



**Northern Illinois
University**



Modeling, Growth, and Characterization of Advanced Photocathode Materials at Northern Illinois University

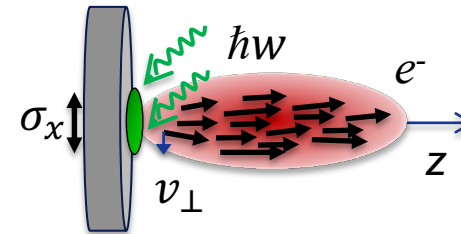
Oksana Chubenko

Department of Physics, Northern Illinois University

Introduction

High-quality electron beams =

- bright beams $B_{4D} \propto \frac{N_{bunch}}{\epsilon_x \epsilon_y} \propto \frac{(E_z)^k}{MTE}$



Photocathode

$$N_{bunch} \propto \sigma_x \sigma_y (E_z)^k$$

$$1 \leq k \leq 2$$

$$\epsilon_{x,y} = \sigma_{x,y} \sqrt{MTE/m_e c^2}$$

High-quality photocathodes =

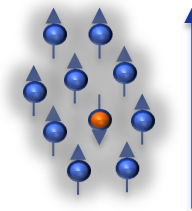
- low mean transverse energy $MTE = \frac{m \langle v_{\perp}^2 \rangle}{2}$
 $MTE \sim k_B T \sim 25 \text{ meV}$ at room temperature \rightarrow $MTE \sim \text{few } 100\text{s meV}$

Factors, limiting MTE:

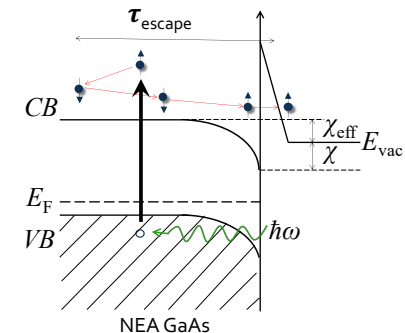
- requirements of the high charge density
- disordered nature of photocathode materials
- surface roughness and work function variations

- high Quantum Efficiency, $QE = \frac{N_{e^-}}{N_{\hbar\omega}}$

- high Electron Spin Polarization, $ESP_0 = \left| \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}} \right|$



- prompt response time



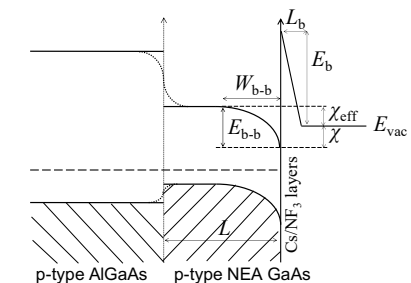
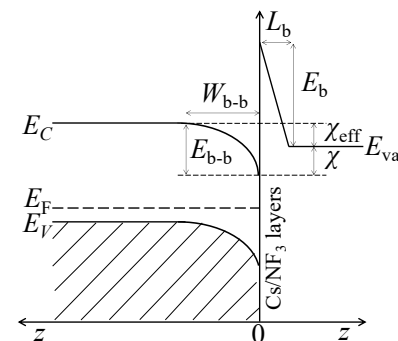
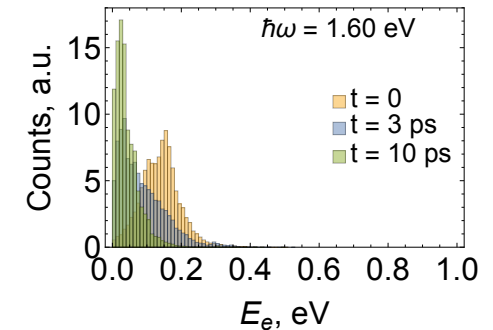
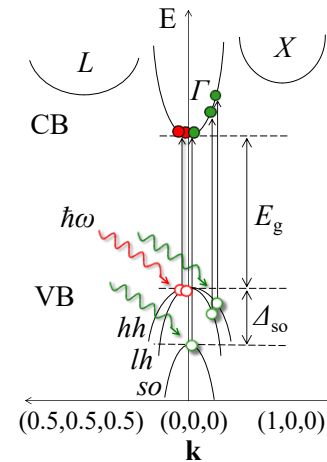
- robustness + long operational lifetime under realistic photoinjector conditions (5-100 MV/m to extract $\sim 50\text{-}1000$ pC/mm² of charge densities/bunch)

Monte Carlo Modeling of Photoemission from Semiconductors

Monte Carlo Modeling of Photoemission from Semiconductors

Advantages of Monte Carlo approach:

- QE, ESP, MTE, response time = $f(\hbar\omega, p, \chi, T)$.
- Accounts for the subtleties of the material band structure.
- Does not require *a priori* assumption about the particle distribution functions.
- Can be easily modified to include different scattering mechanisms to model both steady-state and non-equilibrium conditions.
- Accounts for the surface effects.
- Can be applied to both bulk and thin layers.

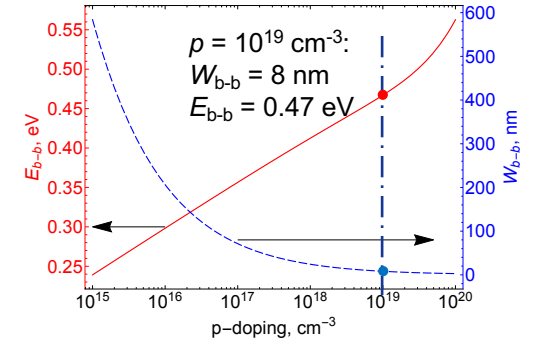
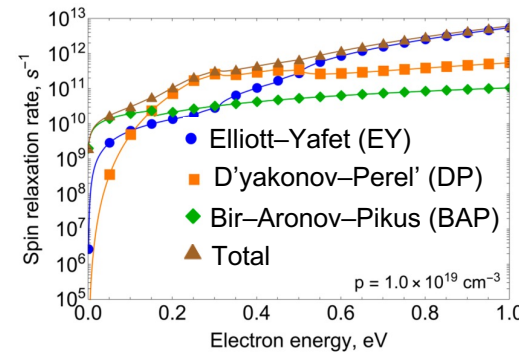
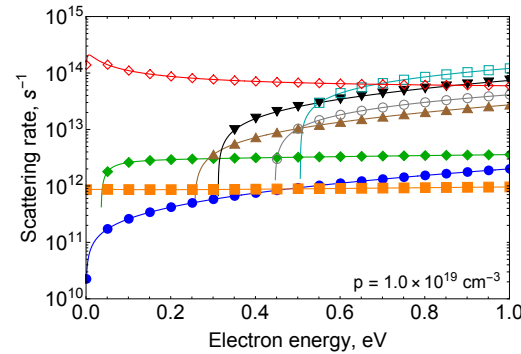
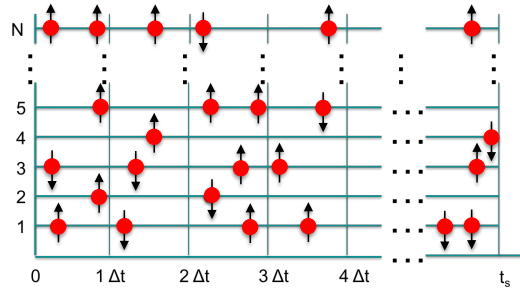


Monte Carlo Modeling of Photoemission from Semiconductors

AAC24 Advanced Accelerator Concepts Workshop

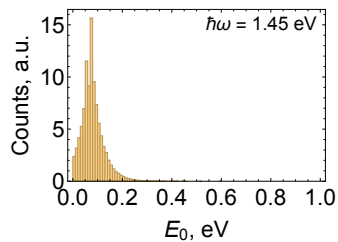
Jul 22, 2024

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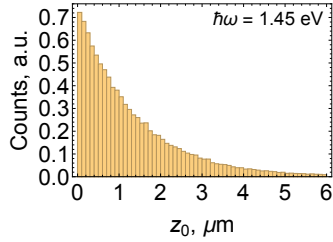


