

# Selected Beam Studies at PITZ in 2017

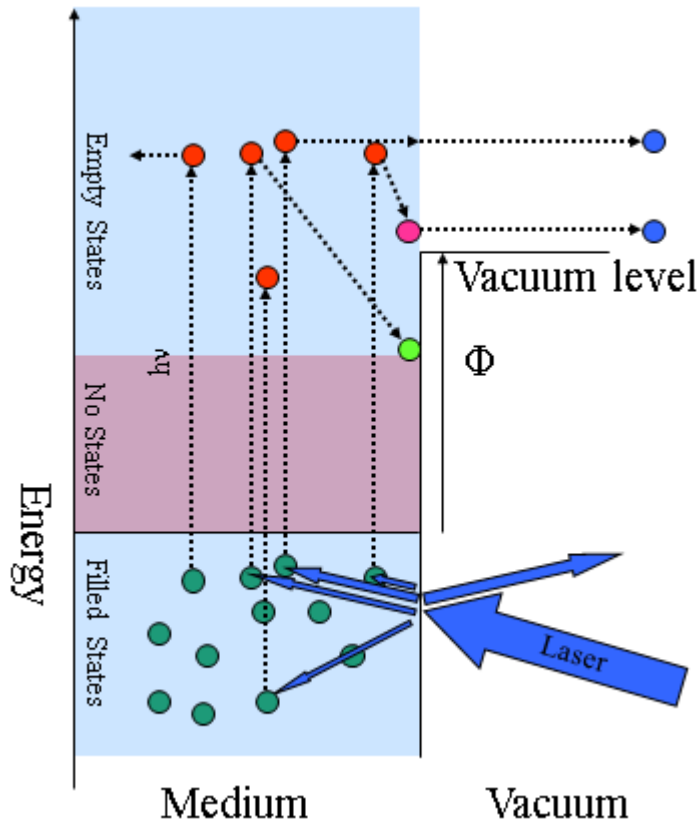
Ye Chen and Mikhail Krasilnikov for the PITZ Team

TEMF-DESY Collaboration Meeting  
06.10.2017, TEMF, Darmstadt, Germany

## 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<sup>-</sup>-phonon scattering (momentum change)
- e<sup>-</sup>-defect scattering (momentum change)
- e<sup>-</sup>-e<sup>-</sup> scattering (energy change, metal)
- Random Walk (Monte Carlo)

## 3. Escape to vacuum

- Overcome work function
  - ✓ E<sub>g</sub>(band gap) + E<sub>a</sub>(electron affinity) for semiconductor
  - ✓ E<sub>g</sub> variation, E<sub>a</sub> variation
  - ✓ Surface potential reduction due to field effect

**For thorough descriptions, see:**

W. E. Spicer, *Phys. Rev.*, 112 114 (1958)

M. Cardona and L. Ley: *Photoemission in Solids 1*, (Springer-Verlag, 1978)

W. E. Spicer & A. Herrera-Gomez, *SLAC-PUB-6306* (1993)

D. H. Dowell et al., *Appl. Phys. Lett.*, 63, 2035 (1993)

J. Smedley, *P3 workshop 2016*

K. L. Jensen, *P3 workshop 2016*

L. Cultrera, *EWPA 2017*

J. Smedley, *EWPA 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)

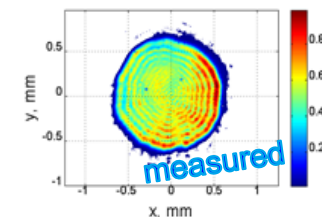


# Space charge dominated PE modeling

## 1. Driving (UV) laser

- Realistic transverse (Virtual-Cathode-based Core+Halo model\*) distributions
- Realistic temporal distributions
- **initializing transient emission process**

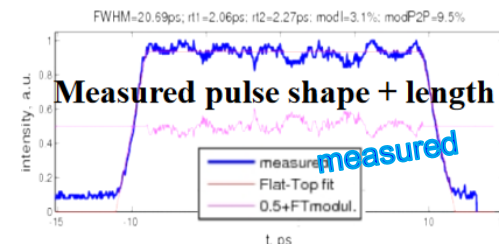
Cathode UV laser spot



## 2. Photocathode

- QE map and QE characterization
- **intrinsic emission homogeneity**

Laser temporal profile



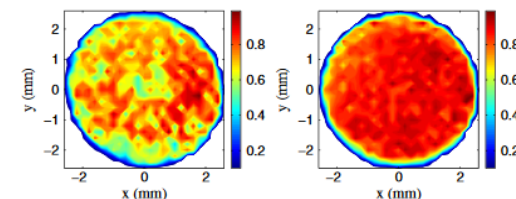
## 3. EM fields in close cathode vicinity

- 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**

QE homogeneity



## 5. Others

- Temperature
- Surface charge limit\*\*
- Secondary emission, etc.

\* C. Hernandez-Garcia et al., NIM A 871 (2017) 97–104

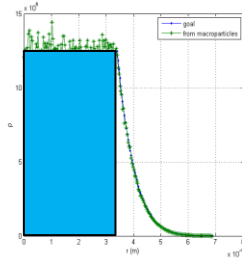
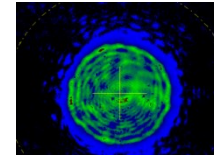
\*\*M. Zolotarev, SLAC-PUB-5896, 1992



