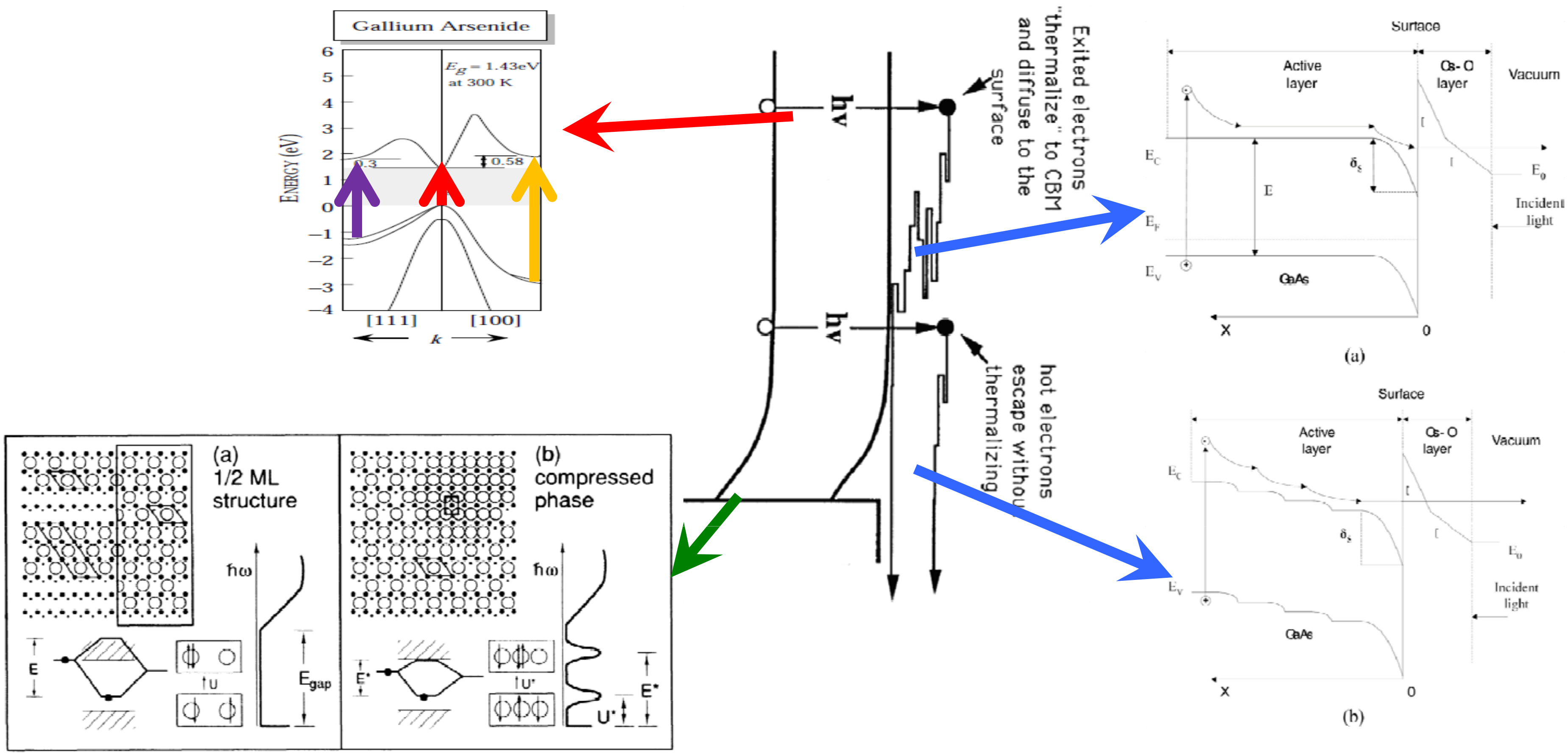
The Design Concept of the Photocathode Itself



- QE is defined by many factors: reflection losses, absorption probability, electron transport to surface, and electron emission
- Cathode is heterogeneous structure: each layer influences the functionality of the others
- All cathodes discussed are semiconductor cathodes: design principles can be applied to all three classes.

Theory Inspired Design of Devices

Basic Energy Sciences (BES) supports **fundamental research** to understand, predict, and **ultimately control matter and energy at the electronic, atomic, and molecular levels** in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.



A Few General Comments about Cathodes of Interest

- General properties:
  - All cathodes of interest are Semiconductors
  - All band gaps are between .6eV and 1.2eV (besides GaN).
- The photo-electron:
  - 400nm photons have a energy of 3.1eV
  - All photo electrons are **HOT-electrons**
- All cathodes are between **20nm-50nm** thick (2-3 absorption length)
- Consequences of cathode thickness:
  - Electron scattering on defects is not essential (may help to thermalize and randomize direction)
  - Interface and surface chemistry determines band banding (nearly not avoidable; also in the case of bi- and multi-alkali.
  - QE can be >100%

The Building Blocks at ANL

Design of Cathode Production Facility

- Prototype Facility for industrial production (ability to tailor wavelength response)

Materials / **Main Focus**

- Glass – Cathode Interface (inclusive conduction layer)
  - Surface morphology
  - Electronic doping levels & Fermi-level
  - Reflection Behavior
- M3Sb (M: K, Na, Cs) (amorphous /crystalline)
  - Poly-crystalline versus crystalline growth
  - Segregation to optimize wavelength optimization
  - Influence of buffer layer on growth and electronic behavior
  - Industrial growth: evaporators, sputter?....
- Ga(In)N (amorphous) Lead: WashU
  - Where does the In go
  - Alternative growth technologies (ALD?)
  - Doping and amorphous growth
- GaAs
  - Wavelength optimization
  - Doping profile optimization
  - Minimizing dark current
  - Development of cost-efficient transfer technology

The Interface between Glass and Cathode
Why is it important

- Morphology and chemical composition (especially surface) have strong influence on growth-characteristics of cathode (crystallite/amorphous, grain boundaries,…)

- Fermi-level will influence band-bending of the cathode

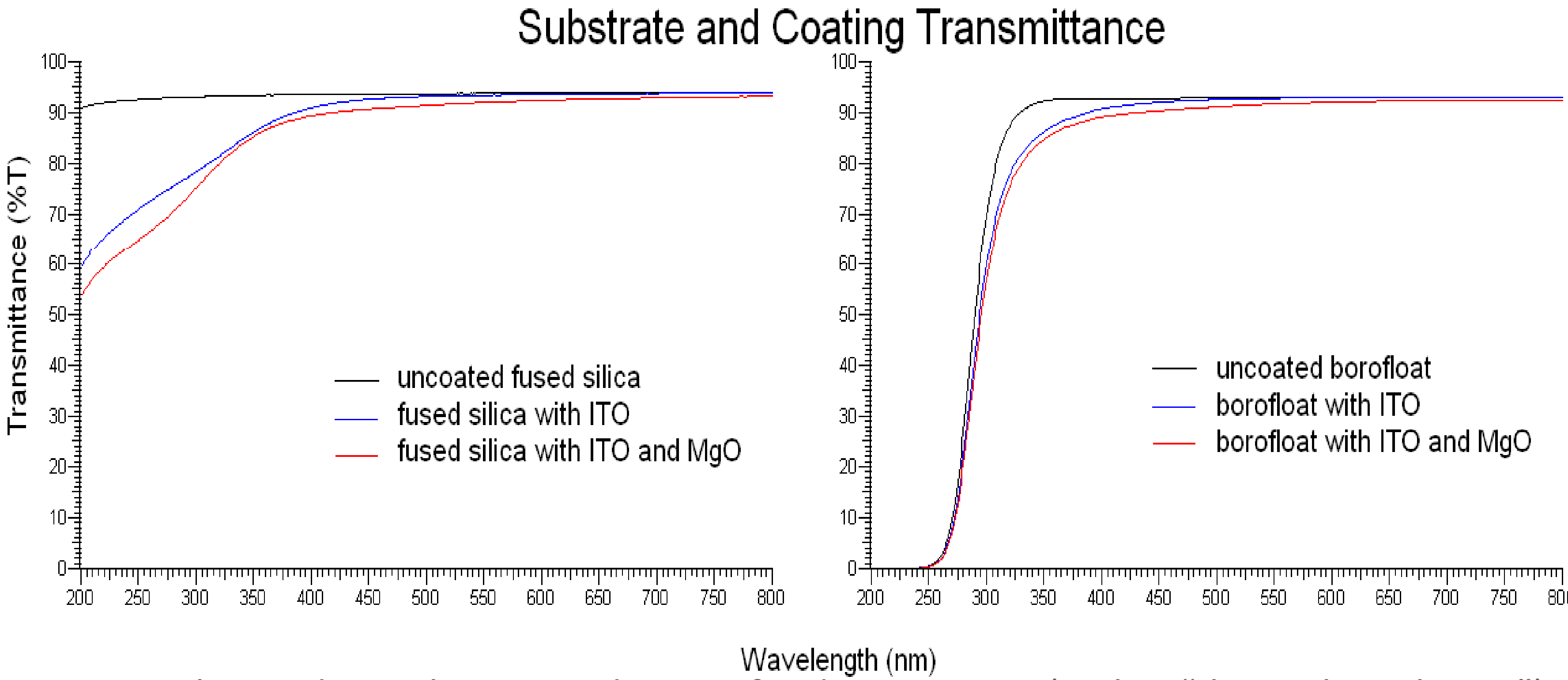
- Large technological importance:
  - Less influence of cleaning procedure of glass-window
  - Less influence of glass composition
  - Conductivity allows higher count rate applications

Optical Properties of Interface Layer

Glass: Fussed Silica or B33

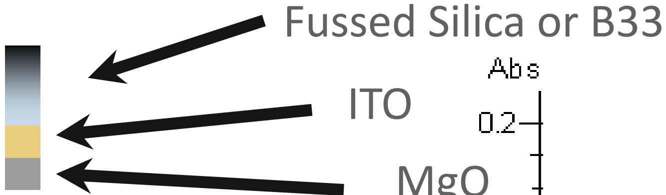
ITO (ALD): 2 monolayer Al2O3 and 4.5nm ITO