Photoexcitation

Initial energy distribution of photoexcited electrons

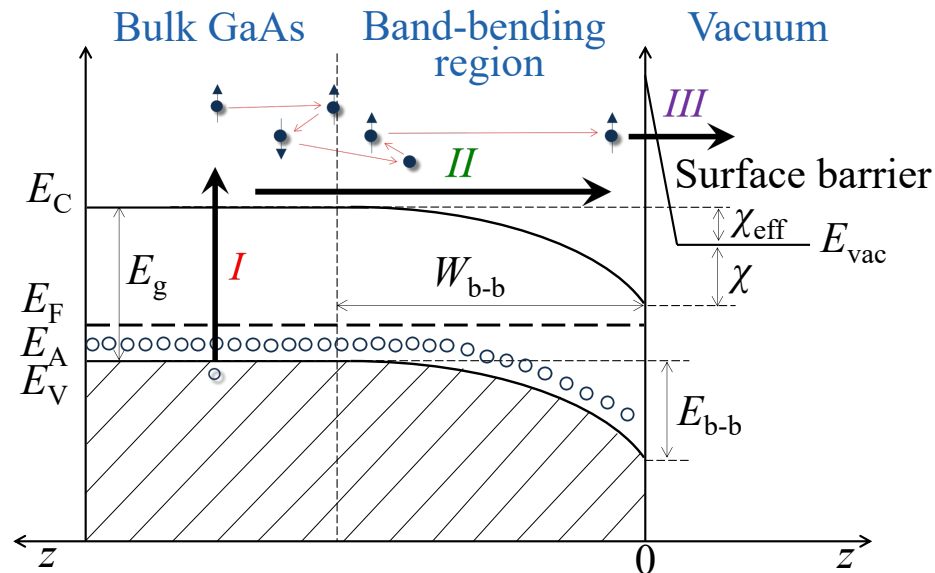
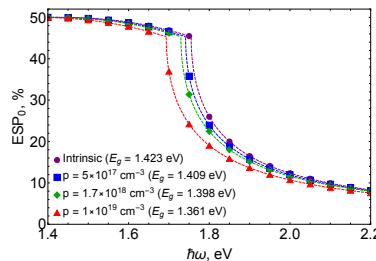


Initial electron distribution in real space

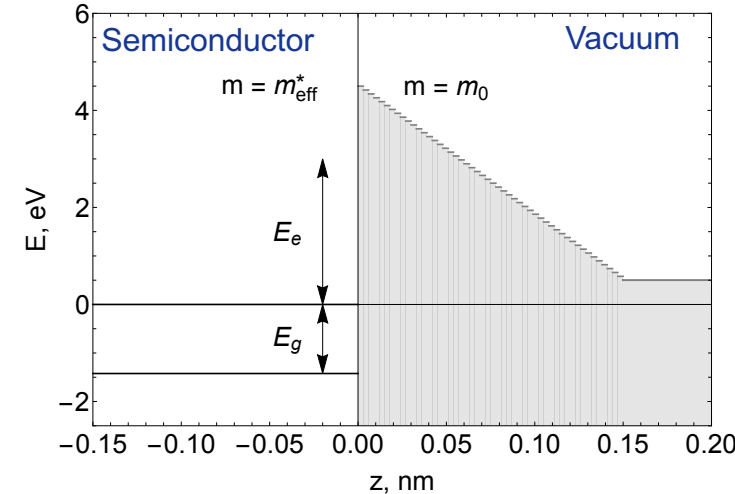


Initial spin orientation of photoexcited electrons

$$ESP_0 = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}}$$



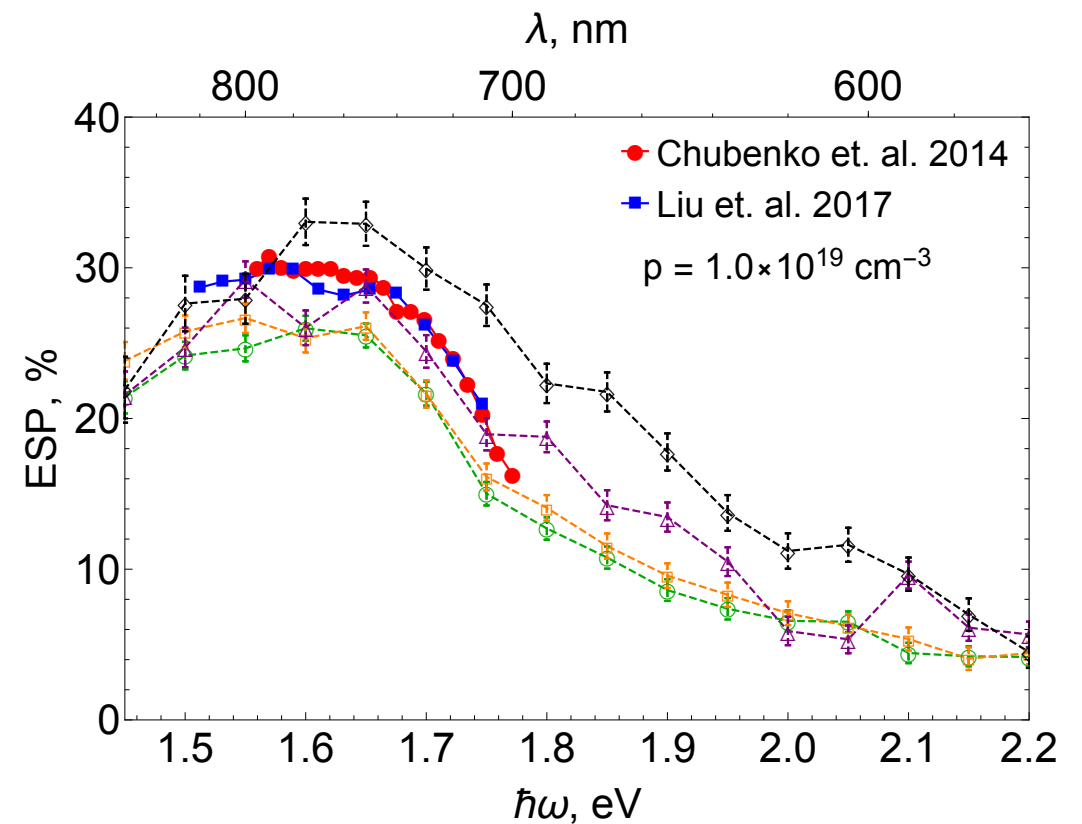
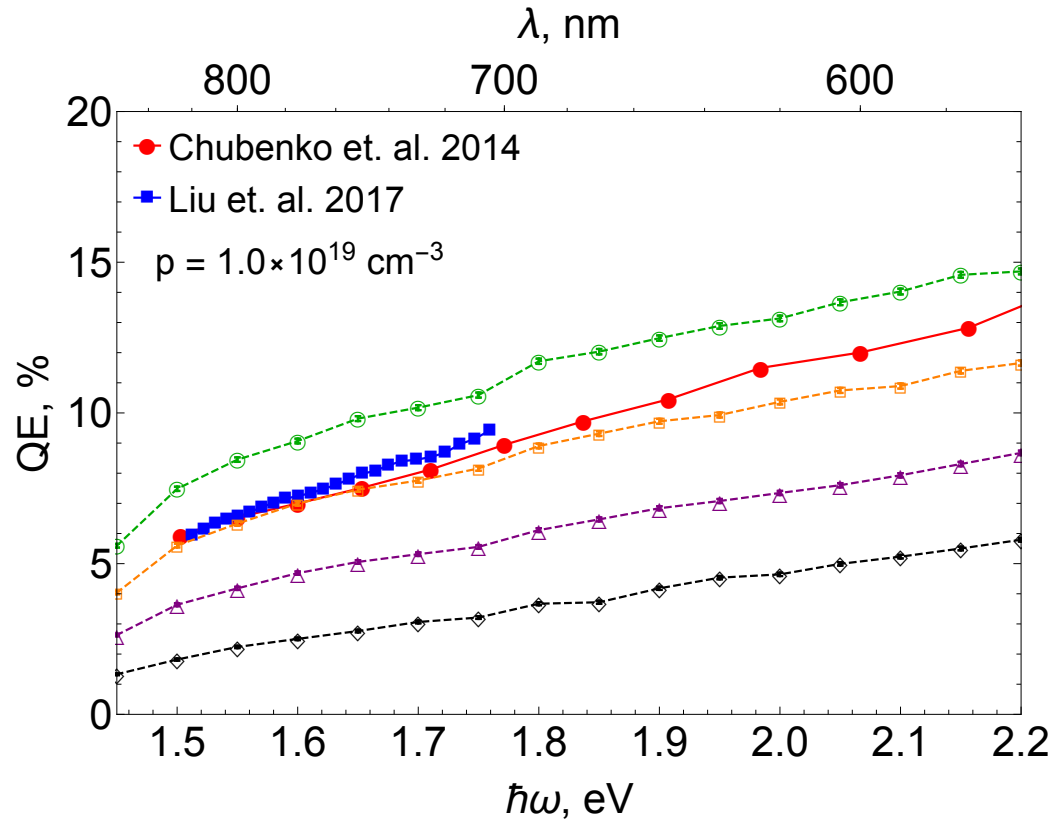
Emission



