Monte Carlo Study of Photoemission Properties of Semiconductor Cathodes for Accelerator Applications

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High-quality photocathodes =

- high quantum efficiency
  \[ QE = \frac{N_{e^-}}{N_{hw}} \]
- high electron spin polarization (for polarized electron sources)
  \[ ESP = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}} \]
- prompt response time + low mean transverse energy (high-brightness applications)
  \[ MTE = \frac{m\langle v_{\perp}^2 \rangle}{2} \]

Electron-Ion Collider (EIC)
- nucleon spin structure
- parity-violating mechanisms

Electron cooling of hadron beams
reduction of emittance of hadron beams

X-ray Free Electron Laser (XFEL)
- protein crystallography
- cell biology

Ultrafast Electron Diffraction (UED)
dynamical changes of material structure

- robustness + long operational lifetime (5-100 MV/m to extract ~ 50-1000 pC/mm² of charge densities/bunch)
Monte Carlo approach for modeling photoemission from semiconductors

Photocathode Physics for Photoinjectors (P3) Workshop at SLAC November 11, 2021

Photoexcitation

Initial energy distribution of photoexcited electrons

Initial electron distribution in real space

Transport

Bulk GaAs

Band-bending region

Vacuum

Surface barrier

Emission

Semiconductor

Vacuum

Advantages of Monte Carlo approach:

- QE, ESP, MTE, and response time can be simulated simultaneously as a function of $\hbar \omega$, $N_a$, $\chi$, $T$.

- 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 approach for modeling photoemission from semiconductors

Provides good agreement with experimental data:


Application to spin-polarized photoemission?

Ultra-short-pulse laser of high fluence

Characteristic behavior of experimental QE and ESP from NEA GaAs.
Monte Carlo study of spin-polarized photoemission from GaAs
Monte Carlo study of spin-polarized photoemission from GaAs

Initial electron spin polarization $ESP_0$:

\[ \hbar \omega \approx E_g \rightarrow ESP_0 = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} = \left\lfloor \frac{3 - 1}{3 + 1} \right\rfloor = 50\% \]

Chubenko et al. J. Appl. Phys. 130, 063101 (2021)
D'yakonov and Perel', Sov. Phys. JETP 33, 1053 (1971)
Spin relaxation mechanisms:

- Elliott-Yafet (EY): takes into account the mixing of wave functions with different spins as a result of spin-orbit interaction.
- D'yakonov-Perel (DP): arises due to the lack of an inversion center in some semiconductors which leads to splitting of the spin states of the CB at $k \neq 0$.
- Bir-Aronov-Pikus (BIP): originates from the exchange interaction of electrons with holes.
Comparison with experiment: QE and ESP from p-type GaAs for different electron affinity levels

Monte Carlo study of spin-polarized photoemission from GaAs

Chubenko et al. J. Appl. Phys. 130, 063101 (2021)

Chubenko et. al. 2014
Liu et. al. 2017

$\rho = 1.0 \times 10^{19} \text{ cm}^{-3}$
Comparison with experiment: QE and ESP from p-type GaAs for different doping densities

Chubenko et al. J. Appl. Phys. 130, 063101 (2021)
High-QE, high-ESP from GaAs-based SuperLattice structures activated to NEA:

Monte Carlo investigation of novel spin-polarized electron sources:

- Effective/fast modeling of spin-polarized photoemission: C + MPI to run in parallel at HPC cluster.
- Good agreement with available experimental data → creates a paradigm for future studies:
  - predict spin-polarized photoemission from other known spin-polarized materials and/or structures, which do not require traditional surface preparation (Luca Cultrera’s talk, Session C).
  - Monte Carlo + ab initio calculations to enable effective exploration of other potential materials to produce spin-polarized electrons.
Monte Carlo study of non-linear photoemission from semiconductor photocathodes
Non-linear effects in metals

**Metals:**

- \( E \)
- \( E_{\text{vac}} \)
- \( \hbar \omega \)
- \( E_F \)

\[
\hbar \omega \approx \phi \quad \Rightarrow \quad \text{MTE} \approx k_B T
\]

Low MTE, but low QE

\[
\hbar \omega \gg \phi \quad \Rightarrow \quad \text{MTE} \approx (\hbar \omega - \phi)/3
\]

High QE, but high MTE

- sub-ps pulse, 1 mJ/cm²
- Non-monotonic MTE

**Semiconductors:**

Ultra-short-pulse laser of high fluence:

1. High density of electron-hole pairs
   - Carrier-carrier (C-C) interactions
   - Non-equilibrium polar optical phonons (NE POPs)
   - Degeneracy effects
   - Screening effects
   - Auger recombination