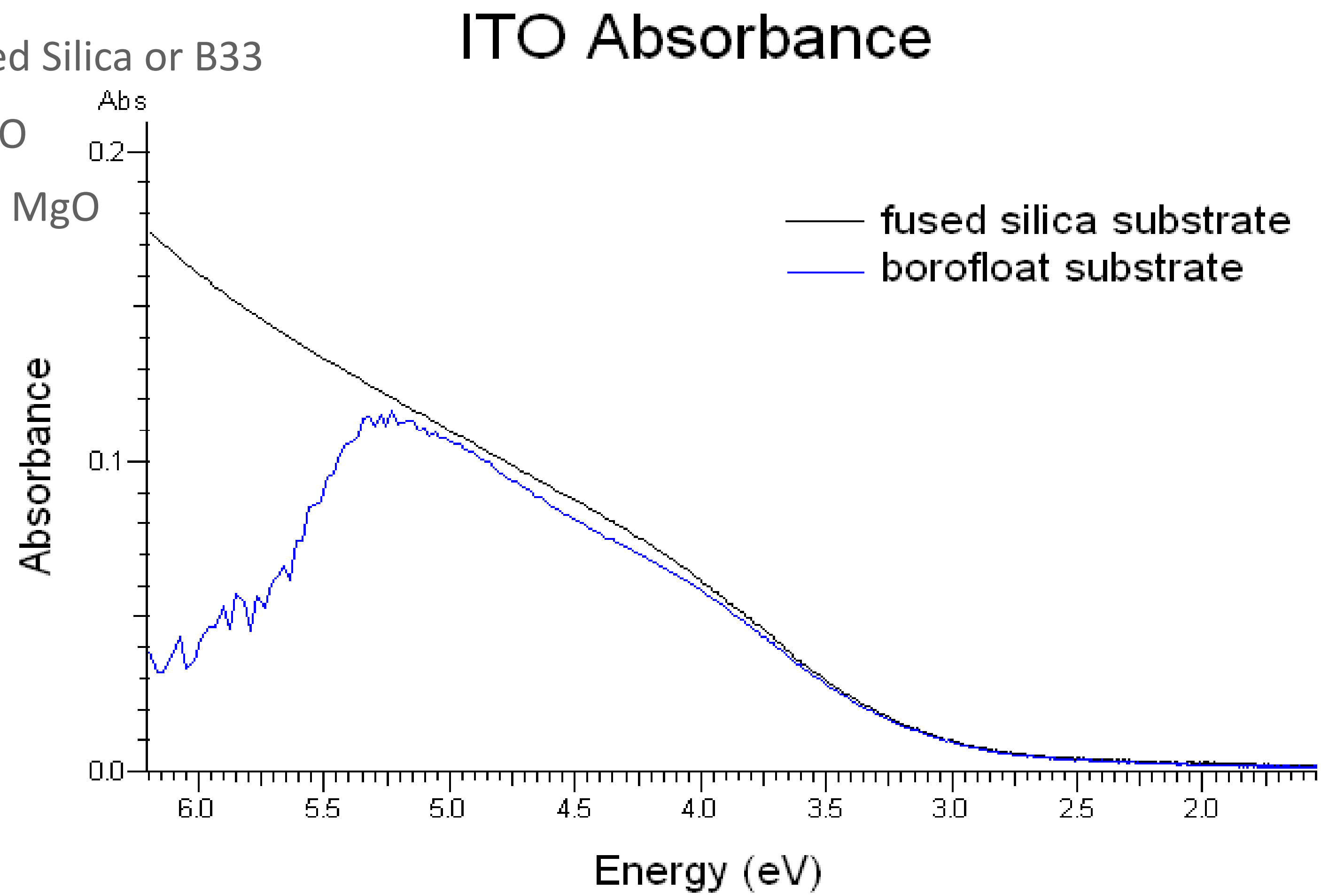
MgO: 5nm MgO layer applied with ALD



- Silica and B33 show no indication for doping states (within “thermal resolution”)
- Additional measurements (thoughts) will be necessary to determine if optical spectroscopy can trace surface states caused by cleaning procedure (increase of signal to noise figure by differential techniques)

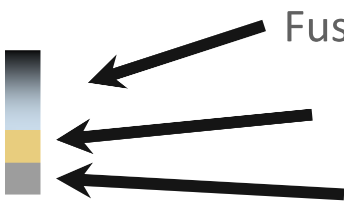
Optical Properties of Interface Layer

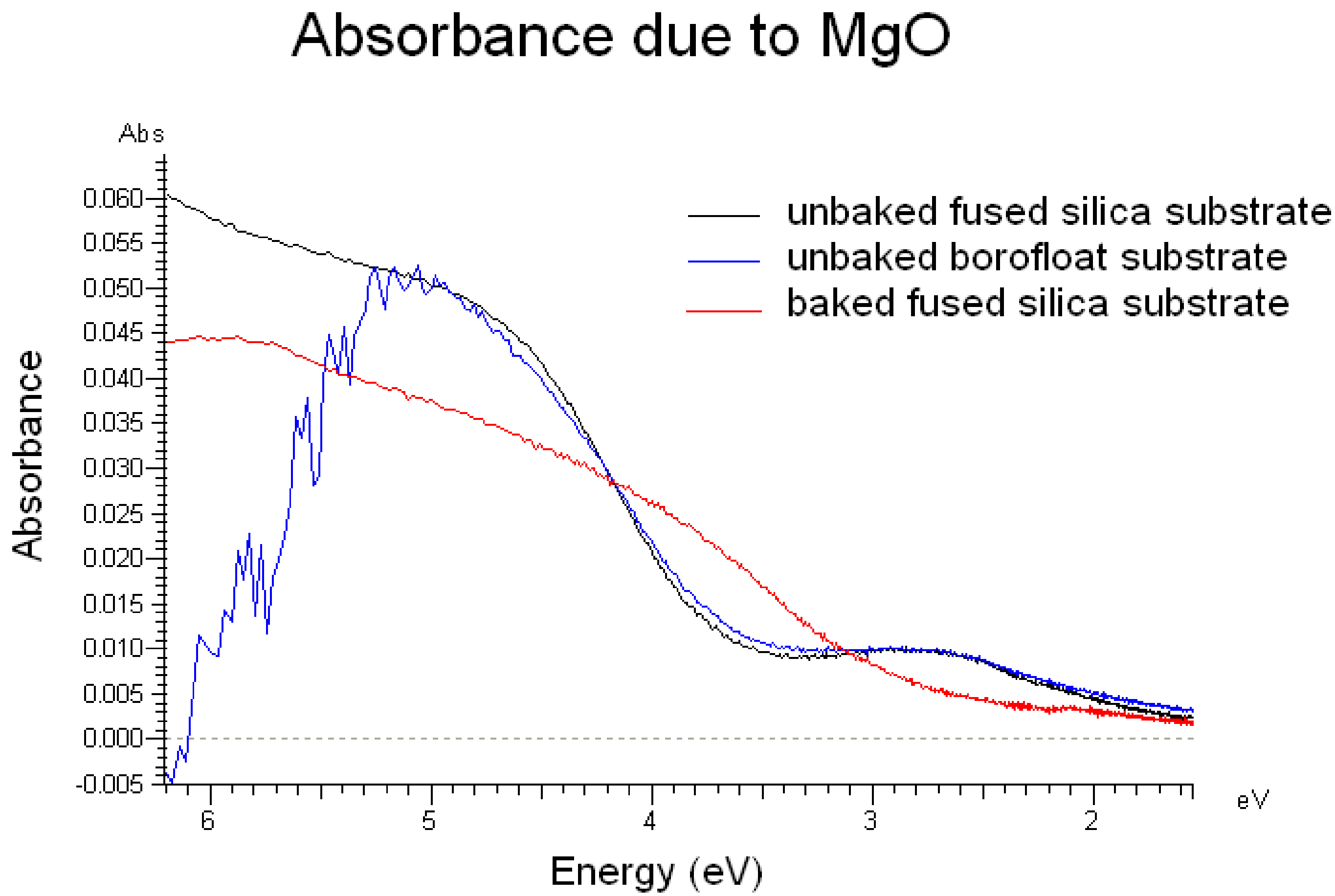




- show no indication for distinct doping states (within “thermal resolution”)
- Continuous increase indicates many doping levels with different energies (additional temperature dependent conductivity measurements will be necessary)

