Towards measurement-based S2E beam dynamics modeling & simulations for XFEL operation
(1. start-up & gun)

Ye Chen
Beam dynamics meeting, Hamburg
November 19, 2019
Outline

- Motivation
- XFEL injector studies in October
- Strategy of studies
- Status: measurement vs. simulation
- Intermediate summary
- Roadmap
Motivation

- **Reduce** discrepancies between measurement & simulation
- **Develop** models to describe effects routinely observed in XFEL operation
- **Optimize** machine parameters for improved FEL performance
- **Explore** new working conditions / working scenarios
Injectors measurements in Oct.

Joint proposal by Yauhen Kot, Mikhail Krasilnikov et al. for XFEL injector studies

Injector Characterization. Proposals for the machine studies.

Yauhen Kot, Igor Zagorodnov, Martin Dohlus, Chen Ye Lining and Mikhail Krasilnikov

I. Goals

1. Characterisation of the gun
   a) Determination of the basic gun “zero” state (GZS) i.e. characterization of the gun in the usual operation mode.
   b) Find out the solenoid calibration \( s_0, s_1 \): \( B_{main} = s_0 + s_1 \cdot I_{main} \)
      (database: SOLA: s0=0, s1=4E-4 T/A, SQLB: s0=0, s1=6E-4 T/A)
   c) Find out generated input charge \( Q_{input} \) at the cathode needed to achieve nominal charge of 250pC after the gun: \( Q(Q_{input}, GZS) = 0.25nC \)
   d) Measure laser pulse energy needed to get \( Q_{input} \)
   e) Measure the emission curve for charge vs laser transmission LT: \( Q=Q(LT) \)
   f) Measure maximum beam mean energy (momentum) gain in the gun vs. gun gradient

2. Characterization of the longitudinal beam profile:
   a) Establish alternative calibration of A1 and AH1 with respect to each other comparing the results of the energy measurement with and without third harmonic module
   b) Document longitudinal beam profile after A1 (with switched off AH1).
   c) Document beam profile after AH1 with A1 operated on crest.
   d) Document longitudinal beam profile for various settings of the chirp, 2\(^{nd}\) and 3\(^{rd}\) derivatives around the usual SASE WP.
**Injector measurements in Oct.**

- **Carried out on 29th-30th.10.2019**

- **Joint efforts:**
  - Beutner, Bolko
  - Krasilnikov, Mikhail
  - Brinker, Frank
  - Scholz, Matthias
  - Chen, Ye
  - Tomin, Sergey
  - Dohlus, Martin
  - Zagorodnov, Igor
  - Kot, Yauhen
  & the XFEL operation team

- **Not everything finished as planned, but managed to measure:**
  1. Schottky scans (Q vs. Φ)
  2. Emission curves (Q vs. Elas)
  3. Phases of MMMG and zero-crossing
  4. Beam momentum after gun (using BK24)
  5. Emittance measurements
  6. TDS measurements
Strategy of measurement-based studies

1. **Identify** realistic (not ideal) beam & machine parameters (w.r.t. theory / used in previous simulations)
2. **Clarify** significance of identified properties (with vs. without)
3. **Demonstrate** parametric dependences of the properties ("from a point to a range")
4. **Develop** models to describe observed behaviours
5. **Implement** models in existing tools
6. **Compare** simulation with measurement for consistency
7. **Transfer** knowledge gained from simulation to machine operation
8. **Optimize** FEL performance

**Resources**

www.desy.de/fel-beam/s2e/codes.html

**Tools**

- Excel/IPRE for XFEL (www.desy.de)
- POM (www.desy.de)
- Data (X-ray) Library for XFEL (www.desy.de)
- Database for XFEL (www.desy.de)
- Inspector Database for EXAFS (www.desy.de)
- Inspector Database for PLASIM (www.desy.de)

**Codes**

- ALICE (Igor.Zagorodnov@desy.de)
- ATTRA (Ives.J.Bohlen@desy.de)
- CTBeam (Martin.Dolbin@desy.de)
- EGMN (Tanguy.Barateau@desy.de)
- Elevate (Markus.Buchholz@desy.de)
- Genie (Martin.J.Linden@desy.de)
- GANTAL (Tanguy.Barateau@desy.de)
- MAD (www.desy.de)
- MCFE (Jens.Tortora@desy.de)
- QField (Martin.Dolbin@desy.de)
Details re-noticed in measurements of Oct.

