Selected Beam Studies at PITZ in 2017

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Contents

- Photoemission modeling in the gun
- Updates on beam asymmetry studies
- Summary & Discussion
Review of Three-Step Photoemission (PE) model

1. Optical excitation of electrons
   - Reflection
   - Transmission
   - Energy distribution DOS

2. Migration of electrons to solid surface
   - $e^-$-phonon scattering (momentum change)
   - $e^-$-defect scattering (momentum change)
   - $e^-$-$e^-$ scattering (energy change, metal)
   - Random Walk (Monte Carlo)

3. Escape to vacuum
   - Overcome work function
   - $E_g$ (band gap) + $E_a$ (electron affinity) for semiconductor
   - $E_g$ variation, $E_a$ variation
   - Surface potential reduction due to field effect

For thorough descriptions, see:

M. Cardona and L. Ley: Photoemission in Solids 1, (Springer-Verlag, 1978)
J. Smedley, P3 workshop 2016
K. L. Jensen, P3 workshop 2016
L. Cultrera, EWPAA 2017
J. Smedley, EWPAA 2017
Motivation of further PE modeling at PITZ

> Explain PE associated measurement-simulation discrepancies in the gun
  - Charge production
  - Slice energy spread
  - Bunch length
  - Beam asymmetries, etc.

> Assist semiconductor photocathode R&D

**Background:**

+ Photocathode R&D usually focuses on *single electron* emission mechanism
+ Operation condition of PITZ for optimized emittance @ transition regime between QE and space charge limited emission regimes
+ Classical electrodynamics seems not sufficient explaining transient PE process
+ Intrinsic emittance modeling not yet thorough

**Our Challenge:** Improved modeling of photoemission process

⇒ At the semiconductor-vacuum interface in the gun how to model quantum mechanics with the presence of strong electromagnetic fields (RF + SPCH = collective effects)
Space charge dominated PE modeling

1. **Driving (UV) laser**
   - Realistic transverse (Virtual-Cathode-based Core+Halo model*) distributions
   - Realistic temporal distributions
   → initializing transient emission process

2. **Photocathode**
   - QE map and QE characterization
   → intrinsic emission homogeneity

3. **EM fields in close cathode vicinity**
   - RF, image charge & space charge
   → time and space dependent cathode work function modulation

4. **Quantum mechanics with the presence of strong EM fields at Semiconductor-Vacuum interface**
   - Surface states
   - Band bending
   → time and space dependent electron affinity variation
   → kinetic energy variation

5. **Others**
   - Temperature
   - Surface charge limit**
   - Secondary emission, etc.

* C. Hernandez-Garcia et al., NIM A 871 (2017) 97–104
**M. Zolotorev, SLAC-PUB-5896, 1992
Status: Core + Halo Model applied to ASTRA simulations

If a uniform distribution is used instead, the charge saturates

Extracted charge with core + halo for 0.8 mm beam diameter with 1.5 ps rms Gaussian temporal at maximum cathode field ($\phi_0=90^\circ$)

- $E_0 = 58\text{MV/m}$
- $E_0 = 44\text{MV/m}$
- $E_0 = 29\text{MV/m}$

If a uniform distribution is used instead, the charge saturates.
ASTRA simulations for **Gaussian** pulses using **Core+Halo**

> BUT for flattop photocathode laser pulses

**measured**

![measured data](image)

**Used in simulations**

![Used in simulations](image)

**Charge vs. laser pulse energy**

- **measured**
- **simulated (homogeneous)**
- **simulated (Core+Halo)**

![Charge vs. laser pulse energy](image)

**X-Y**

- $\phi_{\text{gun}}=$ MMMG
- $Q=0.5\text{nC}$
- $\varepsilon_x=0.82$ mm mrad
- $\varepsilon_y=0.84$ mm mrad

**X-X', Y-Y'**

- $\phi_{\text{gun}}=$ MMMG
- $Q=0.5\text{nC}$
- $\varepsilon_x=1.05$ mm mrad

**simulated**

Parameters "plugged" from measurements:

- $\phi_{\text{gun}}=$ MMMG
- $Q=0.5\text{nC}$
- $\varepsilon_x=1.05$ mm mrad

**MaxB[T]=-(A+B*0.982*Imain[A])**

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Status: ASTRA simulations for 2011 case using Core+Halo