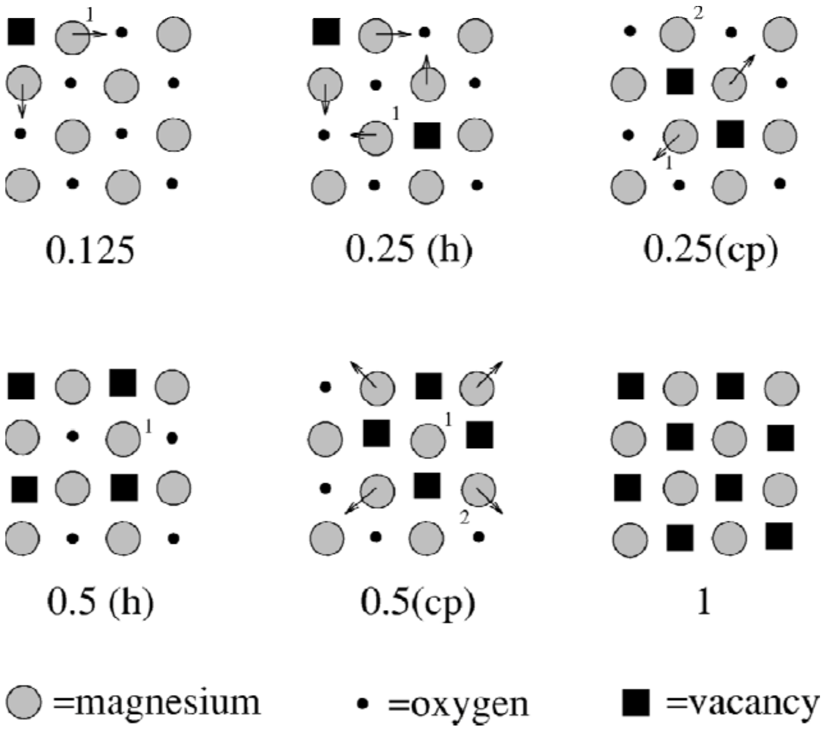
Optical Properties of Interface Layer



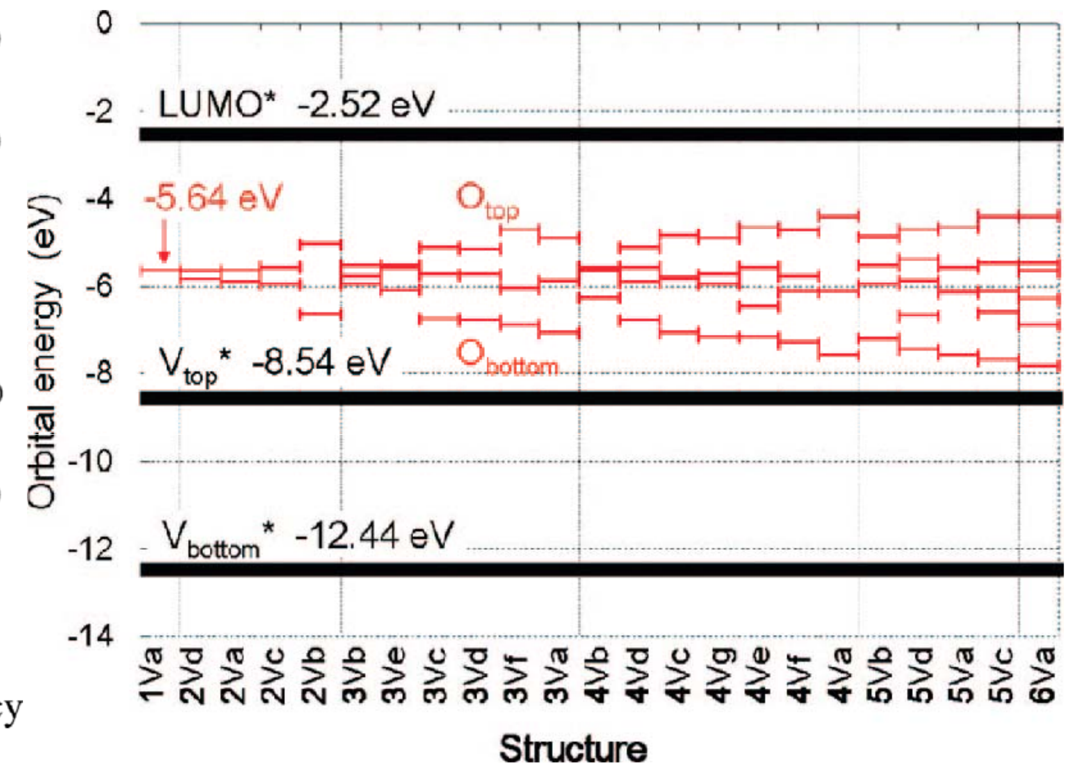


- Bandgap:7.8eV (literature)
- First increase around 5.5eV is according literature
- Peak at 2.7eV is clear indication for doping level (O defect?)
- After temper: absorbance is less!; peak disappears; onset sifts to low energy

Can We Understand the Optical Spectrum?



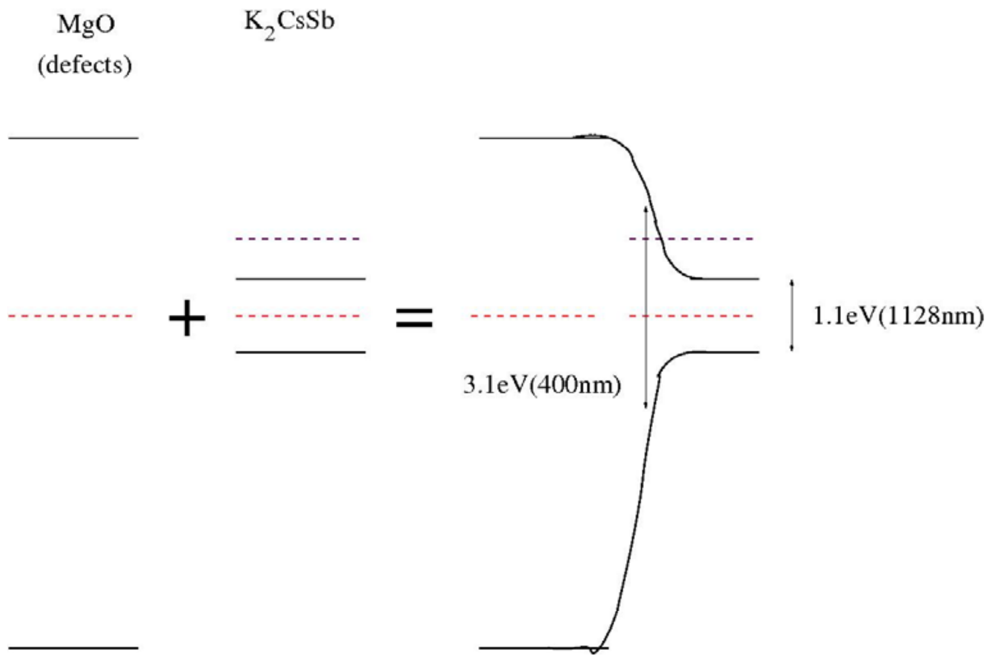
Phys. Rev. B 59, 5178–5188 (1999)

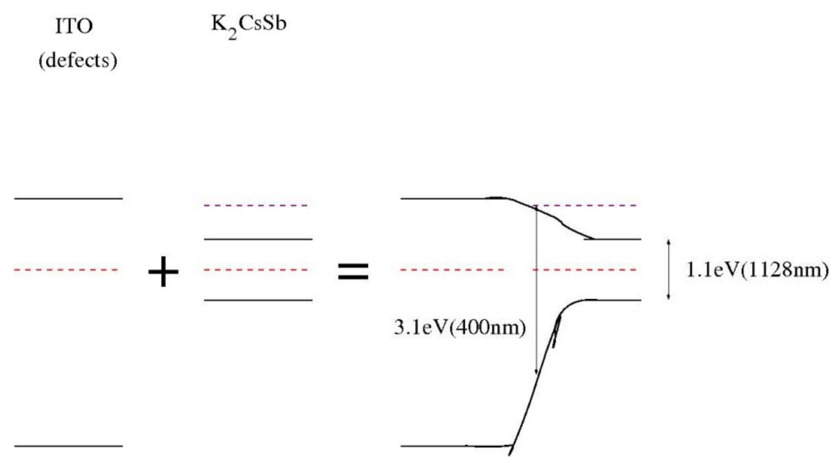


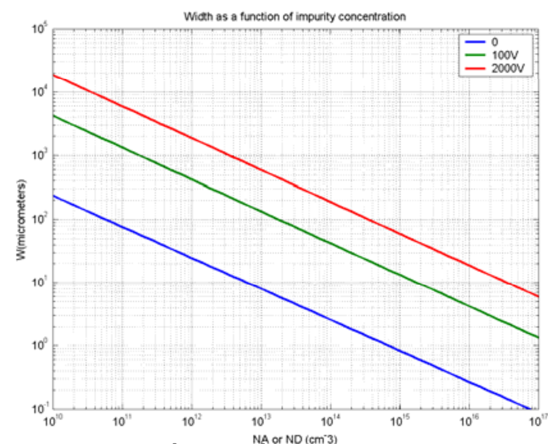
J. Chem. Theory Comput., Vol. 4, No. 7, 2008

- Energy levels of specific defects can be calculated (Insepov & Stegailov)
- Theory includes relaxation effects!
- Width and position of optical transition can be compared
- Defect model helps to do the “right thing” (growth parameters)

The Model: What does that Mean for a Cathode







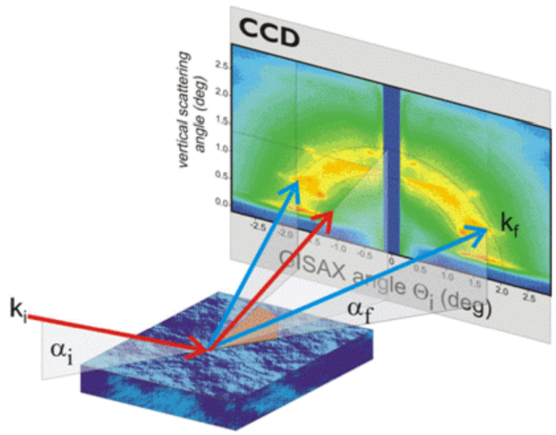
- Will require more simulation and calculation
- Basic understanding on influence on electric fields inside the device possible
- Optical spectroscopy in combination with theory is an essential tool
- Carrier densities will be needed (doping of the cathode)

Influences on Growth?