Spin-polarized photoemission from p-type GaAs activated to Negative Electron Affinity (NEA): I – photoexcitation, II – transport, III – emission.

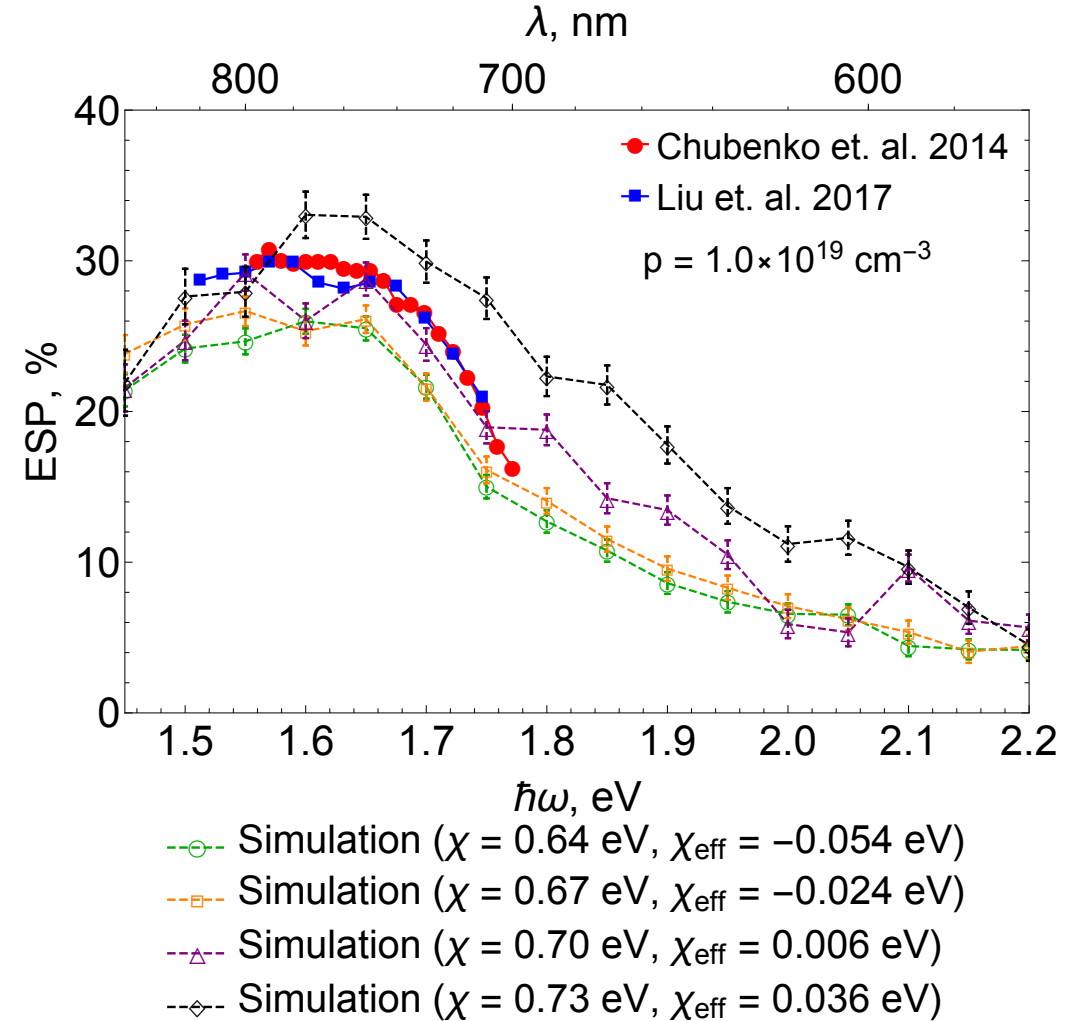
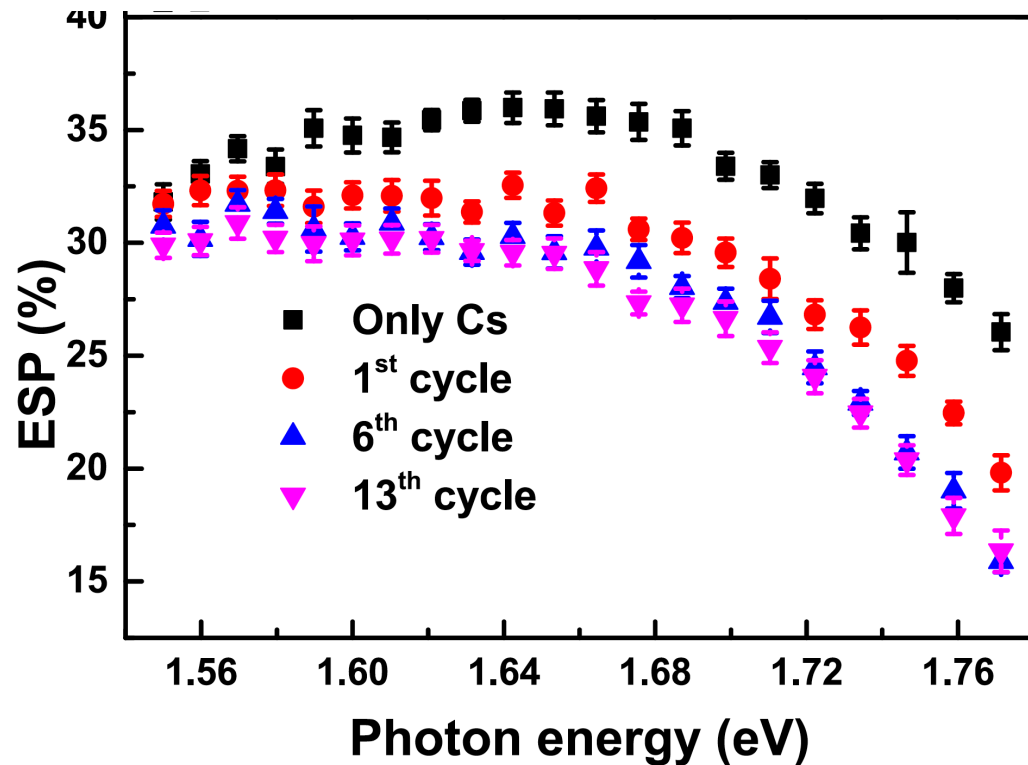
Spin-polarized Photoemission from GaAs