2. High excess energy
   - Additional source of kinetic energy leading to carrier heating

   \[ \text{QE}_{\text{PEA}} \approx 0.01\% \Rightarrow N_y \approx 10^{16} \text{ cm}^{-2} \text{ in a 1-ps pulse} \]
   \[ (P \approx 2.4 \text{ GW/cm}^2) \]
   \[ N_{\text{ex}} \approx 10^{18} \text{ to } 10^{20} \text{ cm}^{-3} \]

**Detailed modeling is required to provide quantitative estimation of the mechanisms limiting beam brightness of semiconductor photocathodes under high laser fluences.**

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Monte Carlo study of laser-induced heating effects in semiconductor photocathodes

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Photoexcitation:

Gaussian laser pulse of different power density $P$

Initial energy distribution of electrons

Initial energy distribution of holes in p-doped GaAs ($N_a = 10^{18}$ cm$^{-3}$)

Ratio of two-photon transition rate $W_2$ to the one-photon transition rate $W_1$ for various laser power densities inside GaAs (ab initio calc. by J. Kevin Nangoi).
**Transport:**

- **Pauli exclusion principle**

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**“Equilibrium” Monte Carlo for electrons**

- **Equilibrium** Monte Carlo for electrons
- Acoustic phonon
- Eq. polar optical phonon (absorption)
- Eq. polar optical phonon (emission)
- Intervalley $F\rightarrow L$ (absorption)
- Intervalley $F\rightarrow L$ (emission)
- Intervalley $F\rightarrow X$ (absorption)
- Intervalley $F\rightarrow X$ (emission)
- Ionized impurity

**“Equilibrium” Monte Carlo for holes**

- **Equilibrium** Monte Carlo for holes
- Acoustic phonon
- Polar $hh\rightarrow hh$ (absorption)
- Polar $hh\rightarrow hh$ (emission)
- Polar $hh\rightarrow hh$ (absorption)
- Polar $hh\rightarrow hh$ (emission)
- Nonpolar $hh\rightarrow hh$ (absorption)
- Nonpolar $hh\rightarrow hh$ (emission)
- Nonpolar $hh\rightarrow hh$ (absorption)
- Nonpolar $hh\rightarrow hh$ (emission)
- Nonpolar $hh\rightarrow so$ (absorption)
- Nonpolar $hh\rightarrow so$ (emission)
- Ionized impurity

**Non-equilibrium polar optical phonons (NE POPs)**

- $P = 0.01 \text{ GW/cm}^2$
- $\hbar\omega = 1.9 \text{ eV}$

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**Hole MC by Jai Kwan Bae**
Monte Carlo study of laser-induced heating effects in semiconductor photocathodes

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Preliminary results:

\[ \langle E_{\text{internal}} \rangle = \frac{3}{2} k_B T \]

\[ P = 0.01 \text{ GW/cm}^2 \]
\[ t_r = 1 \text{ ps} \]
\[ \hbar \omega = 1.45 \text{ eV} \]

\[ P = 0.1 \text{ GW/cm}^2 \]
\[ t_r = 1 \text{ ps} \]
\[ \hbar \omega = 1.45 \text{ eV} \]
Monte Carlo study of laser-induced heating effects in semiconductor photocathodes

Preliminary results:

Low-electron-affinity semiconductor photocathodes are better candidates to operate under high laser fluences.*

*Preliminary
Summary and future directions

The detailed Monte Carlo model of photoemission has been developed to model main electron emission characteristics of semiconductor photocathodes. The model provides good agreement with experimental data for bulk NEA GaAs.

The work in progress to study effects of non-linear photoemission on QE and MTE of thin GaAs structures for high-current high-brightness applications. The model can be modified further to study non-linear effects in other bright photocathodes like alkali antimonide semiconductors.

The developed Monte Carlo model is the semi-classical approach, which is applicable when the applied and/or built-in potentials vary slowly on the scale of electron’s wavelength (~ 29 nm in GaAs), otherwise the wave phenomena such as reflections and tunneling are present and carriers must be treated quantum mechanically. Therefore, the full quantum methods like Non-equilibrium Green’s Function Technique or Wigner Monte Carlo can be employed to enable modeling of nanostructured photocathodes.
Monte Carlo study of spin-polarized photoemission:
Siddharth Karkare (ASU)
Dimitre A. Dimitrov (LANL)
Jai Kwan Bae (Cornell University)
Luca Cultrera (BNL)
Ivan Bazarov (Cornell University)
Andrei Afanasev (GWU)

Monte Carlo study of laser-induced heating effects:
Jai Kwan Bae (Cornell University)
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Jared Maxson (Cornell University)
Tomas A. Arias (Cornell University)
Ivan Bazarov (Cornell University)
Dimitre A. Dimitrov (LANL)
Siddharth Karkare (ASU)

Thank you!