- Trajectory change while A1/AH1 phase scan
- Beam momentum determination (accuracy)
- Gun coupler kick (compensation)
- Gun quads operation (instruction)
- Gun solenoid calibration (needs precision)
- Injector laser diagnostics (not really ideal)

LH set-up
TDS-based bunch shape & length
Longitudinal phase space reconstruction
Realistic bunch / bunch properties for FEL simulation

\[ B_{main} = s_0 + s_1 \cdot I_{main} \]

(database: SOLA: s0=0, s1=4E-4 T/A, SOLB: s0=0, s1=6E-4T/A )

Running
Trigger: 200 Hz
ACR: 5.589 psi
Pulse fit (Gaussian): 6.945 psi
MSE: 5.258E-5

Orbit change
BPM before A1
Head-tail > 100um
Pz after gun?
Gun power measurements

- **Mhfpw10xfelgun**: ~5.2 MW
- **Directional coupler**
  (LLRF calibration based?)
  - **Directional Coupler**
  - **Pfor. 5.40 MW**
  - **Deviation exists**

**Latest XFEL database** 01. 2018
- Set-point power
- Measured power
- Beam momentum after gun
- Cathode field gradient
  - e.g. Power ≈ 5.21MW
  - $P_z \approx 6.67$ MeV/c
  - $E_{cath} \approx 58.35$ MV/m

**Table 1: Results of momentum measurements at XFEL**

<table>
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<tr>
<th>sp power</th>
<th>power in coupler@XFEL [MW]</th>
<th>power R&amp;S@XFEL [MW]</th>
<th>momentum, MeV/c</th>
<th>gun phase, deg</th>
<th>Iain, A</th>
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</table>

Credits*: I. Isaev, M. Krasilnikov, R. Niemczyk

European XFEL

\[
P_{RF_{XFEL}}[MW] = 0.00148 \cdot (E_{cath}[MV/m])^2
\]

\[
P_{RF_{R&S}}[MW] = 0.00153 \cdot (E_{cath}[MV/m])^2
\]
Low-charge measurement of zero-crossing phase

- 10 experiments each at BPM24 and TORA25
- Measured zero-crossing phase ~ 2 deg SP

Graph showing measured charge and charge accuracy at BPM24 and TORA25.
Low charge dynamics can be well described, $Q = f_1 + f_2 + \text{constant}$

\[
f_1 = a^* \exp \left\{ - \left( \frac{(\Phi + b)}{c} \right)^2 \right\}
\]
\[
f_2 = d^* (E_{\text{rf}})^e
\]

- $a = -0.005385$
- $b = 0.04175$
- $c = 3.749$
- $d = 0.01435$
- $e = 0.5716$

(determined Schottky power index)

constant = 0.003898
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Measurement of MMMG phase

**Measured MMMG at ~ -46 deg SP**
(47 ~ 48 deg w.r.t. zero-crossing)
Simulation of beam momentum after gun

- Laser intensity SP (Qin=320pC) indicated from a measured emission curve (→Slide 15)
- Simulated Pz ~ 6.66 MeV/c at MMMG
- Simulated MMMG: ~46 deg from zero-crossing
  → ~ consistent with the measured one
- Charge at MMMG ≈ 230 pC
  → 20 pC (8%) off measured 250 pC

fit: Pz[MeV/c] = 6.659 e^{-( \varphi[deg]-220.5 \over 104.4}^2
Diagnostics of injector laser ('Laser 2')

Measured laser temporal profiles

- **Streak camera measurement**
  - Gaussian-like shape
  - 7.345 ps FWHM
  - 3.126 ps RMS

- **Autocorrelation measurement**
  - Gaussian-like shape
  - 6.945 ps FWHM
  - 2.955 ps RMS

  → close numbers off by 5%
  → a bit noisy in the AC case

Credits: Lutz Winkelmann

Measured transverse laser distributions

Laser beam on virtual cathode

- BSA SP = 1.0 mm

Standard 29-30.10.2019

→ 'irregular' shape w.r.t. standard case
→ unclear cause
→ **charge-weighted map** used to represent realistic trans. distro for simulations
Simulations: Uniform Trans. Distro vs. Measured Trans. Distro

- Gun phase set at MMMG
- (“an extreme case”) Using irregular trans. laser distribution results in up to 35% deviation w.r.t. using an uniform one

→ Different dynamics at Working Points (WP) for 250 pC
  - Linear regime in ideal simulation
  - Nonlinear regime already when using measured trans. distro
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Simulations vs. Measurement