Comparison with experiment: QE and ESP from p-type GaAs for different electron affinity levels



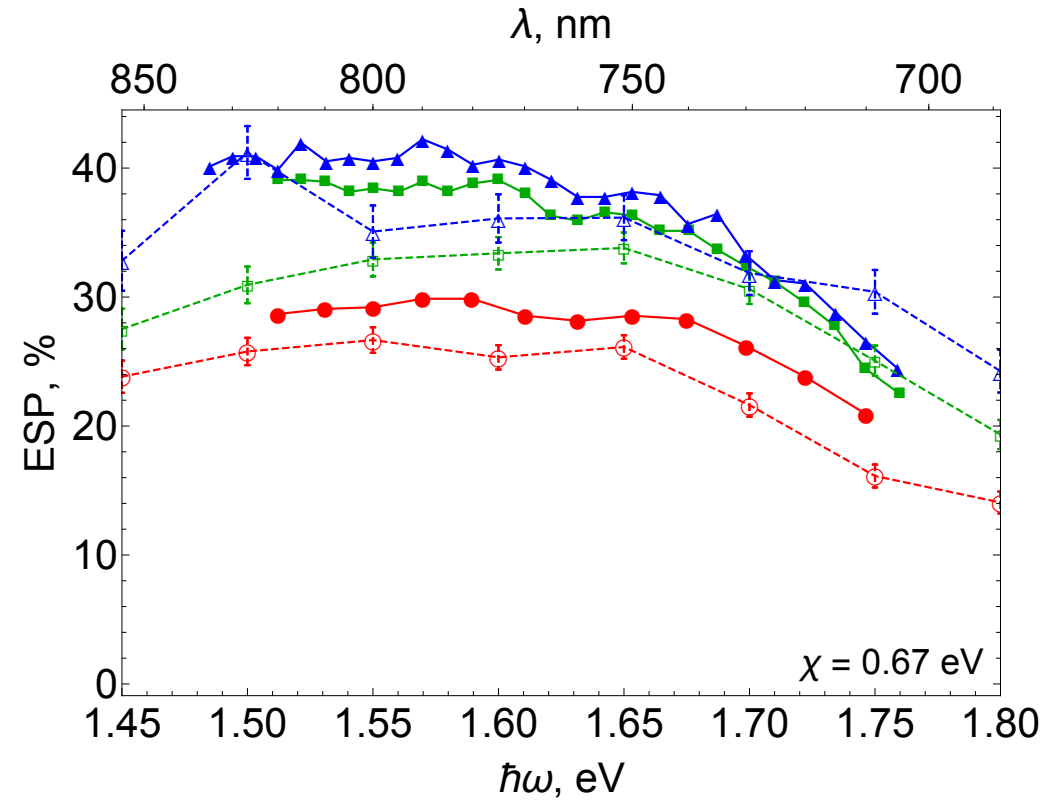
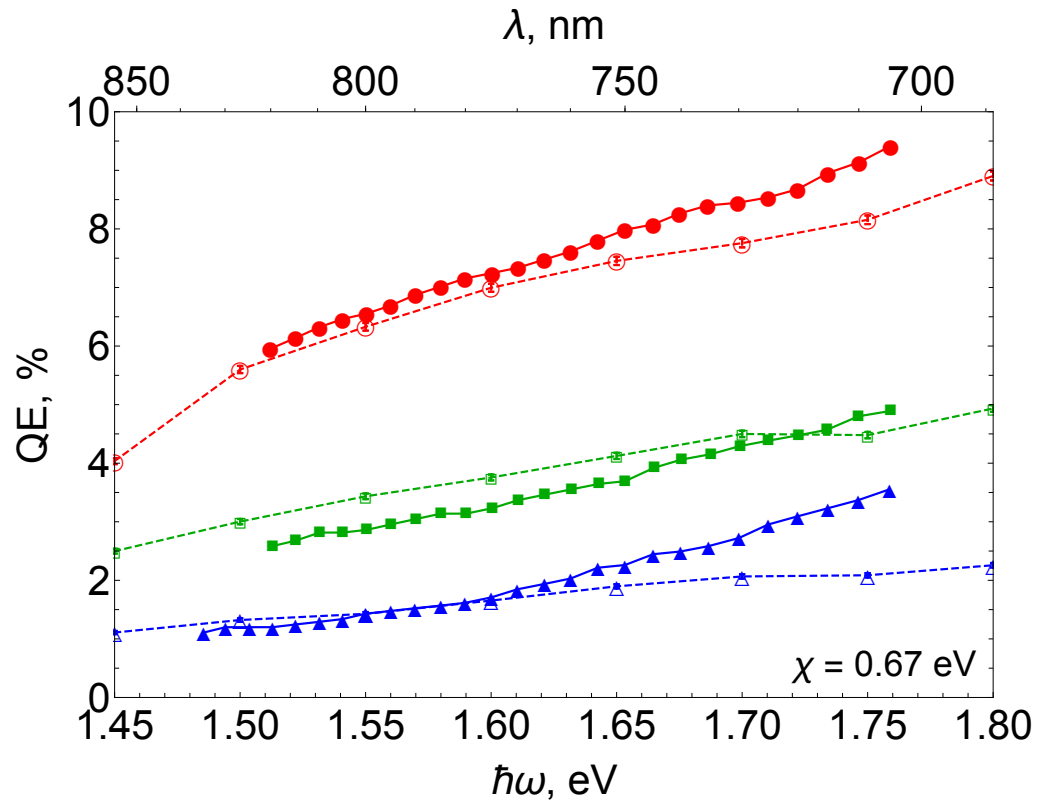
- Simulation ($\chi = 0.64 \text{ eV}$, $\chi_{\text{eff}} = -0.054 \text{ eV}$)
- Simulation ($\chi = 0.67 \text{ eV}$, $\chi_{\text{eff}} = -0.024 \text{ eV}$)
- △— Simulation ($\chi = 0.70 \text{ eV}$, $\chi_{\text{eff}} = 0.006 \text{ eV}$)
- ◇— Simulation ($\chi = 0.73 \text{ eV}$, $\chi_{\text{eff}} = 0.036 \text{ eV}$)

Introduction



Introduction

Comparison with experiment: QE and ESP from p-type GaAs for different doping densities



- Liu et. al. 2017 -○- Simulation ($p = 1 \times 10^{19} \text{ cm}^{-3}$, $\chi_{\text{eff}} = -0.024 \text{ eV}$)
- Liu et. al. 2017 -□- Simulation ($p = 1.7 \times 10^{18} \text{ cm}^{-3}$, $\chi_{\text{eff}} = 0.012 \text{ eV}$)
- ▲ Liu et. al. 2017 -△- Simulation ($p = 5 \times 10^{17} \text{ cm}^{-3}$, $\chi_{\text{eff}} = 0.039 \text{ eV}$)

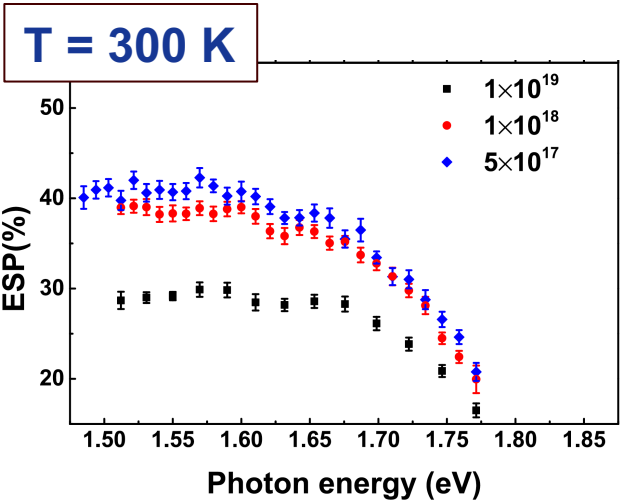
Future applications of Monte Carlo model

- ✓ Effective/fast modeling of spin-polarized photoemission: C + MPI to run in parallel at HPC cluster.
- ✓ Good agreement with available experimental data.
- ✓ Required model parameters from Density Functional Theory (DFT) calculations.