> BUT for flattop photocathode laser pulses

<table>
<thead>
<tr>
<th>measured</th>
<th>Used in simulations</th>
</tr>
</thead>
</table>

**Charge vs. laser pulse energy**

- measured
- simul. (laser rms size 0.3mm)
- simul. (laser rms size 0.4mm)

**Parameters “plugged” from measurements:**
- $\phi_{\text{gun}} = \text{MMMG} + 6^\circ$
- $Q = 0.97 \text{nC}$
- $\varepsilon_x = 2.5 \text{ mm mrad}$

**Simulated**

- $\phi_{\text{gun}} = \text{MMMG} + 6^\circ$
- $Q = 1 \text{nC}^*$
- $\varepsilon_x = 0.72 \text{ mm mrad}$
- $\varepsilon_x = 0.60 \text{ mm mrad}$

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Status: PE modeling using a 3D full EM Lienard-Wiechert (LW) approach*

- **LW Approach with 3D emission process**
  - LW solution for the electromagnetic field of a charged particle in arbitrary motion
  - Full particle trajectory stored and used for field computation
  - Field-induced work function modification:
    \[
    \Delta \Phi_f(\mathbf{r}_\perp, t) = \sqrt{\frac{q^3}{4\pi \varepsilon_0}} [E_{rf}(\mathbf{r}_\perp, t) + E_{sc}(\mathbf{r}_\perp, t)]
    \]
  - Charge production per simulation time step:
    \[
    dQ(\mathbf{r}_\perp, t) = \Delta t \int \int_S \frac{P_l(\mathbf{r}_\perp, t)}{h \nu} QE(\mathbf{r}_\perp, t) dS
    \]
    \[
    QE = \frac{(1 - R_w)(1 + \frac{h \nu - \Phi_w}{E_a})^2}{2(p_0 + 1)(1 + \frac{E_a}{h \nu - \Phi_w})^2}
    \]
    K. Jensen, 2007

- **Status**
  - Dynamic generation of emitted particle distribution at cathode according to time-dependent emission models, taking into account full electromagnetic fields (RF + space-charge) during emission
  - Charge production in **QE limited regime** agrees with measurements
  - In **space charge dominated regime**, remaining deviations w.r.t. simulations probably due to:
    - Ideal beam distributions initially plugged in the simulations or/and time dependent work function variation resulting from quantum mechanics

*E. Gjonaj, TEMF, TU Darmstadt
Further PE modeling: band bending $\rightarrow$ space charge layer

> **Surface states**

- Due to lattice translational symmetry broken @cathode surface
- Surface band lying **within bandgap** of the bulk (fewer bonds)
- Possessing **charging character**

> **Surface states $\rightarrow$ band bending**

- Charge carriers falling into surface states $\rightarrow$ "**surface charged**"
- Matching fermi level at bulk and surface $\rightarrow$ band bent
- Band bending $\rightarrow$ **space charge layer formed** (from surface into the bulk)

> **Characteristics**

- Band bends **quadratically**
- **Local curvature proportional to local space charge density**
- Bending amount and width depending also on **material properties**

$$E_{bb} \propto \frac{\rho_{sc}(r, t)d^2}{\varepsilon}$$

Further modeling approach needed
PE modeling: interpretation of surface space charge layer

For Cs$_2$Te
- Donor-like surface, acceptor-like bulk
- Band bends downwards at surface

Electrons may be extracted from
- Valence band (VB)
- Surface band (SB)

\[ \text{ratio of VB and SB (emitted) electrons changes } E_{\text{kin}} \text{and } \varepsilon_{\text{th}} \]

Surface space charge layer may affect electron affinity
\[ \text{time and space dependent } E_a \propto \rho_{\text{sc}}(r,t) \]

UV@257nm $\rightarrow$ $E_{\text{ph}} \approx 4.82 \text{ eV}$

- Intrinsic cathode work function $\Phi_w = E_g + E_a$
- Work function due to presence of strong space charge densities @cathode surface

\[ \Phi_w \rightarrow \Phi'_{w,SB} = E_g - E_{SB} + E_a - E_{bb}[\rho_{sc}(r_\perp,t)] - \Delta \Phi_f(r_\perp,t) \]

\[ \Phi_w \rightarrow \Phi'_{w,VB} = E_g + E_a - E_{bb}[\rho_{sc}(r_\perp,t)] - \Delta \Phi_f(r_\perp,t) \]

\[ \Delta \Phi_f(r_\perp,t) = \sqrt{\frac{q^3}{4\pi\varepsilon_0}[E_{rf}(r_\perp,t) + E_{sc}(r_\perp,t)]} \]

\[ Q E = \frac{(1 - R_w) \sqrt{1 + \frac{hv - \Phi_w}{E_a}}}{2(p_0 + 1)(1 + \frac{E_a}{hv - \Phi_w})^2} \]