# Status: Core + Halo Model applied to ASTRA simulations

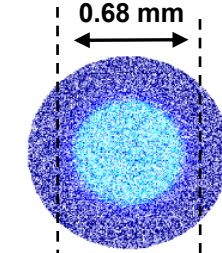
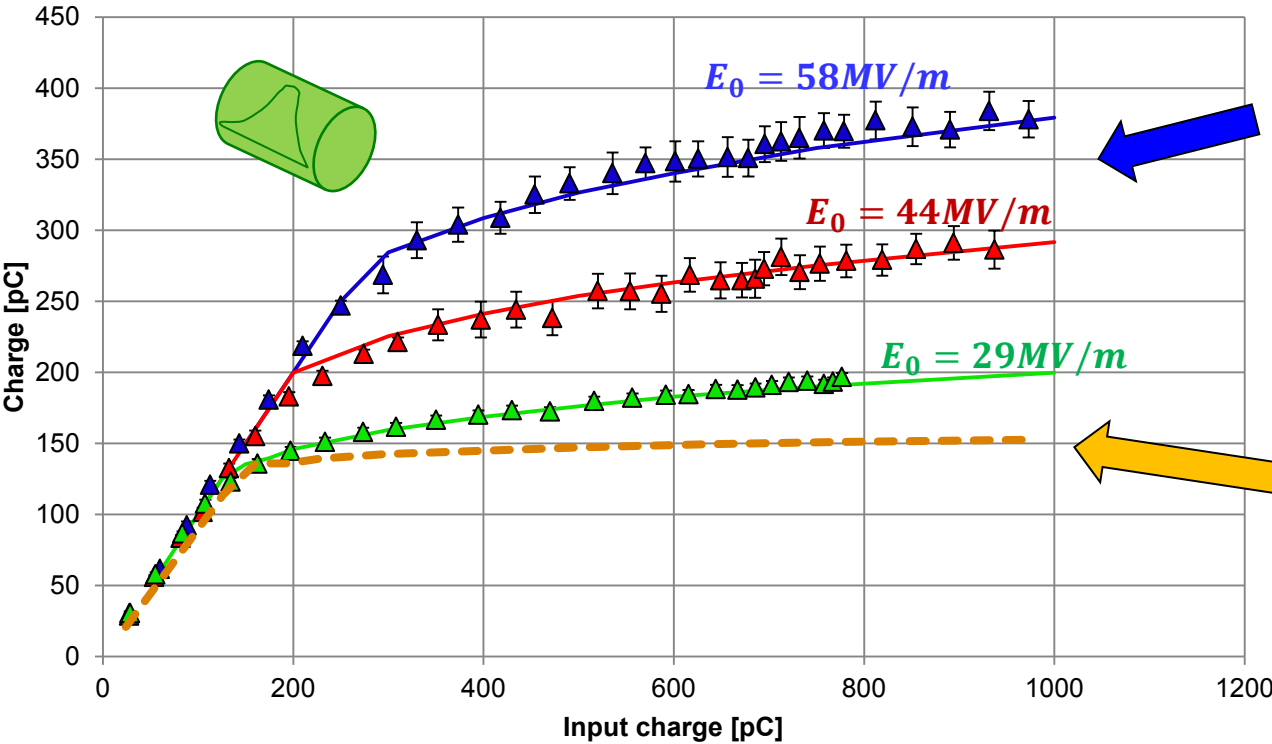
If a uniform distribution is used instead, the charge saturates

Laser radial distribution image

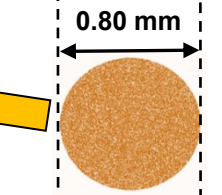


Transverse radial profile core + halo

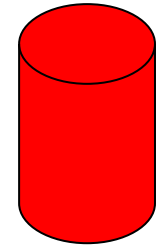
Extracted charge with core + halo for 0.8 mm beam diameter with 1.5 ps rms Gaussian temporal at maximum cathode field ( $\phi_0=90^\circ$ )