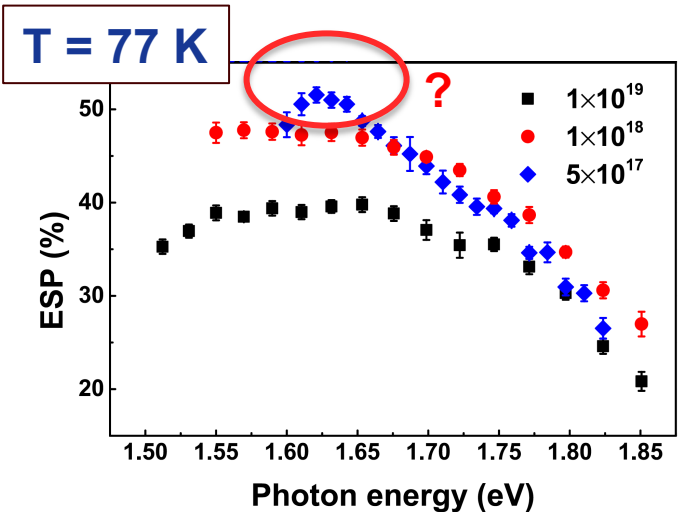
The developed Monte Carlo model establishes a paradigm for future studies of spin-polarized photoemission.

Future applications of Monte Carlo model

$ESP_0 = 50\%$



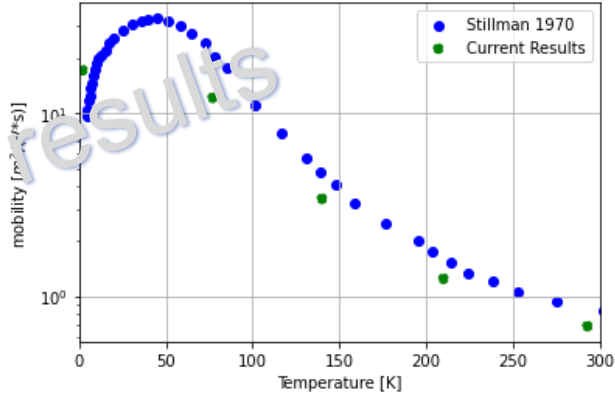
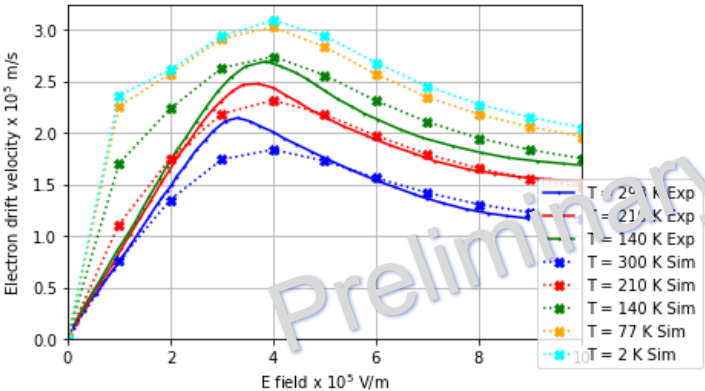
Liu et al. Appl. Phys. 122, 035703 (2017).



T = 2 K



Temperature effects on spin-polarized photoemission from bulk GaAs



Future applications of Monte Carlo model

High-QE, high-ESP from GaAs-based SuperLattices

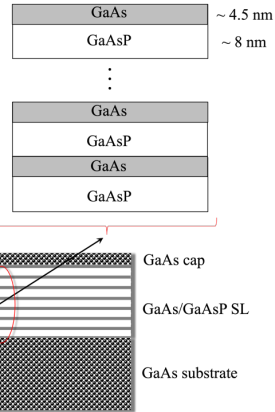


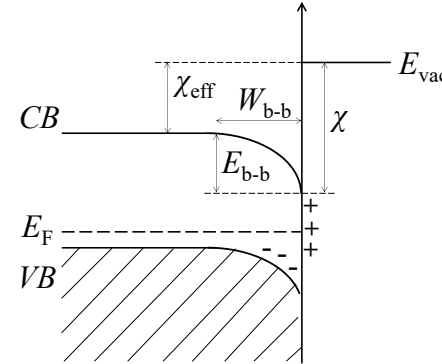
TABLE I. Figure of merit for polarized electron sources.

Cathode	Reference	P (%)	QE (%)	P^2QE (%)
GaAs-GaAsP _{0.36}	SLAC/SVT ¹⁵	86	1.2	0.89
GaAs-GaAsP _{0.38}	Nagoya ²⁰	92	1.6	1.35
Al _{0.19} In _{0.2} GaAs-Al _{0.4} GaAs	St. Peterburg ¹⁸	92	0.85	0.72
GaAs-gaAsP _{0.35} (with DBR)	JLab/SVT	84	6.4	4.52

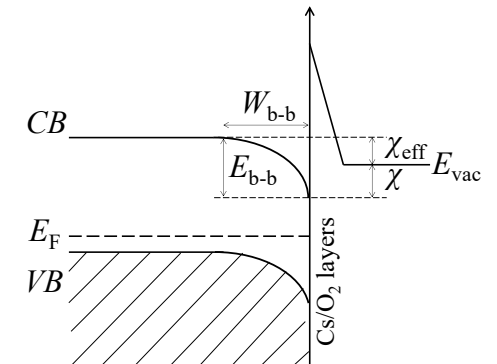
Liu et al. Appl. Phys. Lett. **109**, 252104 (2016)

Require traditional Cs-based activation to NEA

p-doped GaAs:

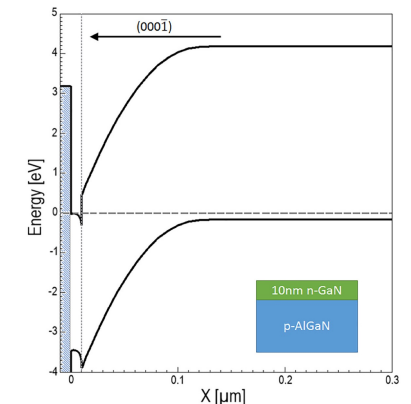


p-doped GaAs activated to NEA:



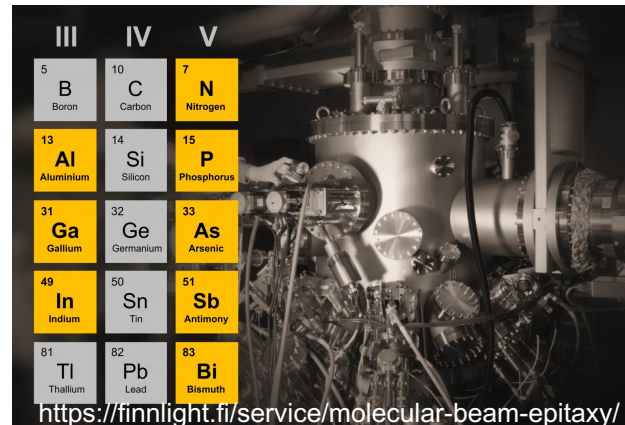
Spin-polarized photoemission from materials with inherently low/negative electron affinity levels

- Polarization band engineering to achieve an effective NEA condition without the use of Cs at the surface of GaN photocathode structures.
- Monte Carlo + DFT to study spin-polarized photoemission from III-Nitride materials.