- Intrinsic emittance
\[ \quad \text{If } \varphi \leq \varphi_{\text{max}} = \arccos\sqrt{E_a/E_{\text{kin}}} \]
\[ \varepsilon_{n,\text{rms}} = \frac{r}{2} \sqrt{\frac{2E_{\text{kin}}}{m_0c^2}} \sqrt{\frac{2 + \cos^3\varphi_{\text{max}} - 3\cos\varphi_{\text{max}}}{2(1 - \cos\varphi_{\text{max}})}} \]

- Kinetic energy $E_{\text{kin}}$ varied accordingly

\[ \rightarrow \text{optimization w.r.t. space charge} \]
Updates on beam asymmetry studies
(RF coupler kick simulations &
Gun quadrupole for compensating beam asymmetries)

+ Igor Isaev
Motivation of beam asymmetry studies

Possible sources of the beam asymmetry:

- Vacuum mirror
- Stray magnetic fields
- Related to the laser polarization
- Particular cathode
- ...  
- RF coupler field asymmetry
- Solenoid imperfections (anomalous quadrupole fields)

Ongoing activities

- coupler kick simulations
- solenoid field simulations
- simulations with rotational quads model for fitting measurements
- gun quadrupole designs and simulations
- gun quads compensation
Updates on coupler RF kick studies (no solenoids)

Kick characterization

- Field calculation done under optimum operation condition of the gun (mini.S11 by adjusting inner conductor length)
- 3D field map used for later particle tracking simulations
- RF dynamics → no solenoids, no space charge  
  
Y. Chen et al., FEL2017 proceedings, WEP005

Vertical displacement at $z = 0.3$ m and kick strength as a function of the gun phase

Beam centroid tracking using field map
Updates on coupler RF kick studies (no solenoids)

Kick quantification

- Beam centroid positions on cathode plane

- Using field map tracking a set of particles on the cathode plane though kick region till door-knob transition region

- Fitting multipole expansion form of the integral kick using simulation results

**Multipole expansion of the integral kick**

\[
P_X = P_{0x} + (K_{RF} + K_N)X + K_S Y \\
P_Y = P_{0y} + (K_{RF} - K_N)Y + K_S X
\]

- **Vertical dipole kick** ~4.576 keV/c, time dependent
- **Quadrupole kick strength estimation**
  - Normal quadrupole component ~1.0e-5 keV/c/μm
  - Skew quadrupole component ~5.0e-6 keV/c/μm

- (20-ps) Bunch tail sees higher kick strength than the head by 0.05 mrad @ 6.5MW
Electron beam X-Y asymmetry compensation with gun quads (0.5nC, Gaussian photocathode laser pulse)

Electron beam measurements without gun quadrupoles

Graphs showing beam measurements at different locations and configurations.

Gun quads copy installed at EXFEL and prepared for FLASH

M. Krasilnikov et al., FEL2017 proceedings, WEP007

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Summary

➢ Further **photoemission modeling** towards **quantum mechanics** with the presence of **strong space charge densities** at cathode surface
  ▪ current status
  ▪ further modeling approaches

➢ **Coax coupler RF kick** characterized and quantified under **optimized operation** conditions of the gun
  ▪ **Time dependent vertical dipole kick**, ~0.65 mrad (MMMG phase, 6.5MW)
  ▪ Small quadrupole kick estimated

➢ **Beam asymmetry compensation** with gun quadrupoles optimization
  ▪ Promising results → "**round beam, round emittance**"

**Thank you very much!**
Backup: Updates on "Pz modulation" studies

> (?) Cathode laser temporal profile

- Long Gaussian (11-11.5ps FWHM, Lyot filter in) → Pz modulation observed
- Short Gaussian (~2ps FWHM, Lyot filter out) → not yet observed

→ Lyot filter, the source of modulation?

> (?) Emission mechanism

Emitted charge → fields on surface that affects subsequent emissions
→ "oscillations induced by a sudden influx of charge can persist".

Demonstration for Cu and Cs\textsubscript{3}Sb using MICHELLE