Generated ASTRA input distribution core + halo



Nominal ASTRA input uniform distribution

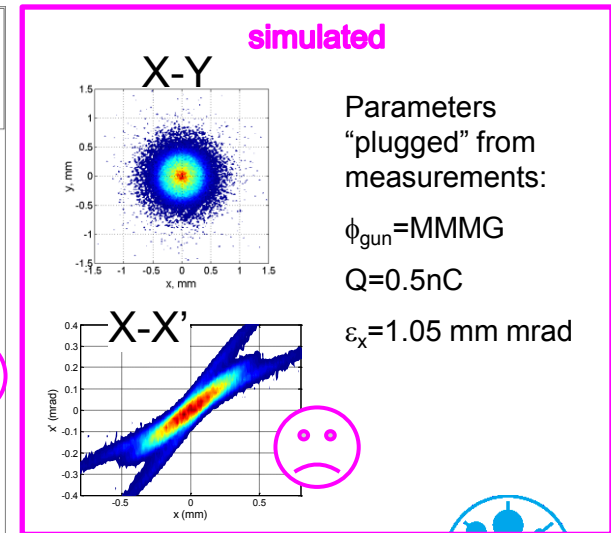
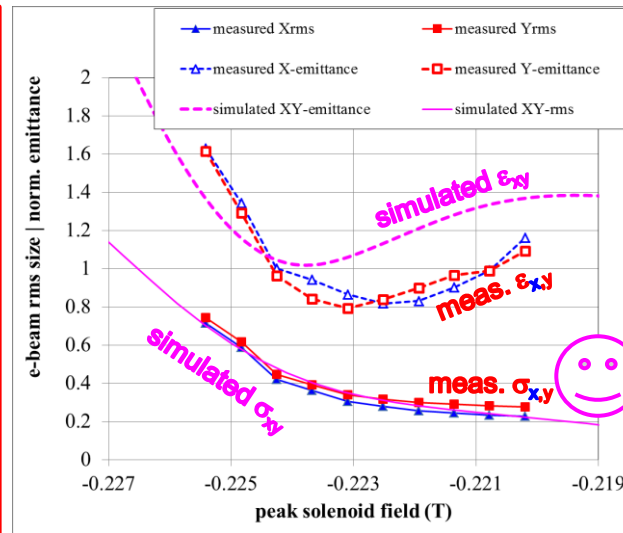
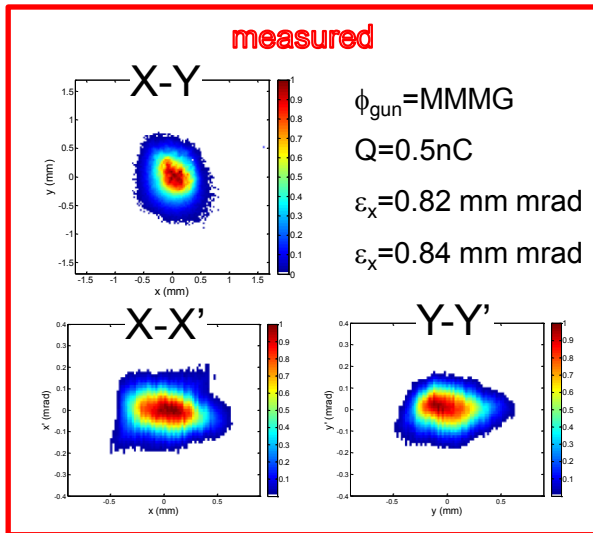
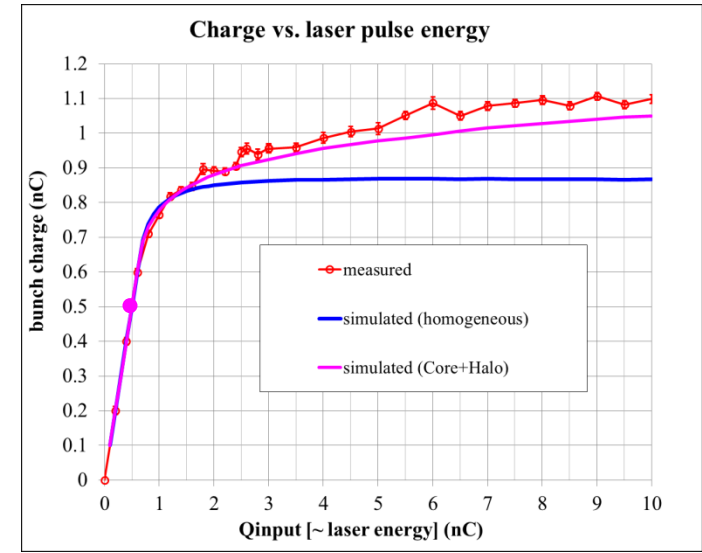
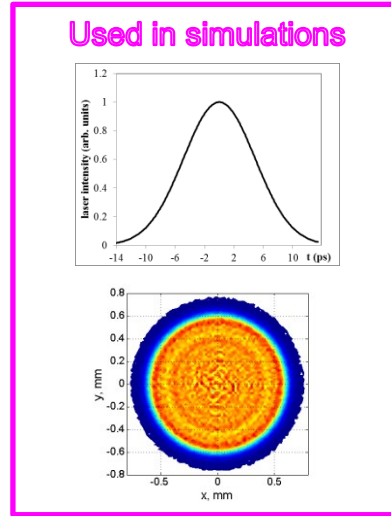
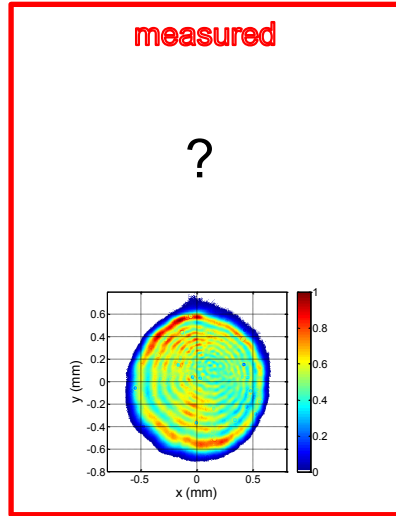
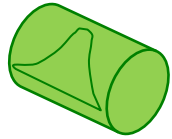