Future applications of Monte Carlo model

Highly efficient GaAs-based SL structures are fabricated using an expensive MBE

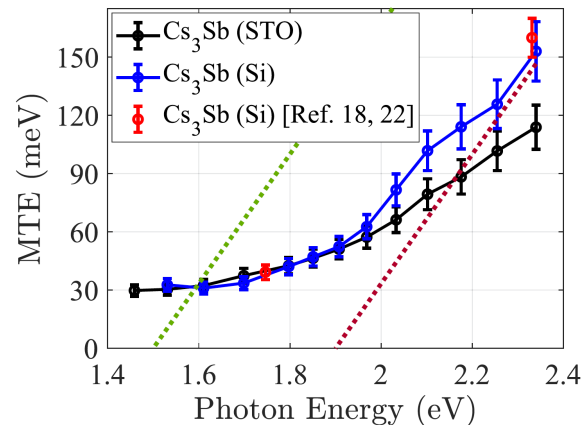
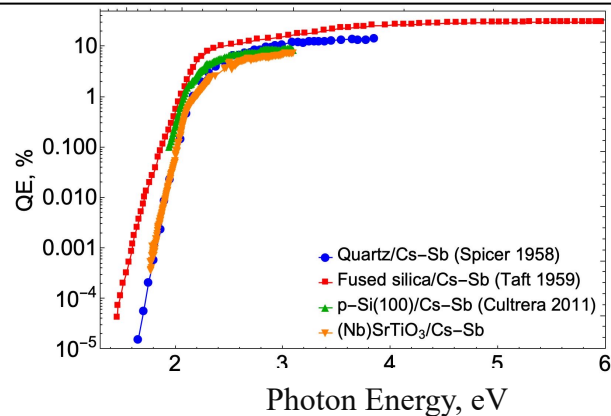


Spin-polarized photoemission from CdTe and other II-VI semiconductors

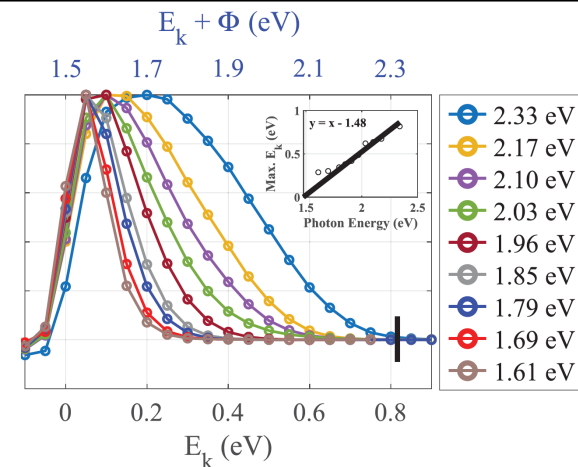
	GaAs	CdTe
Direct bandgap	yes	yes
Cs-based activation	yes	yes
Surface quality	high	high
p-doped	yes	yes
Spin-orbit coupling	strong	moderate
Cost	MBE, expensive	ALD, cheap
Accessibility	limited	accessible

Future applications of Monte Carlo model

Cesium antimonide films: thermal-limit MTE and relatively high QE at photoemission threshold

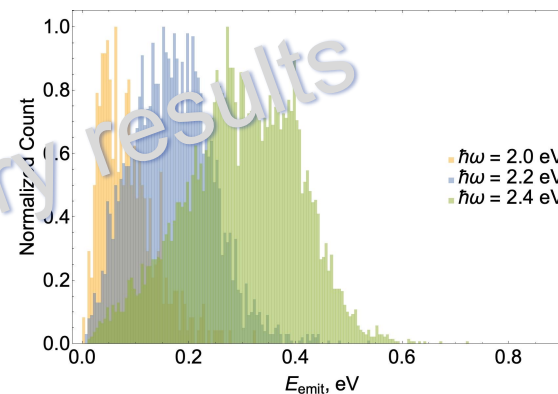
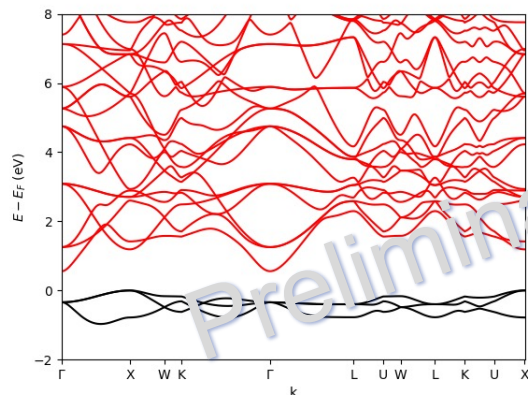


Electron energy losses in thin films



Kachwala et al., Appl. Phys. Lett. **123**, 044106 (2023).

Photoemission from alkali antimonide films (e.g., Cs₃Sb)