Discrepancy drops to 10% when using measured trans. distro, but still…

- Simulated saturation WP2: 38%
- Measured saturation WP3: 22%

→ WP for 250pC in nonlinear regime

For more accurate simulation one needs to consider e.g.
- 'virtual cathode' formation in strong space charge density case
- photoemission model (field dependency of QE on cathode surface)
- to use a tool with 3D space charge solver from the cathode
Phase dependency of charge: measured Schottky scan

**Measured Schottky Scans**

- **QE (source) limited**
- **Space charge limited**

**The corrected behaviour fits the expected low-charge extraction mechanism versus phase**

**NB: influence of noise threshold**

**Drop due to the noise threshold settings**

**Raw data (no filter)**
Simulation vs. Measurement: Schottky scan

- Laser intensity SP (Qin = 320 pC) indicated from the measured emission curve
- Using measured trans. laser distributions
- Laser pulse length ∼ 2.96 ps rms
- $P_z \approx 6.66$ MeV/c
- **Stronger saturation** compared to measurement
- Large discrepancies exist for higher phases
Simulation vs. Measurement: Schottky scan

From the simulated emission curve Laser intensity SP (Qin = 400 pC) indicated for 250pC at MMMG → smaller discrepancies for other phases?

Increasing laser intensity by ~20% renders better agreements for [MMMG-50, MMMG+46] degrees → more charge actually produced in the measurements through field effects (i.e. higher effective QE for given laser pulse energy) and / or space charge force overestimated in simulations

Measured behaviours for higher phases (<MMMG-60) not yet clear
Reference to simulations performed in July 2019 (for the PITZ case)

With emission model incorporated in a 3D space charge code

- Measured, laser energy (LE) 1
- Measured, LE 2
- PE modelled, LE 1
- PE modelled, LE 2
- Simulated, LE 1
- Simulated, LE 2

Charge production corrected by photoemission (PE) model
Particle dynamics considered in a 3D SP-CH tracking code
Inefficient (heavy) simulations
Better agreements with measurements
Effect of gun coupler kick: measured orbit change along train

Cross-checked orbit change over long bunch trains due to gun coupler kick

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<td>156 / 160</td>
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</table>

Simulation results reported in doi:10.3204/PUBDB-2018-05590

Simulated Head-tail kick difference:
~ 0.112 mrad (300us)

Simulated orbit change at BPM24 ~ 78 um

Effect stronger for longer train operation

Kick compensation (→ MSK involved)
Intermediate Summary

- Simulations performed for measurements in Oct. (gun part)
  - BSA1.0, PL 2.96 ps rms, PS Gauss
  - Gun SP 55.6, Prf ≈ 5.2 MW@200μs
  - Simulated Pz ≈ 6.66 MeV/c, Ecath ≈ 58.4 MV/m
  - Simulated MMMG@46 deg from zero-crossing

- Status of measurement vs. simulation
  - Simulated charge at MMMG 20 pC lower, i.e. 8% at 250pC
  - ............. emission curve roughly 10% lower
  - ............. MMMG (w.r.t. zero-crossing) phase ~same (uncertainly from measured 0 phase)
  - ............. phase scan for [MMMG-50, MMMG+46] ~10-15% lower
  - ............. charge extraction vs. phase slippage not yet understood
  - ............. orbit change along bunch train still consistent with current XFEL observations

- Results suggest:
  - Relative increase of laser intensity by 20% leads to fairly good agreements with measured charge extraction behaviours vs. RF phase & laser intensity \(\rightarrow\) more charge actually produced on the cathode (\(\rightarrow\) QE model) and / or space charge force overestimated (\(\rightarrow\) new tool)
  - Use measured trans. & temp. laser distro for simulation
  - Current XFEL machine working point in strong space charge dominated regime (\(\rightarrow\) more careful modelling required)
  - Given asymmetric bunches at cathode & possible numerical issues, Krack 3 should be used
Roadmap

1. Measurements for XFEL injector re-characterization (→ done)
2. Corresponding gun simulations and comparisons with a set of measurements (→ done)
3. Reconstruction of measured longitudinal phase space by Igor (→ ongoing)
4. Try to improve simulations by Krack 3 simulation (→ ongoing)
5. Investigate trajectory change while A1 / AH1 phase scan (→ e.g. use Martin’s kick model)
6. Benchmark projected & sliced emittance under (measured-) nominal conditions
7. TDS & longitudinal phase space by injector exit (→ compare with Igor’s data)
8. Use e-bunches with measured properties for S2E simulations (→ ocelot + Genesis)

Thank you for your attention.