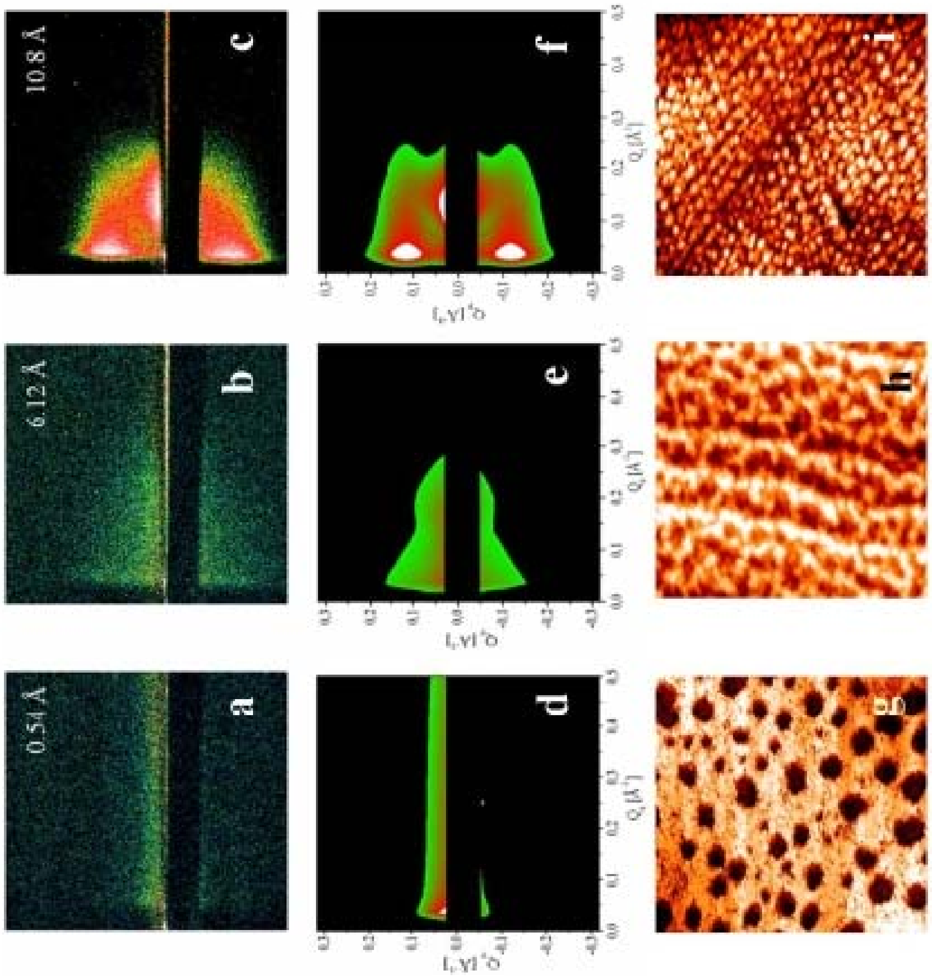
- We are here on the starting point
- Analytical tools (first applied to multialkali):
  - Exsitu AFM will determine the morphology
  - XAFS (X-ray Absorption Fine Structure): elemental composition and chemical bonding
    - Exsitu experiments: samples will be prepared by Burle-tool
    - In-situ setup with time resolved gracing incident techniques (depth sensitivity)
  - Gracing incidence scattering techniques
    - Ex-situ
    - In-situ
- Depending on funding situation: These measurements can be compared with simulations

Surface X-ray Scattering Techniques

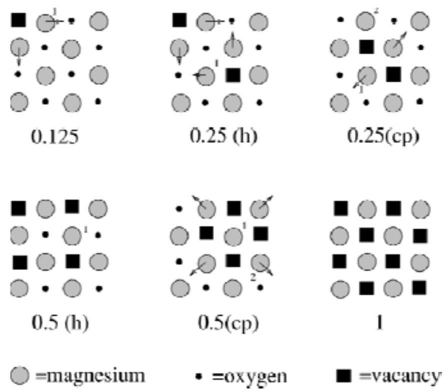
GISAXS investigation of quantum dots

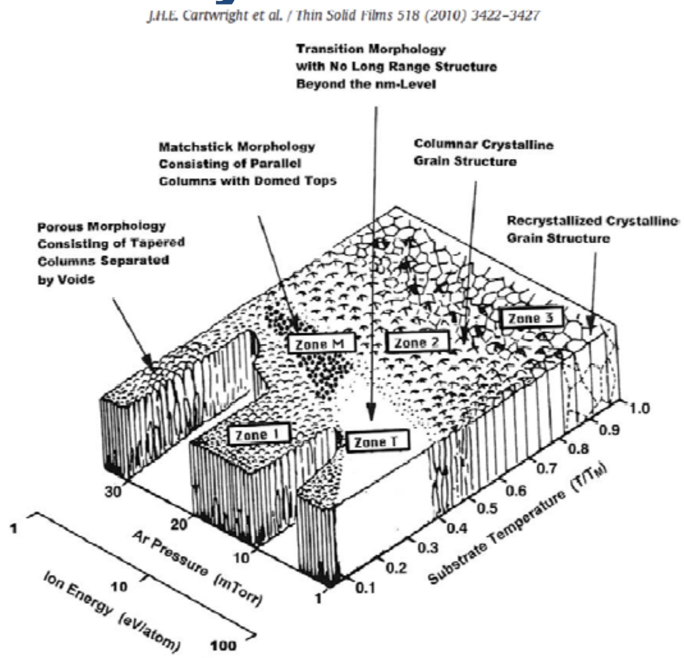


general GISAX-setup



What can the Theory Do?





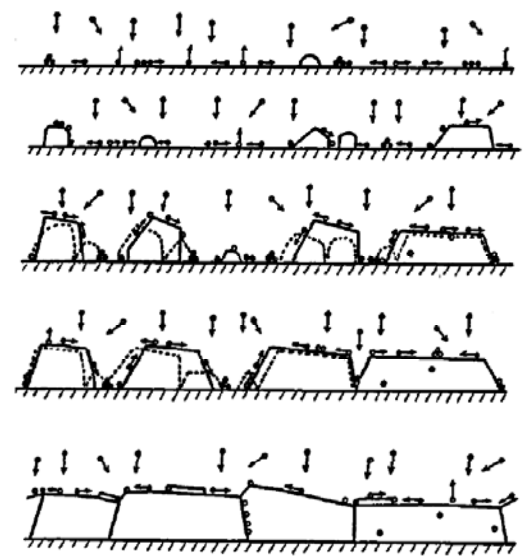


FIG. 1. Schematic diagram illustrating fundamental growth processes controlling microstructural evolution: nucleation, island growth, impingement and coalescence of islands, grain coarsening, formation of polycrystalline islands and channels, development of a continuous structure, and film growth (see Ref. 9).

Petrov, JVSTA 21 (2003) S117

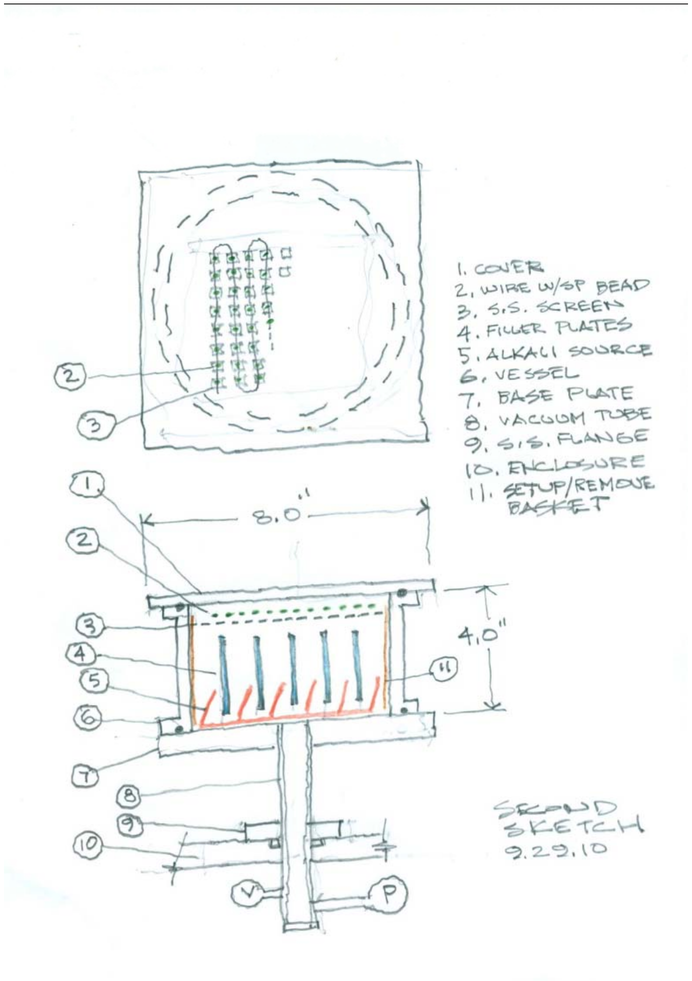
- Microscopic model and calculation of the required energy levels of substrate
- Growth simulation allows to develop microscopic model of growth
- Prediction and guidance in growth parameters and surface manipulation