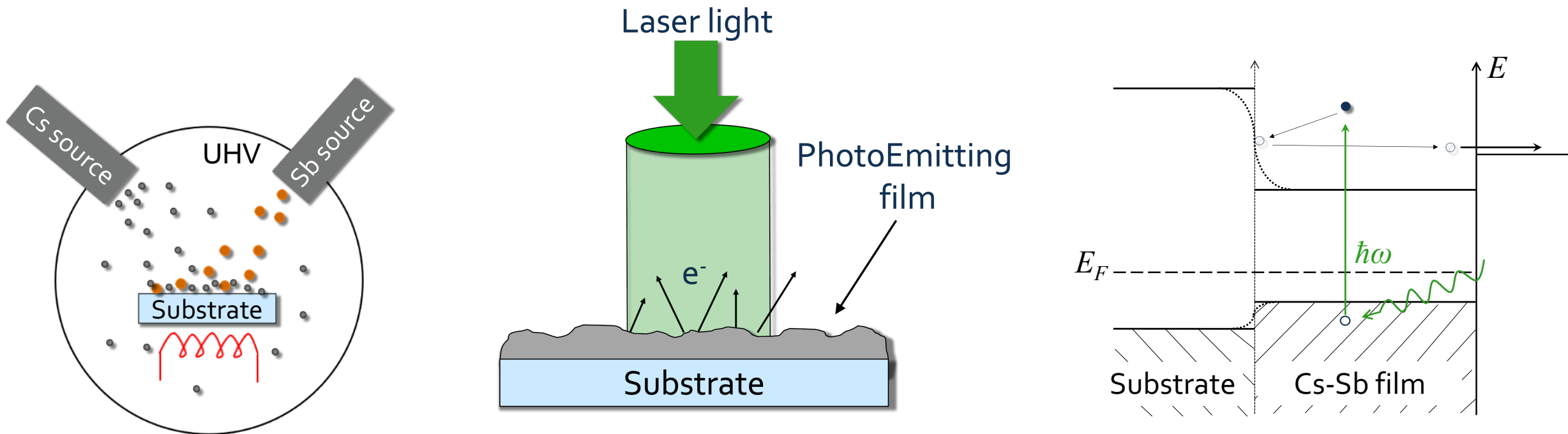


Growth and Characterization of Alkali Antimonide Photocathodes

Cesium-antimonide photocathodes

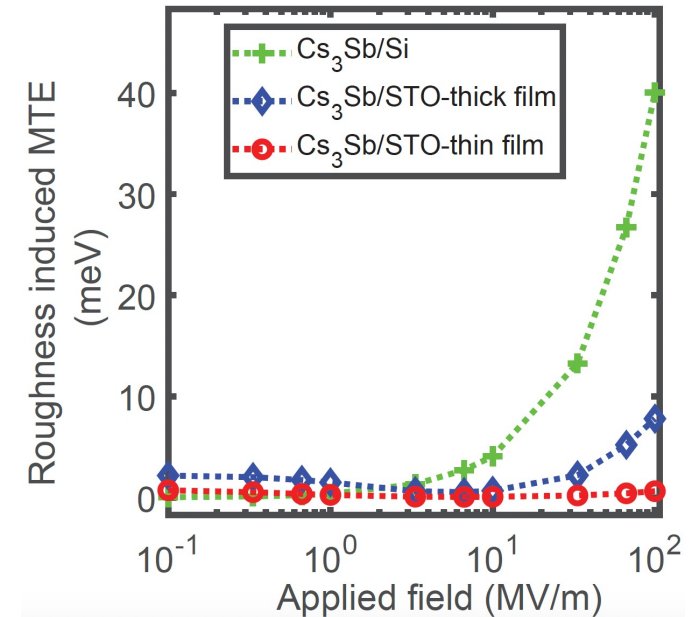
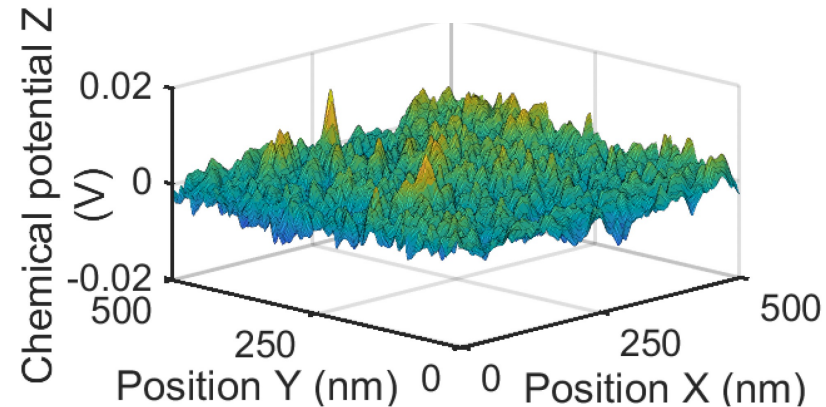
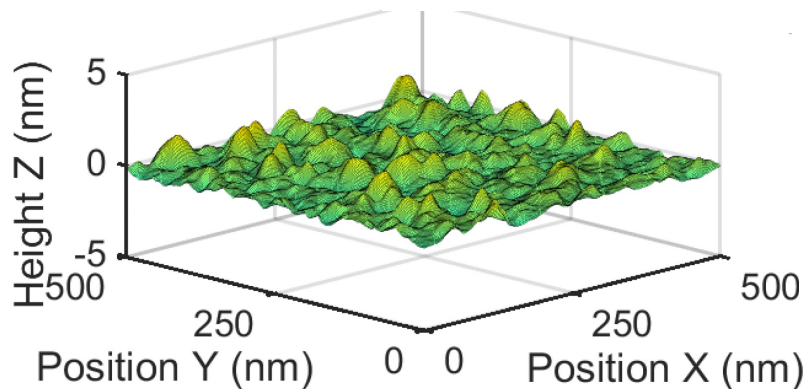
Cesium-antimonide photocathodes:

- can be easily deposited through thermal evaporation at moderate temperatures
- photoemit in a visible wavelengths range



Cesium-antimonide photocathodes

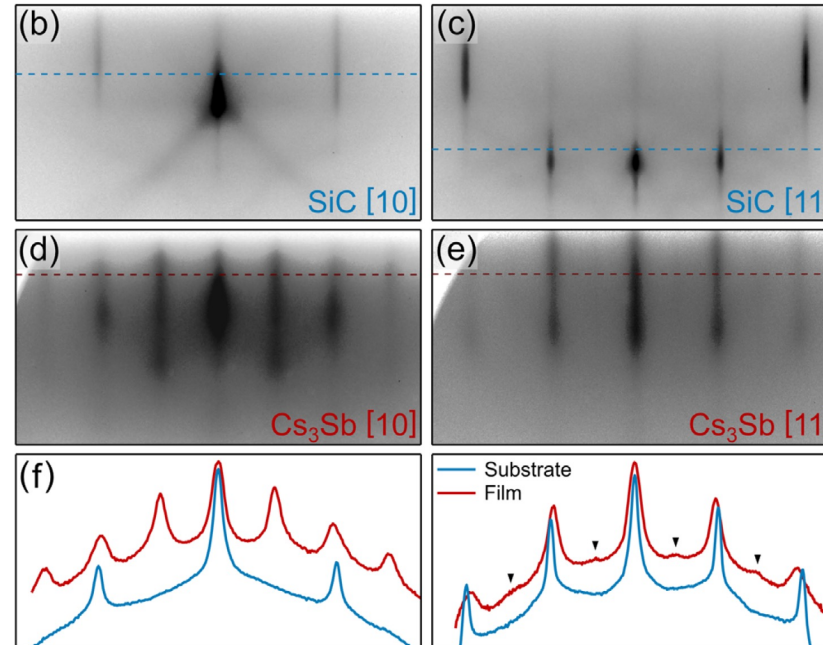
- Surface roughness and work function variation can limit MTE!



Cesium-antimonide films grown on lattice-matched single crystal strontium titanate (STO) substrates demonstrate roughness-induced MTE < 10 meV even at large applied fields.

Cesium-antimonide photocathodes

- Disordered crystal structure can limit MTE!



RHEED images of an annealed SiC substrate and a 10 u.c. Cs₃Sb film.

First-to-date demonstration of epitaxial growth of cesium-antimonide films on lattice-matched single crystal SiC substrates.

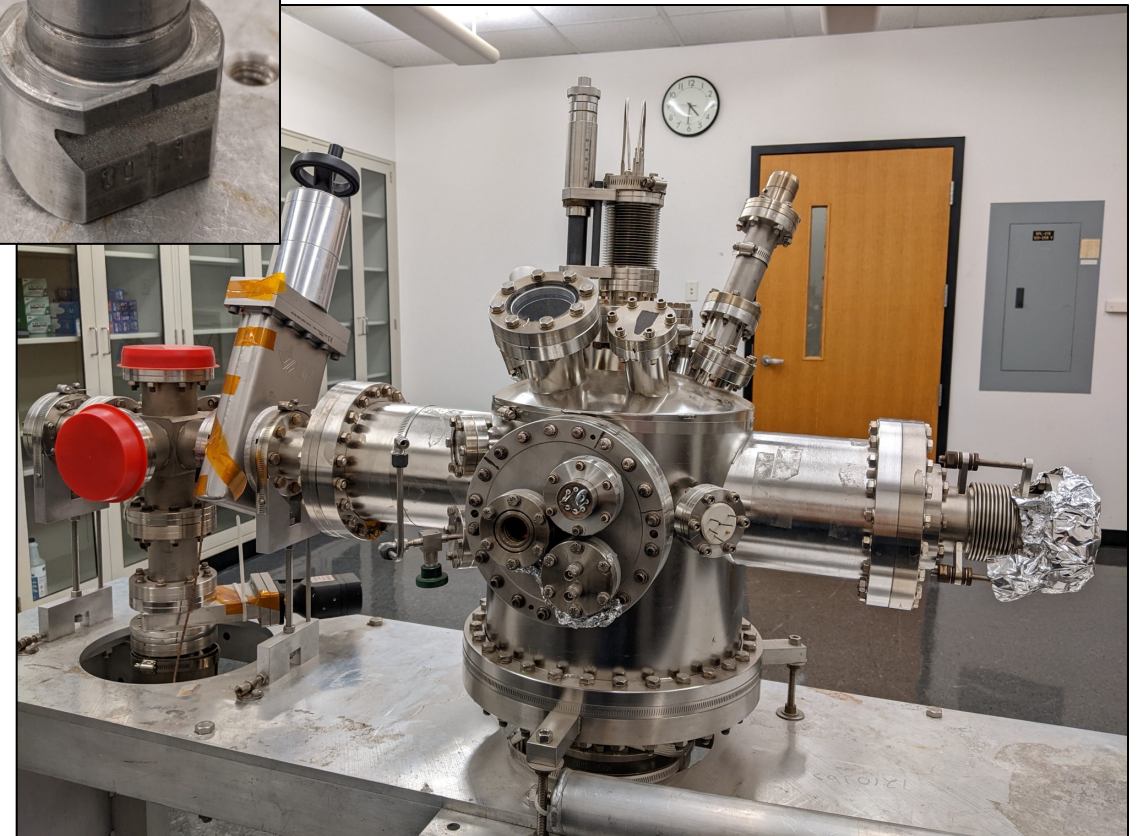
Growth of alkali-antimonide films at NIU