Nominal transverse uniform radial profile



# ASTRA simulations for Gaussian pulses using Core+Halo

➤ BUT for flattop photocathode laser pulses

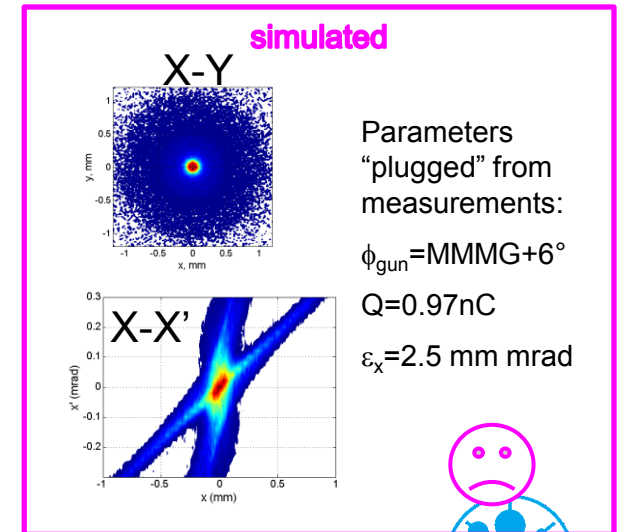
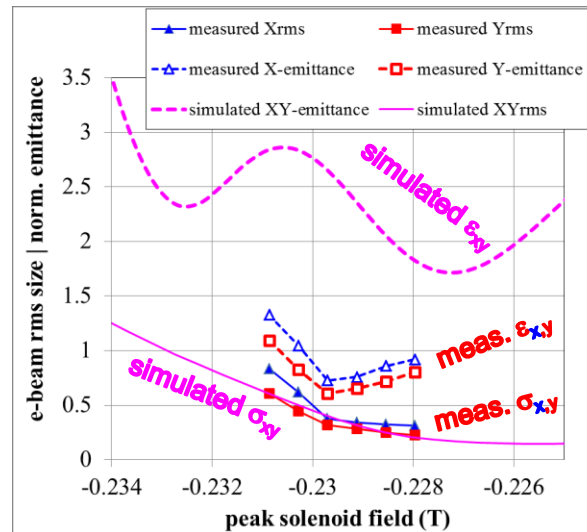
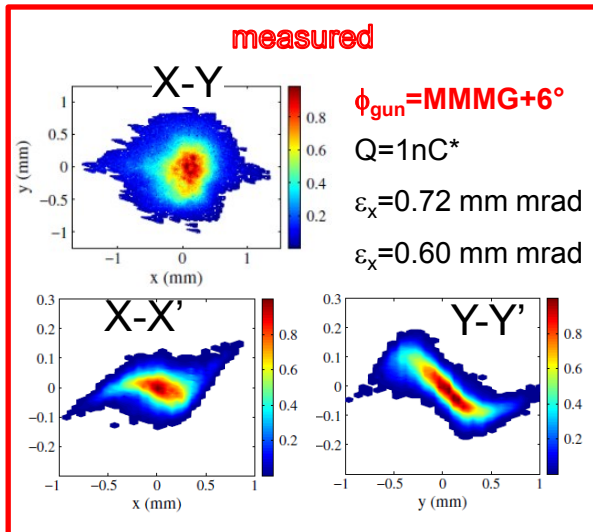
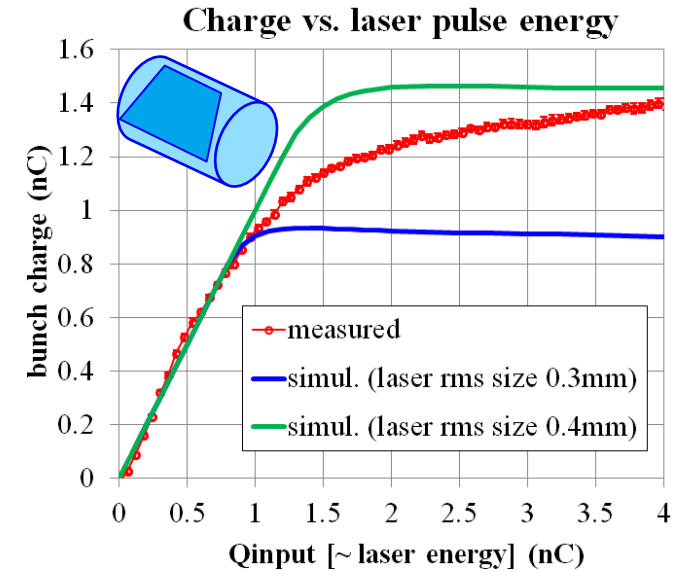
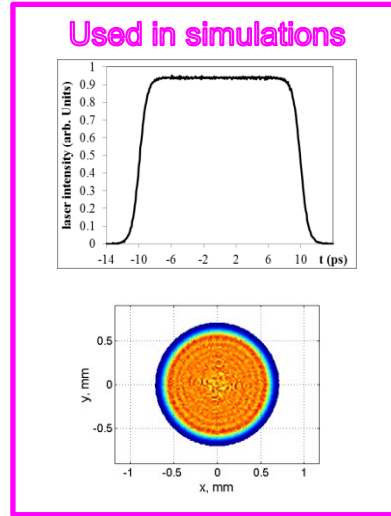
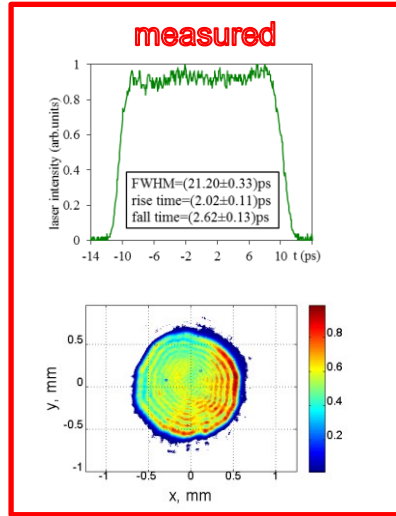


$$\text{MaxB[T]} = -(A + B * 0.982 * I_{\text{main}}[\text{A}])$$



# Status: ASTRA simulations for 2011 case using Core+Halo

➤ BUT for flattop photocathode laser pulses





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

\*E. Gjonaj, TEMF, TU Darmstadt

## ➤ 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:

$$\Delta\Phi_f(r_{\perp}, t) = \sqrt{\frac{q^3}{4\pi\epsilon_0} [E_{rf}(r_{\perp}, t) + E_{sc}(r_{\perp}, t)]}$$

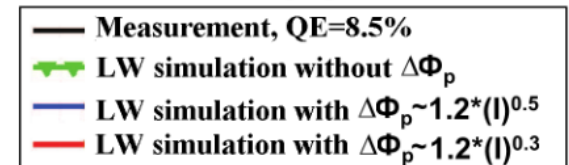
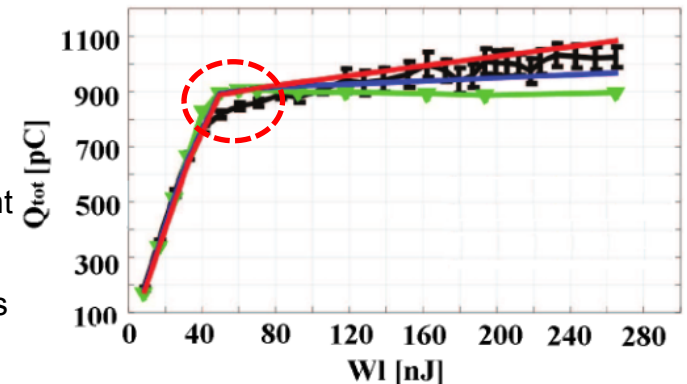
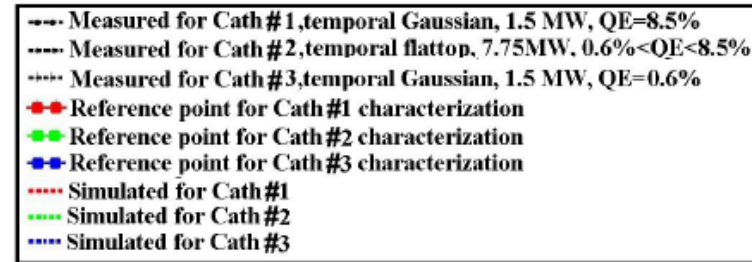
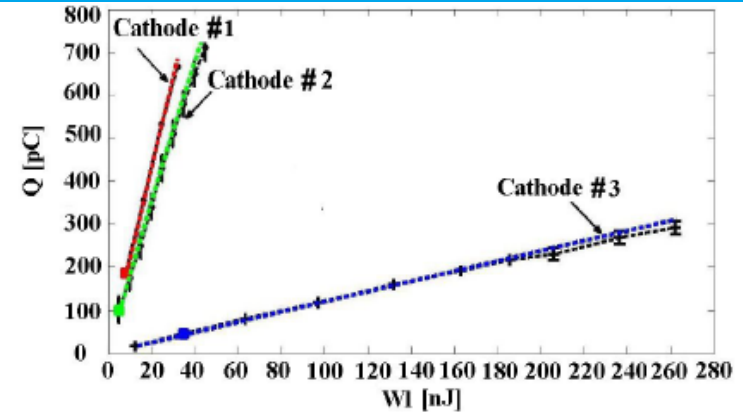
- Charge production per simulation time step:

$$dQ(\mathbf{r}_{\perp}, t) = \Delta t \iint_S q \frac{P_l(\mathbf{r}_{\perp}, t)}{h\nu} QE(\mathbf{r}_{\perp}, t) dS$$

$$QE = \frac{(1 - R_w) \sqrt{1 + \frac{h\nu - \Phi_w}{E_a}}}{2(p_0 + 1) \left(1 + \frac{E_a}{h\nu - \Phi_w}\right)^2} \quad \text{K. Jensen, 2007}$$