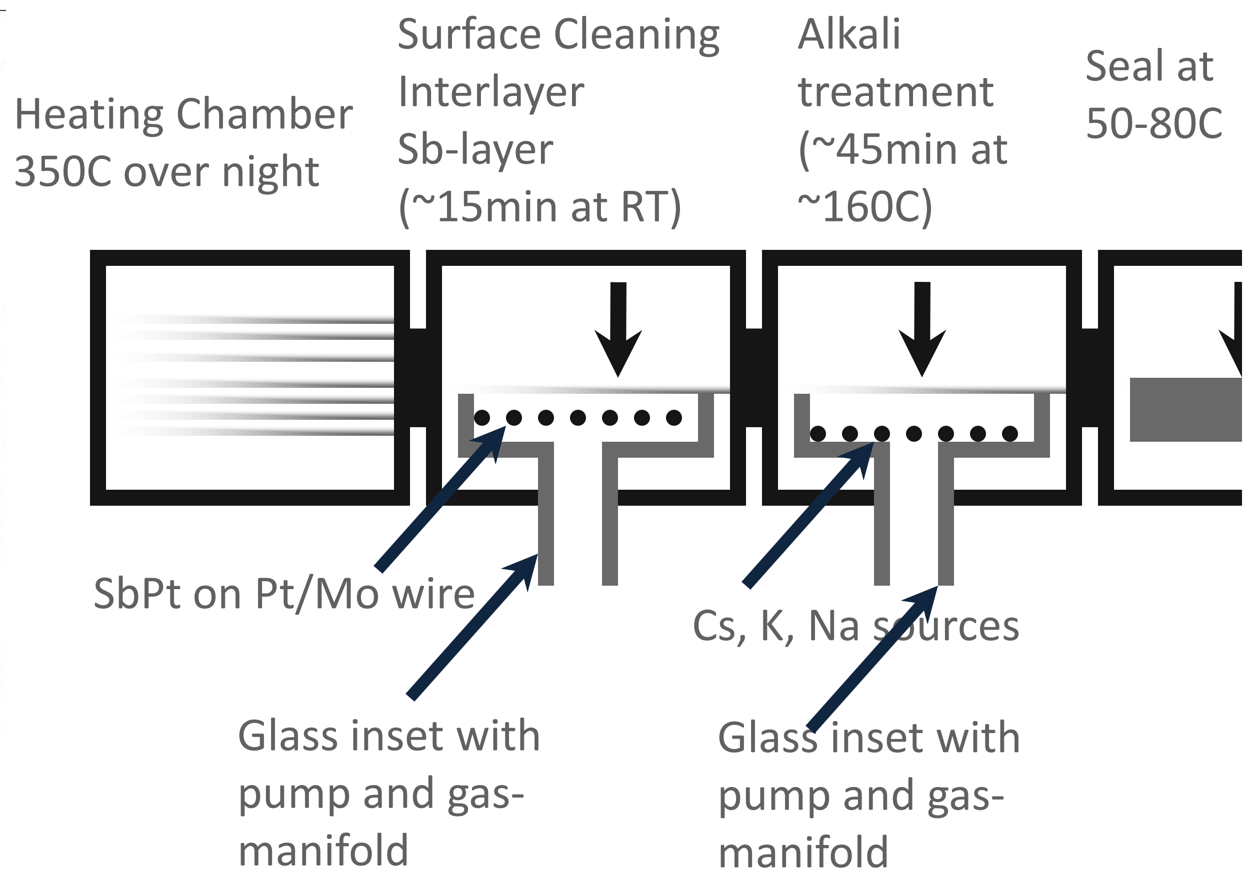
Be aware: The cathode is only ~20nm thick!

M_3Sb (M: K, Na, Cs)- Cathodes

- "Good" knowledge of what is known:
  - Influence of gas-pressure on growth
  - Island growth-film growth transition at 12nm thickness
  - Vertical phase-segregation yield to band banding
  - Under-layer shifts cathode to red
  - PMT-cathodes are with high probability amorphous
  - Band structure calculations of different compounds
- First PMT-like cathode made at Burle with Burle equipment
- Clear plan how to come from a PMT-cathode (amorphous) to a transfer cathode
  - PMT-like cathodes will be used for first analytical tests (especially interlayer)
  - 4"x4" design for evaporator compatible with Burle equipment with "removable" cathode
  - Integration of Burle-concept into transfer-cathode fabrication center
  - The center will allow to take out samples which can be transferred to characterization centers (under UHV)

Short Glance on the Idea (more by Zikri)





One master plate will allow to process cathode and take 1cm diameter test samples

The Growth and Characterization Tools used for M_3Sb (M: K, Na, Cs)- Cathodes

- Growth:
  - Burle equipment (available in about 3month)
    - Exact recipe test
    - Engineering issues of evaporators
    - “Transfer-test”
  - Growth & Characterization Chamber (5-6 month)
    - Modifications of recipe
      - Cleaning procedure (ion/atomic source)
      - Base pressure influence on growth and functionality
      - Evaporation versus sputter
      - Sequential versus co-evaporation
    - Study of inter layer influence
      - Morphology
      - Electronic properties
      - Indirect structural properties
  - Production facility (9-12 month)
    - Homogeneity test
    - Recipe test

The Growth and Characterization Tools used for M_3Sb (M: K, Na, Cs)- Cathodes

- Characterization:
  - In-situ characterization of growth and characterization chamber
    - Optical spectroscopy (UV-VIS) with cryo-capability (200nm-1600nm)
      - Transmission and reflection
      - Angle dependence
    - Electrical characterization
      - QE
      - Photo-conductivity
      - Temperature dependent I-V curves
      - Lateral and transversal conductivity
  - Ex-situ (non vacuum) characterization
    - AFM
    - UV-VIS
  - Structural probes
    - Gracing incidence X-ray techniques (in collaboration with John Smedley (BNL) and APS)
      - First beamtime in December
    - Depth and lateral analysis by Igor (more by himself)

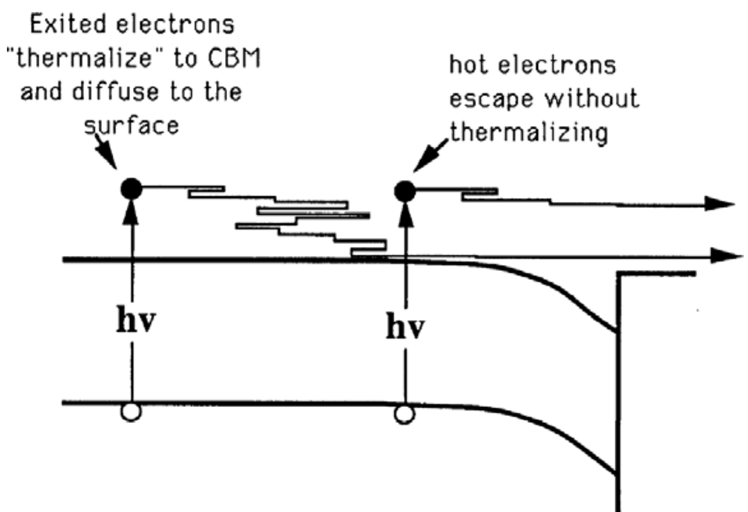
GaN

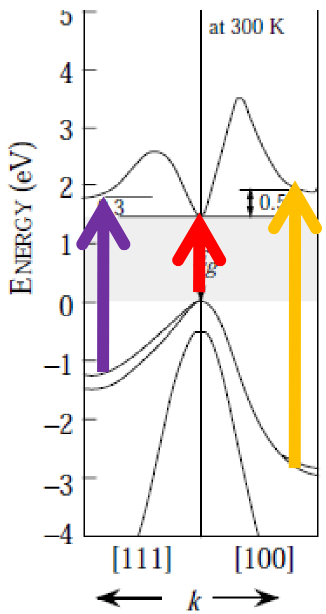
- Will be presented by Jim Buckley

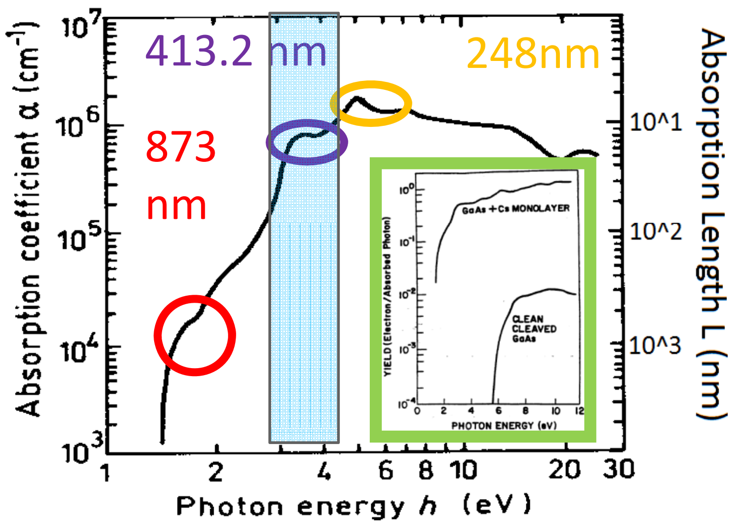
GaAs: The Main Challenges

- Wavelength optimization
- Doping profile optimization
- Minimizing dark-current
- Transfer and bonding technology

Wavelength Optimization of Layer Thickness: The Optimization Criteria

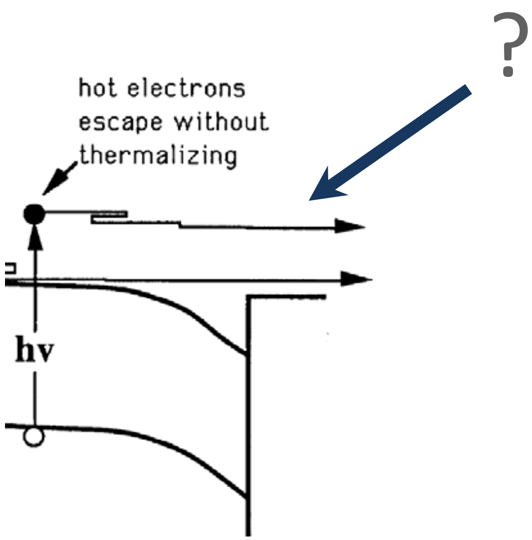


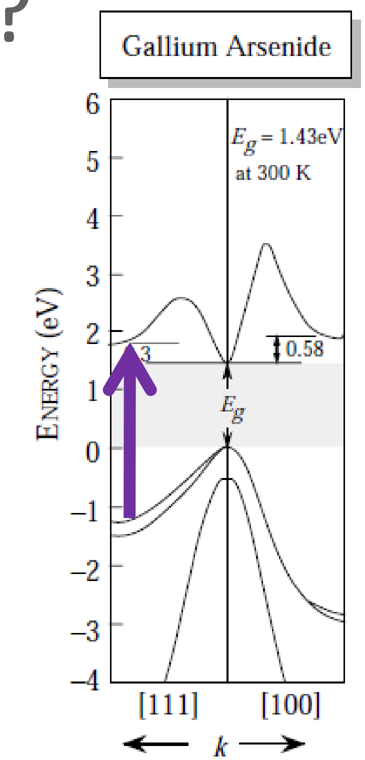




- Efficiency depends on
  - Probability to absorb photon
  - Probability to reach surface
  - (Probability to escape from surface is thickness independent)
- Case GaAs (only an example)
  - Direct bandgap in IR (typical application)
  - Typical absorption length for IR: 1µm
  - Absorption length for 400nm: **30nm-100nm**
- Consequences:
  - Cathode has to be by a factor 10 thinner!
  - Photoelectron has defined kinetic energy
  - Thickness is thinner than mean free path-length
  - Crystallographic direction matters
  - Defect density, strain, …. at the interface between cathode and window matters!