NIU photocathode growth system:

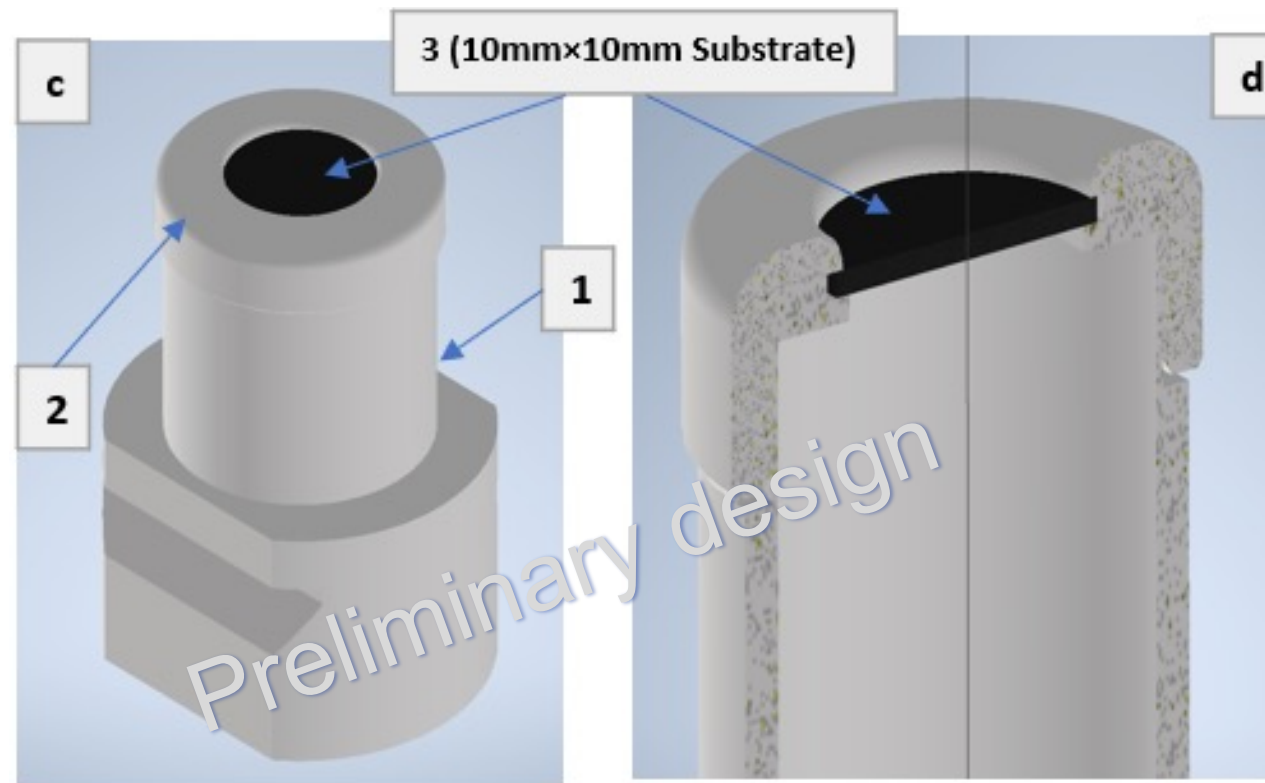
- Was previously used to grow Cs-Te at Fermilab.
- Uses old INFN-type photocathode plug.

Growth system updates

- Replace SAES strip Cs sources with long-lasting effusion cells (MBE Komponenten) with cesium molybdate pellets (SAES Getters)
- *In situ/operando* characterization with the RHEED system required for the epitaxial growth of cesium antimonide photocathodes







Growth of alkali-antimonide films at NIU



Prototype of the INFN-style plug with substrate insertion capability

Alkali-antimonide photocathodes (Cs-Sb, Na-K-Sb):

- Low MTE 
- High QE 
- Thin films → prompt response time 
- Robustness + long operational lifetime under realistic photoinjector conditions 

Testing alkali antimonide photocathodes at AWA Facility

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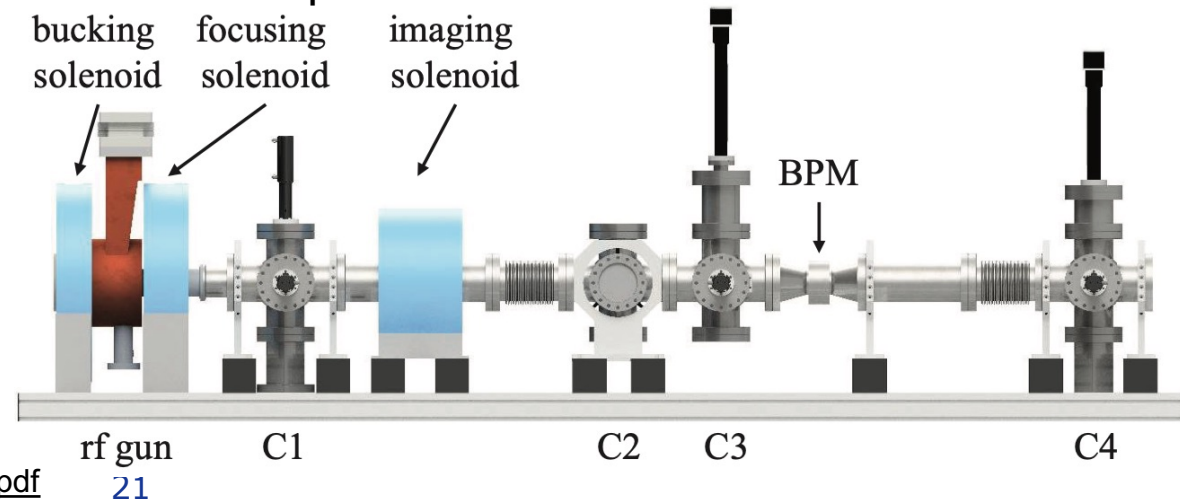
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Argonne Cathode Teststand (ACT):

- L-band 1.3 GHz single-cell photocathode RF gun
- emittance measurement capability
- includes field emission (FE) imaging system to locate emitters with a resolution of $\sim 20 \mu\text{m}$
- currently suitable for testing air-stable materials only
- unique plug design

ACT updates:

- integrate NIU-compatible photocathode plug suitable for testing different photocathode substrates
- develop NIU-compatible load-lock and photocathode transfer systems for testing Cs-containing photocathodes
- update the pump system to achieve $\sim 10^{-10}$ Torr
- possibility of adding the deflecting cavity for photocathode response time measurements



Summary

- A comprehensive R&D photocathode program is currently under development at NIU.
- Located close to two national labs (Argonne and FermiLab).
- Three PhD students are actively working on different aspects of photocathode R&D.

Introduction

Grad students:

John Callahan (NIU)
Daniel Franklin (NIU)
Tariqul Hasan (NIU)
Joniel O Mendez-Nieves (joins NIU this Fall)

Collaborators:

Siddharth Karkare (ASU)
Luca Cultrera (BNL)
John Power (ANL)
Scott Doran (ANL)
Eric Wisniewski (ANL)
Gongxiaohui Chen (ANL)
Philippe Piot (ANL)
Eric Montgomery (Euclid)



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Thank you!