## ➤ 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





# Further PE modeling: band bending → 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**

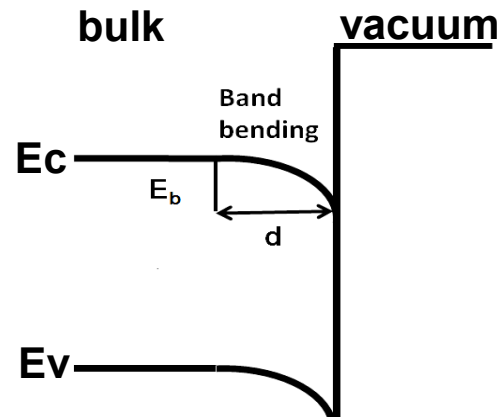
## > Surface states → band bending

- Charge carriers falling into surface states → **"surface charged"**
- Matching fermi level at bulk and surface → band bent
- Band bending → **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**

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



➔ Further modeling approach needed

# PE modeling: interpretation of surface space charge layer

## > For Cs<sub>2</sub>Te

- Donor-like surface, acceptor-like bulk
- Band bends downwards at surface

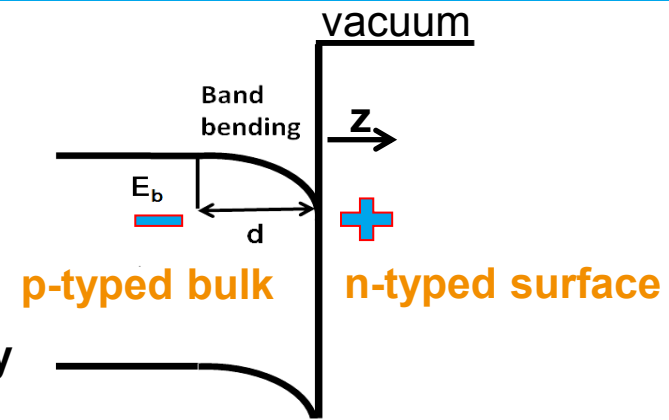
## > Electrons may be extracted from

- Valence band (VB)
- Surface band (SB)

→ ratio of VB and SB (emitted) electrons changes  $E_{kin}$  and  $\epsilon_{th}$

## > Surface space charge layer may affect electron affinity

→ time and space dependent  $E_a \propto \rho_{sc}(r, t)$



UV@257nm →  $E_{ph} \approx 4.82$  eV

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

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

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

Surface band

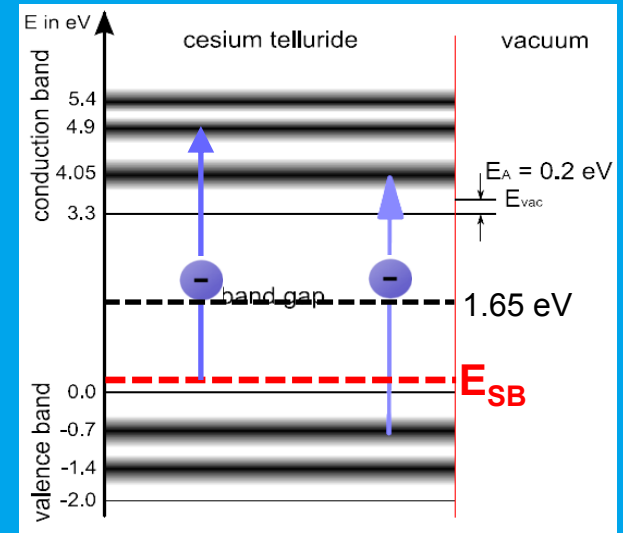
Band bending

Field effect

$$\Delta\Phi_f(r_{\perp}, t) = \sqrt{\frac{q^3}{4\pi\epsilon_0} [E_{rf}(r_{\perp}, t) + E_{sc}(r_{\perp}, t)]}$$

$$QE = \frac{(1 - R_w) \sqrt{1 + \frac{h\nu - \Phi_w}{E_a}}}{2(p_0 + 1) \left(1 + \frac{E_a}{h\nu - \Phi_w}\right)^2} \quad \text{QE: K. Jensen}$$

- ✓ Kinetic energy  $E_{kin}$  varied accordingly



- ✓ Intrinsic emittance

$$\text{If } \varphi \leq \varphi_{max} = \arccos \sqrt{E_a/E_{kin}}$$

$$\epsilon_{n,rms} = \frac{r}{2} \sqrt{\frac{2E_{kin}}{m_0c^2} \frac{1}{\sqrt{3}}} \sqrt{\frac{2 + \cos^3 \varphi_{max} - 3\cos \varphi_{max}}{2(1 - \cos \varphi_{max})}}$$