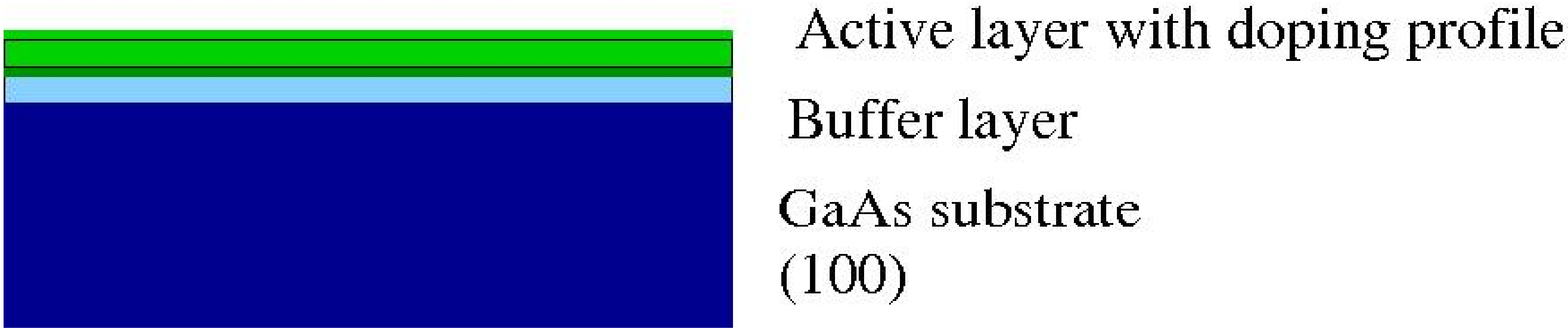
What Happens in a 100nm Thick GaAs Cathode (400nm Photon)

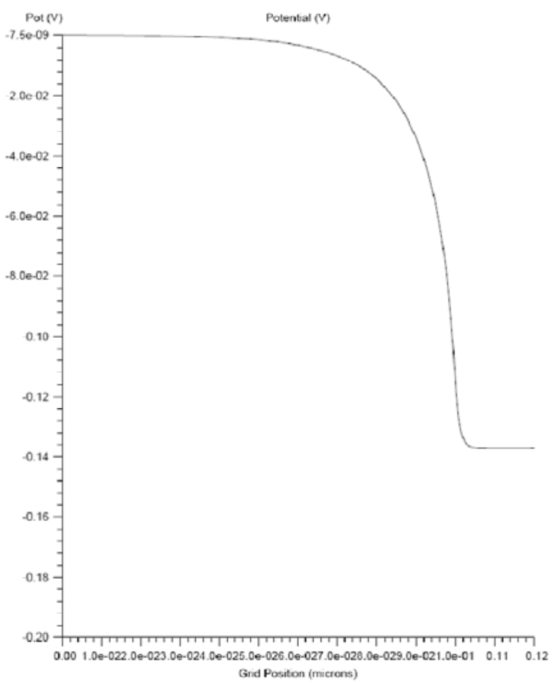




- Answer: **NO**
  - Creation of hot electron
  - Momentum in cathode plane!
    (electron will not reach surface if not scattered)
- Result:
  - Low QE
  - Very slow
- Solution:
  - Increasing scattering probability
    (can be done: tuning band structure to phonon distribution)
  - Better: creating internal electric field gradient
    - By doping gradient (what we have done)
    - Or by external electric Field.

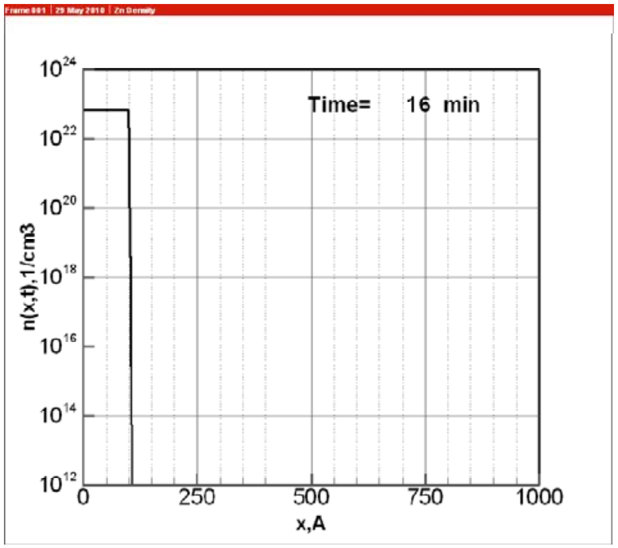
The Doping Profile: The First Steps

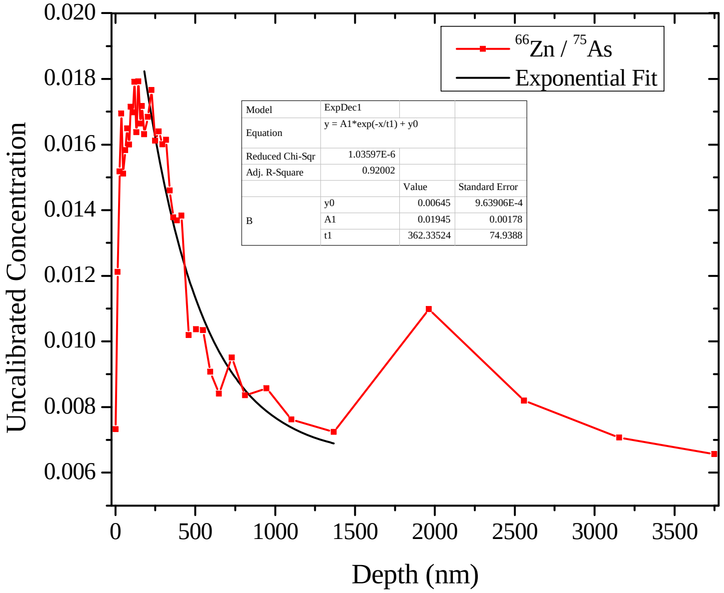




- Doping profile
  - Electric field distribution can be calculated by commercial simulation programs
  - Typical potential difference 0.1-0.2eV
- Influence on timing behavior
  - Theoretical potential possible which allows transient time independent from absorption position!
  - Optimization possible even for very hard x-rays?

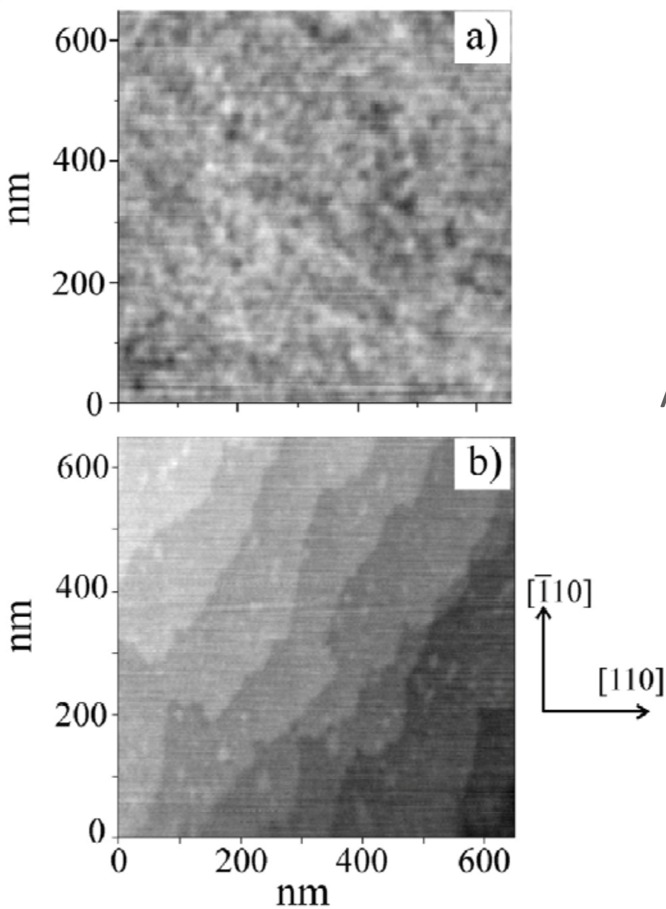
Is the Doping Profile Stable During Processing