→ optimization w.r.t. space charge

# Updates on beam asymmetry studies

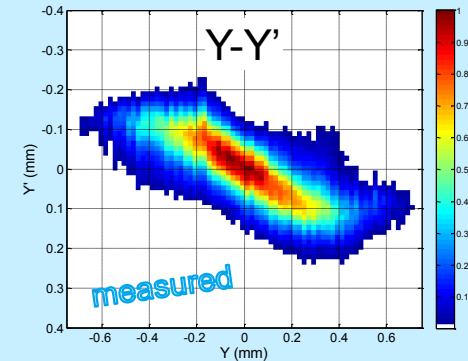
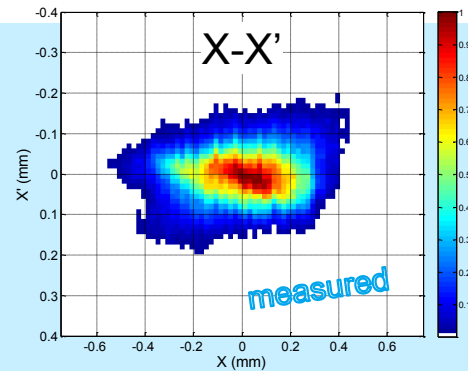
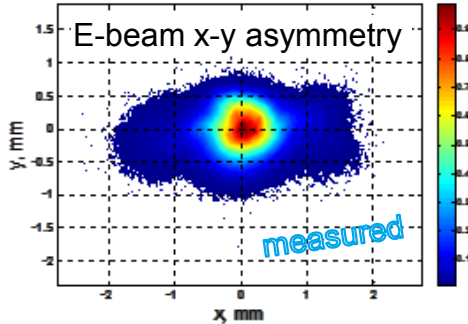
(RF coupler kick simulations &  
Gun quadrupole for compensating beam asymmetries)

+ Igor Isaev

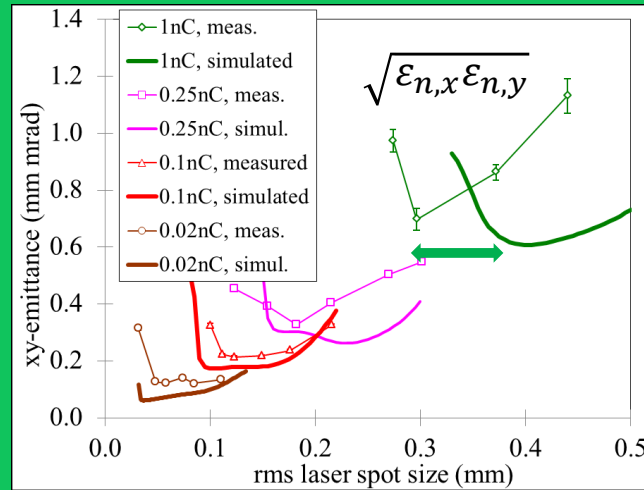


# Motivation of beam asymmetry studies

## Asymmetry $\rightarrow$ kick?



## Space charge



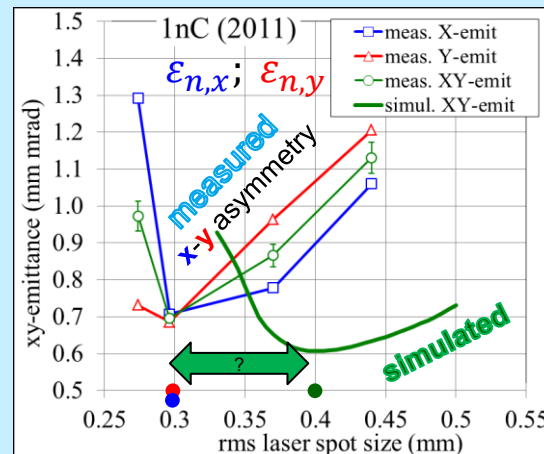
M. Krasilnikov et al., PRSTAB 15, 100701, 2012.

## 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

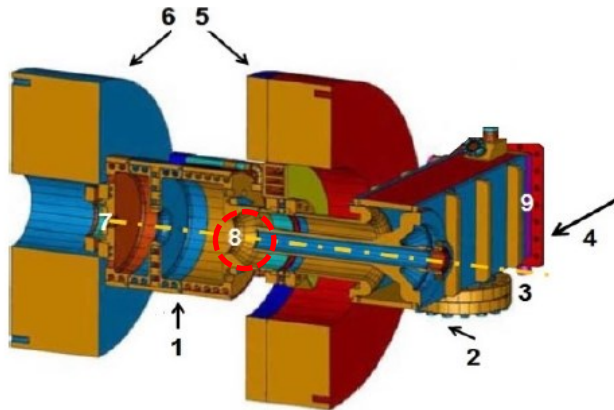
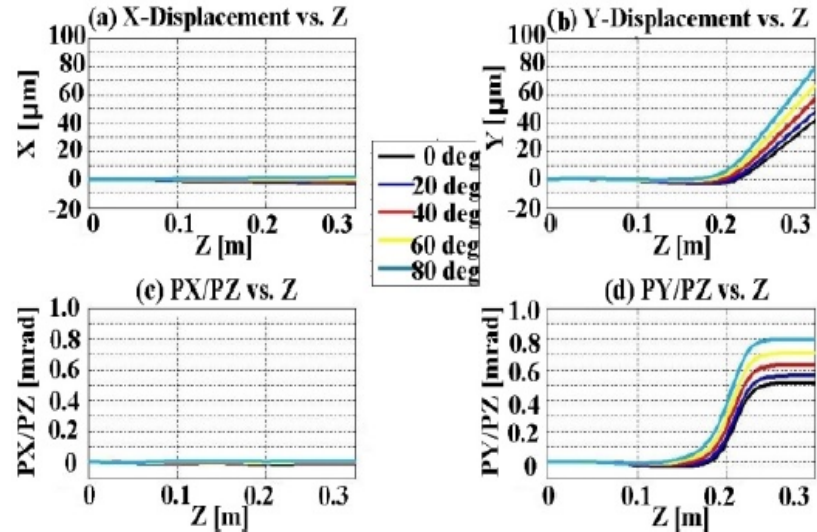


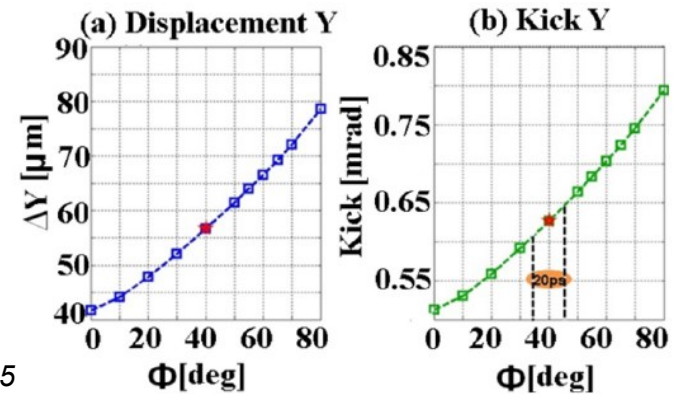
Figure 1: Sketch of the PITZ gun with coaxial RF coupler: 1-gun cavity, 2-door-knob transition, 3-cavity axis, 4-RF feeding direction, 5-main solenoid, 6-bucking solenoid, 7-cathode, 8-end of coaxial line and 9-reference position of WG port for simulations. Note that this sketch is rotated by 90 degrees compared to the computational model used in the follow-up simulations.