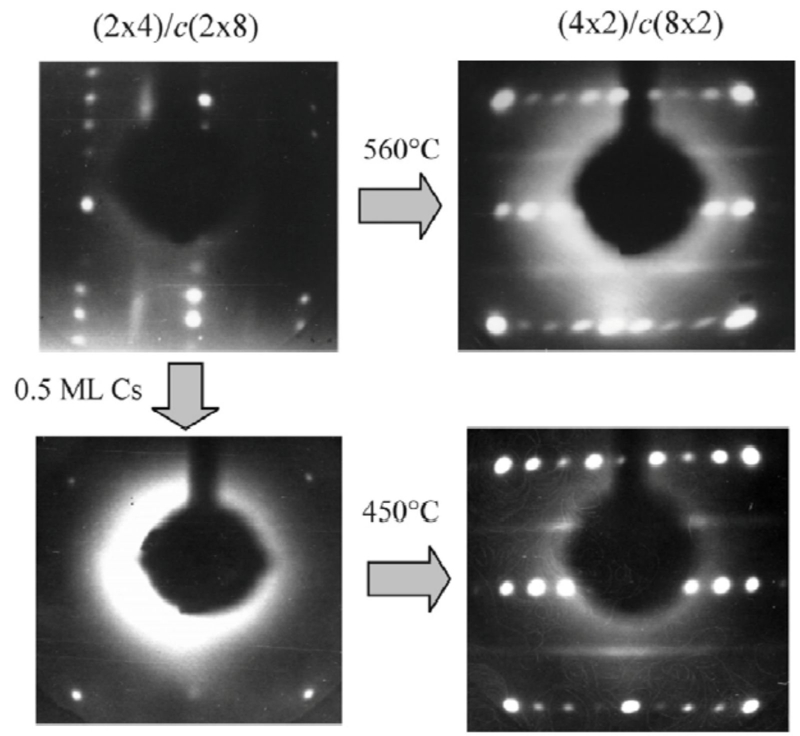


- Approach:
  - Minimizing process temperature
  - Using simulations to predict doping profile after processing
  - Calibrating simulations with selected samples using SIMS (Igor & Slade)
- Status:
  - First simulations done by Zeke Insepov
  - In the process of creating SIMS measurements

The Emission Layer:
The Standard Cleaning and Activation of GaAs



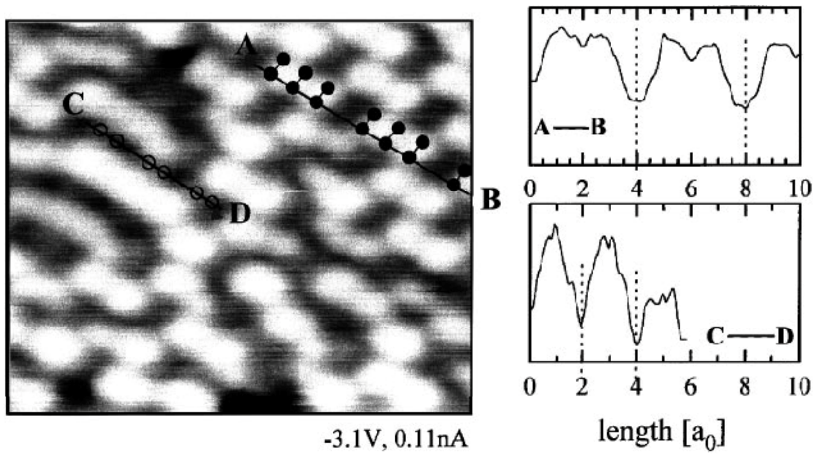
As-rich



Ga-rich

e-J. Surf. Sci. Nanotech. Vol. 5 (2007) 80-88

The Activation and Dark Current



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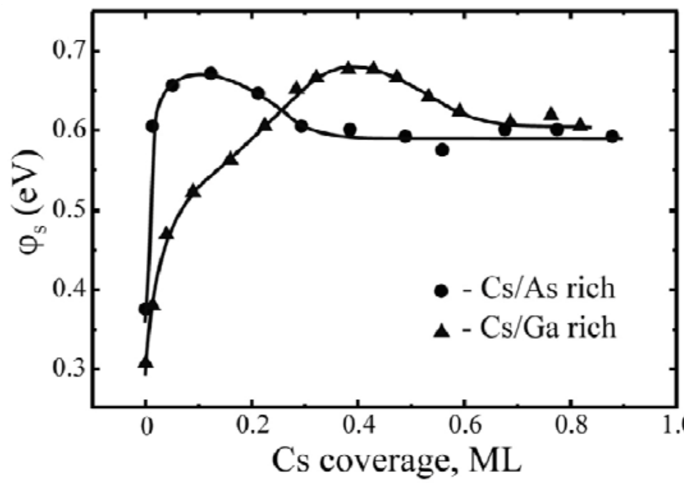
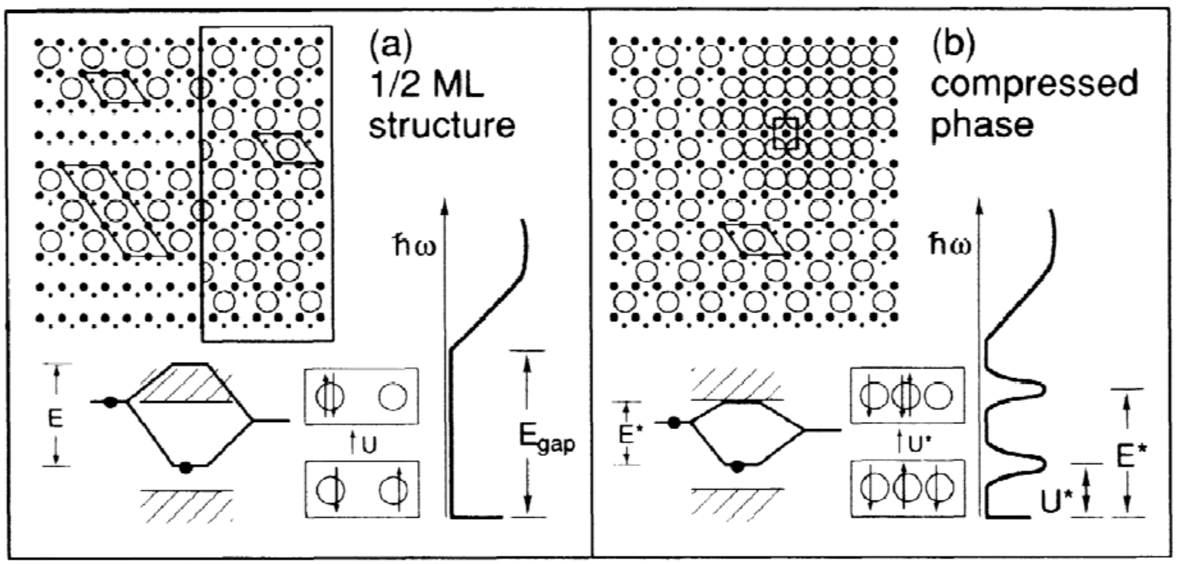
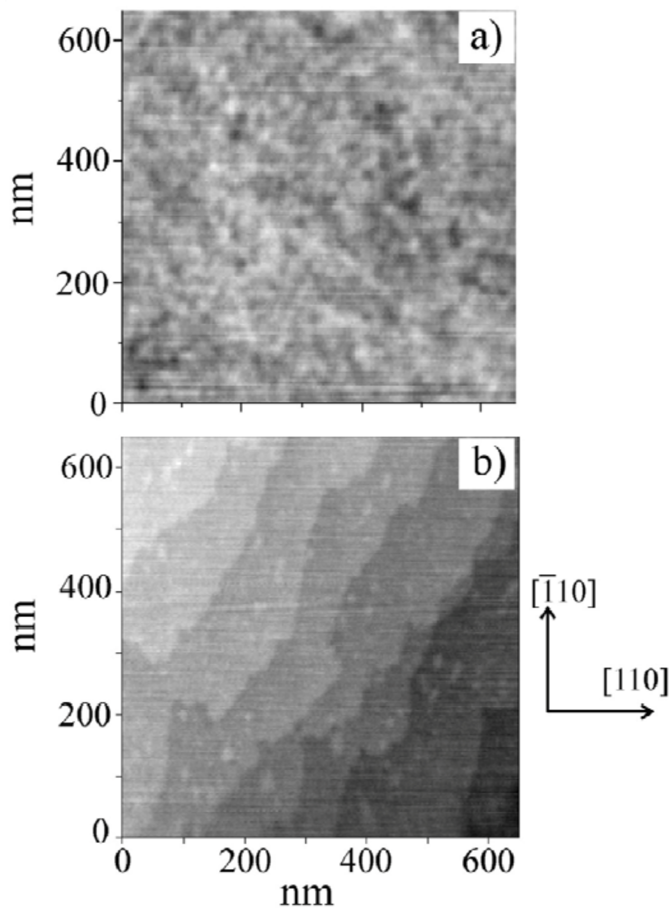




Phys. Rev. Lett. 81, 721–724 (1998)

- Exact details of surface and Cs contribution determines electronic states of activation layer
- Dark counts are highly effected by these details
- Effects of morphology unknown
- Long term stability depends on exact composition

Where We are Now?



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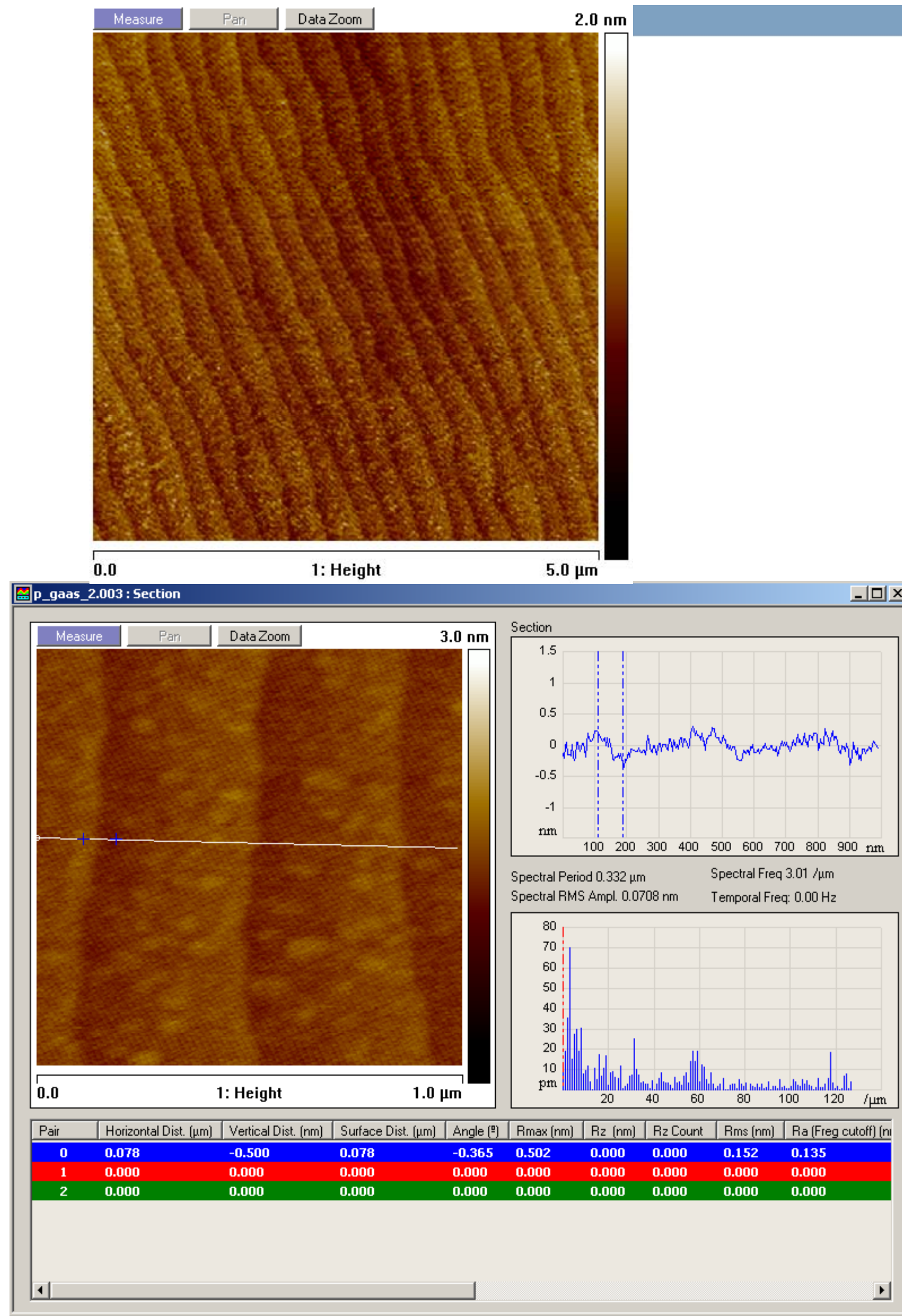
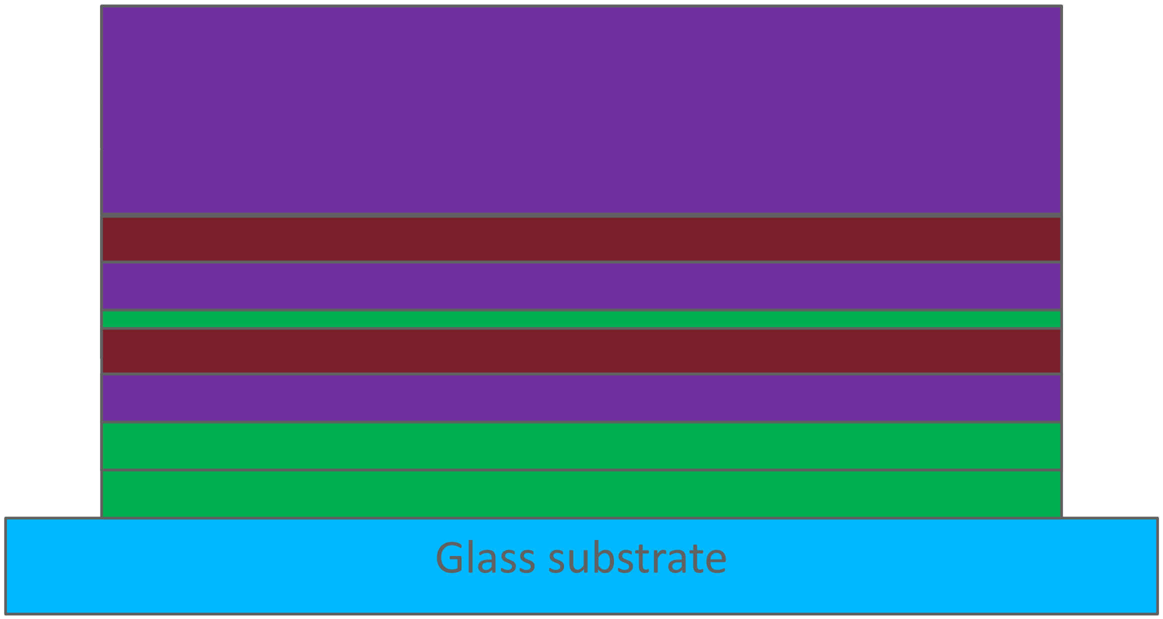


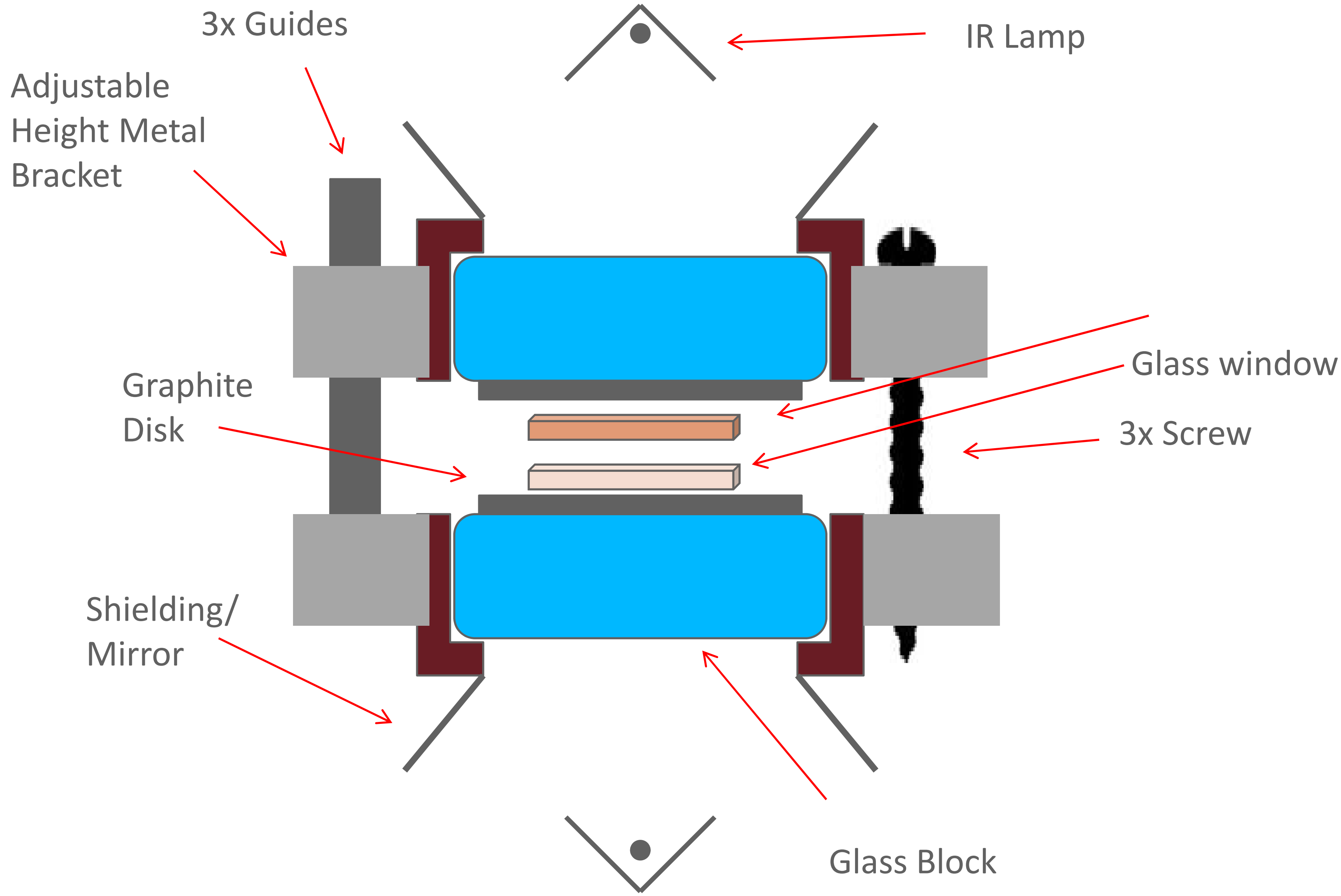
The Transfer and Bonding Technology



First test structured are made and characterized (roughness and shape errors (10x10mm^2)

1. Grow thin layer of sacrificial AlGaAs
2. Growth of photocathode, with layers inverted
3. Deposition of intermediate bonding layers (i.e. SiO_2, $S_{ix}N_x$)
4. Wafer bonded to a glass substrate predeposited bonding layers
5. Bulk of substrate is etched/CMP away
6. Sacrificial layer removed
7. Photocathode ready for activation

Bonding Apparatus Schematic



Conclusion & Take-Home-Message

- The selected cathode systems are:
  - M_3Sb (M: K, Na, Cs)- Cathodes
  - GaAs (in collaboration with UIUC)
  - GaN (in collaboration and under lead of WashU)
- All cathodes of interest follow the same physics principle
  - Similar band structure results in similar thickness requirements
  - Design principles can be transferred between
  - Materials science aspects are different for the three groups
  - Optical, electrical and many structural properties are known: clear program what has to be done
- ANL is focused:
  - Creating proto-type production facility with most cost-efficient recipe
  - Creating the foundations that we will be able to cover the full spectral range after 2 years
  - Providing microscopic and macroscopic characterization tools
  - Providing state-of-the-art theory support utilizing collaborations
- Communication with other institutions:
  - First test using the interlayer-study