- 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*

## Beam centroid tracking using field map



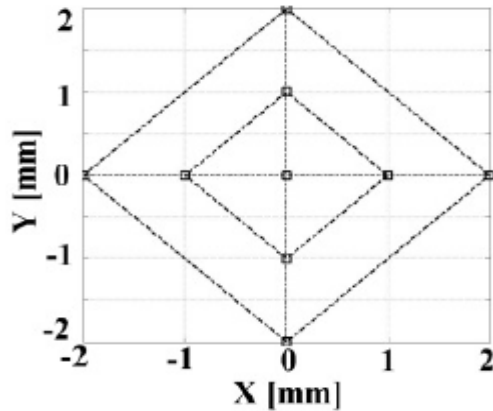
## Vertical displacement at $z = 0.3$ m and kick strength as a function of the gun phase



# Updates on coupler RF kick studies (no solenoids)

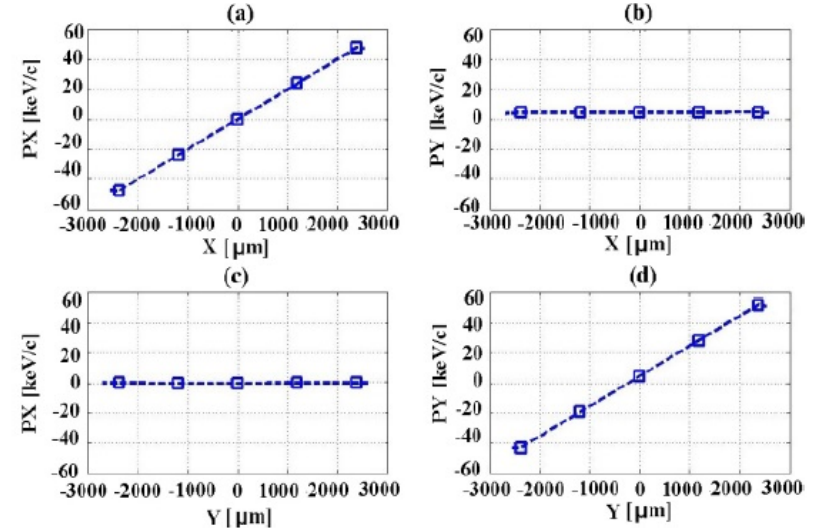
## > Kick quantification

Beam centroid positions on cathode plane



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

Particle tracking simulation results for multipole expansion based quantification of the integral kick



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

### Multipole expansion of the integral kick

$$P_X = P_{0x} + (K_{RF} + K_N)X + K_S Y$$

$$P_Y = P_{0y} + (K_{RF} - K_N)Y + K_S X$$

$X, Y$ : particle offsets from the axis at the location of the integral kick

$P_X, P_Y$ : particle transverse momenta in the horizontal and vertical direction

$P_{0x}, P_{0y}$ : horizontal and vertical dipole kicks

$K_{RF}$ : RF focusing strength of cylindrical symmetric mode

$K_N$  and  $K_S$ : normal and skew quadrupole kick strength

✓ 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



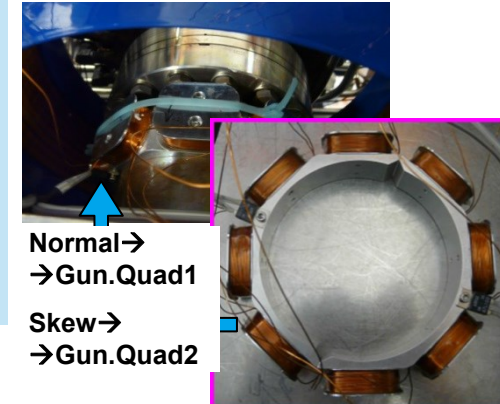
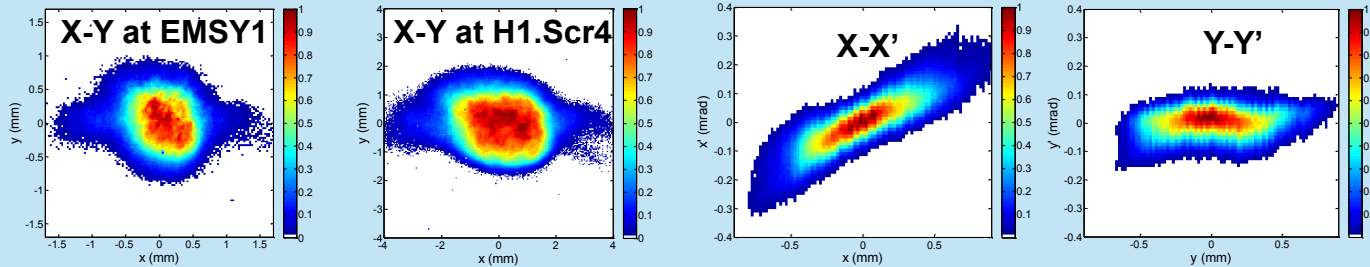


# Electron beam X-Y asymmetry compensation with gun quads

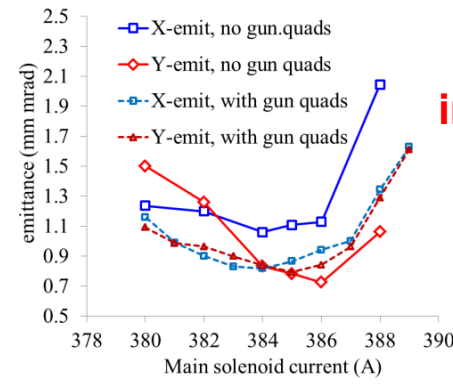
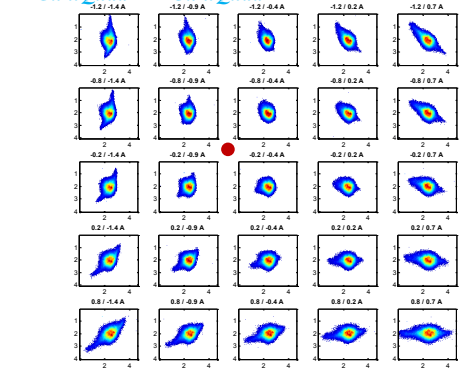
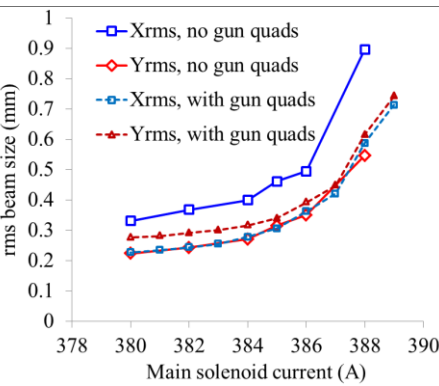
(0.5nC, Gaussian photocathode laser pulse)

measured

## Electron beam measurements **without** gun quadrupoles



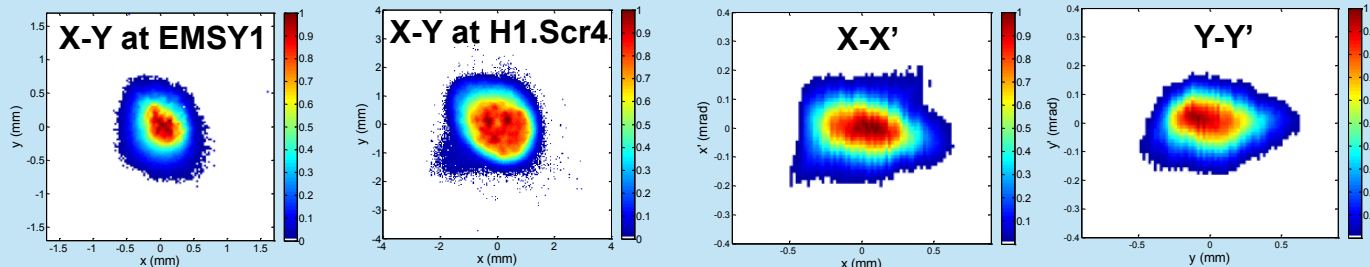
## ( $I_{Gun.Quad1}$ ; $I_{Gun.Quad2}$ ) scan at EMSY1



**Gun quads copy installed at EXFEL and prepared for FLASH**

## Electron beam measurements **with** gun quadrupoles

( $I_{Gun.Quad1} = -0.6A$ ;  $I_{Gun.Quad2} = -0.5A$ )



|   | No gun quads | With gun quads |
|---|--------------|----------------|
| $I_{main}(A)$                                   | 386          | 384            |
| $I_{gun.quad1}(A)$                              | 0            | -0.5           |
| $I_{gun.quad2}(A)$                              | 0            | -0.6           |
| $\sigma_x @ EMSY1 (mm)$                         | 0.50         | 0.28           |
| $\sigma_y @ EMSY1 (mm)$                         | 0.35         | 0.32           |
| $\epsilon_{x,n} (mm mrad)$                      | <b>1.13</b>  | <b>0.82</b>    |
| $\epsilon_{y,n} (mm mrad)$                      | <b>0.73</b>  | <b>0.84</b>    |
| $\sqrt{\epsilon_{x,n}\epsilon_{y,n}} (mm mrad)$ | <b>0.91</b>  | <b>0.83</b>    |





# 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**,  $\sim 0.65$  mrad (MMMMG phase, 6.5MW)
  - Small quadrupole kick estimated
- > **Beam asymmetry compensation** with gun quadrupoles optimization
  - Promising results  $\rightarrow$  "**round beam, round emittance**"

**Thank you very much!**



# Backup: Updates on "Pz modulation" studies

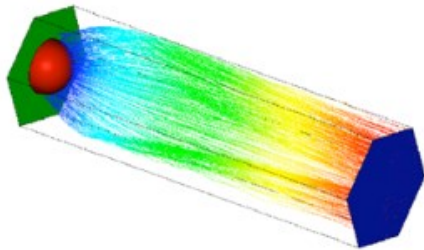
See: M. Krasilnikov, DESY-  
TEMF-Meeting, 01.2017

## > (?)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

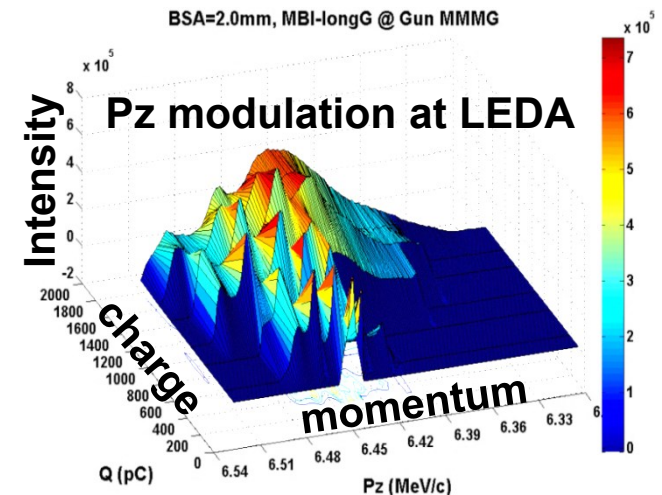


Emitted charge → fields on surface that affects subsequent emissions

→ "oscillations induced by a sudden influx of charge can persist".

Demonstration for Cu and Cs<sub>3</sub>Sb using MICHELLE

- J.J. Petillo et al., *IEE trans. Electron Devices* 52, 742 (2005)
- K.L. Jensen et al., *J.Vac.Sci. Technol.* 26 (2), 831 (2008)



Lyot filter in the  
regenerative amplifier