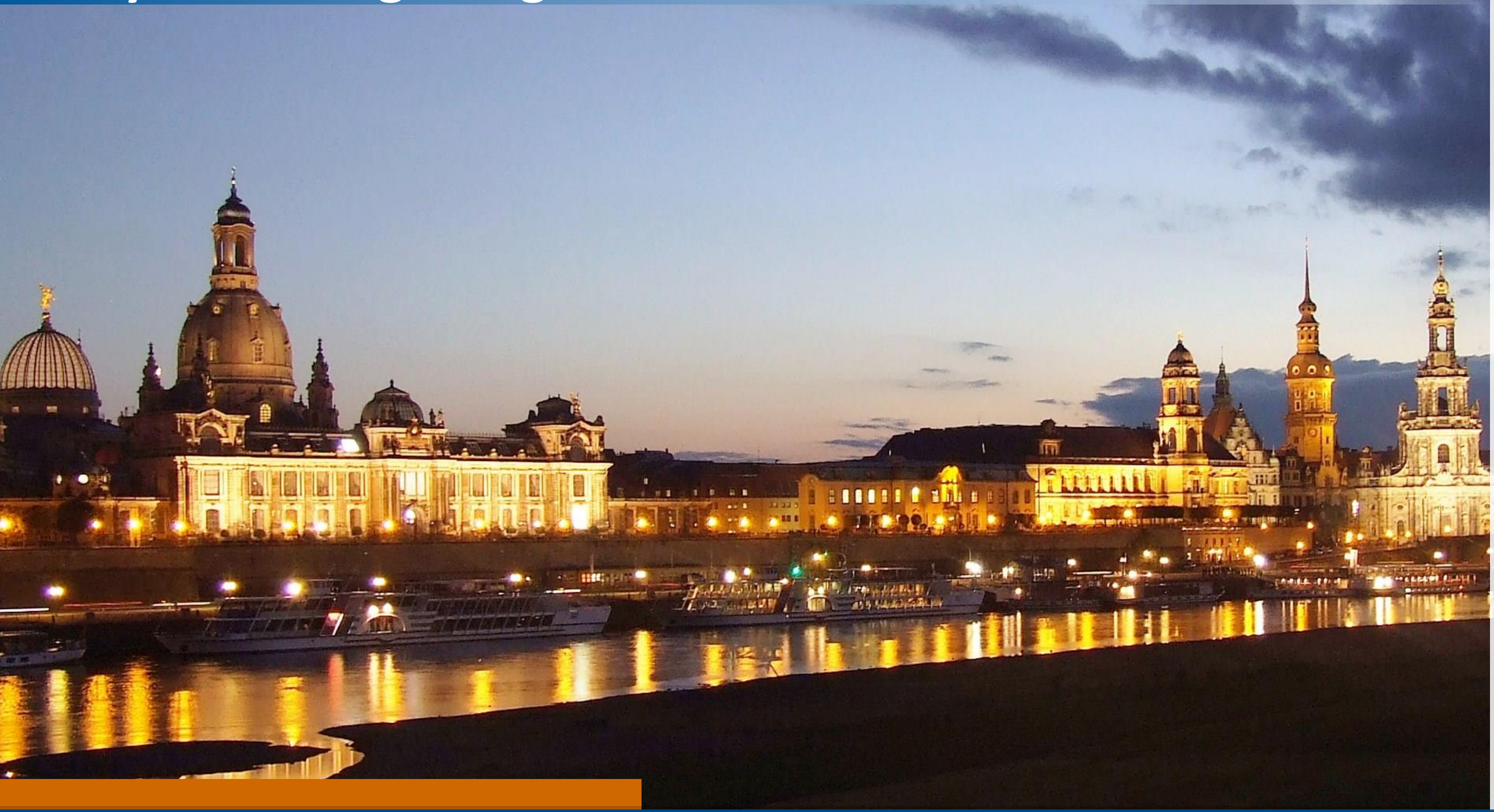
Nanometer probing of ultrahigh intensity ultrashort pulse laser interaction with solid density plasmas, by Small Angle X-Ray Scattering using XFELs



Thomas Kluge

Partially supported by EC FP7 LASERLAB-EUROPE/CHARPAC (contract 284464) and German Federal Ministry of Education and Research (BMBF) (contract 03Z1O511). This work was partially supported by DOE Office of Science, Fusion Energy Science under FWP 100182. The experiments were performed at the Matter at Extreme Conditions (MEC) instrument of LCLS, supported by the DOE Office of Science, Fusion Energy Science under contract No. SF00515.

- **Motivation** for advanced probes and **concept** of Small Angle X-ray Scattering
  - step-like interfaces
  - instabilities
  - Higher Harmonics Generation (HHG)
  - resonant scattering (RCXD)
- **Experimental realization**
  - Wires
  - Gratings

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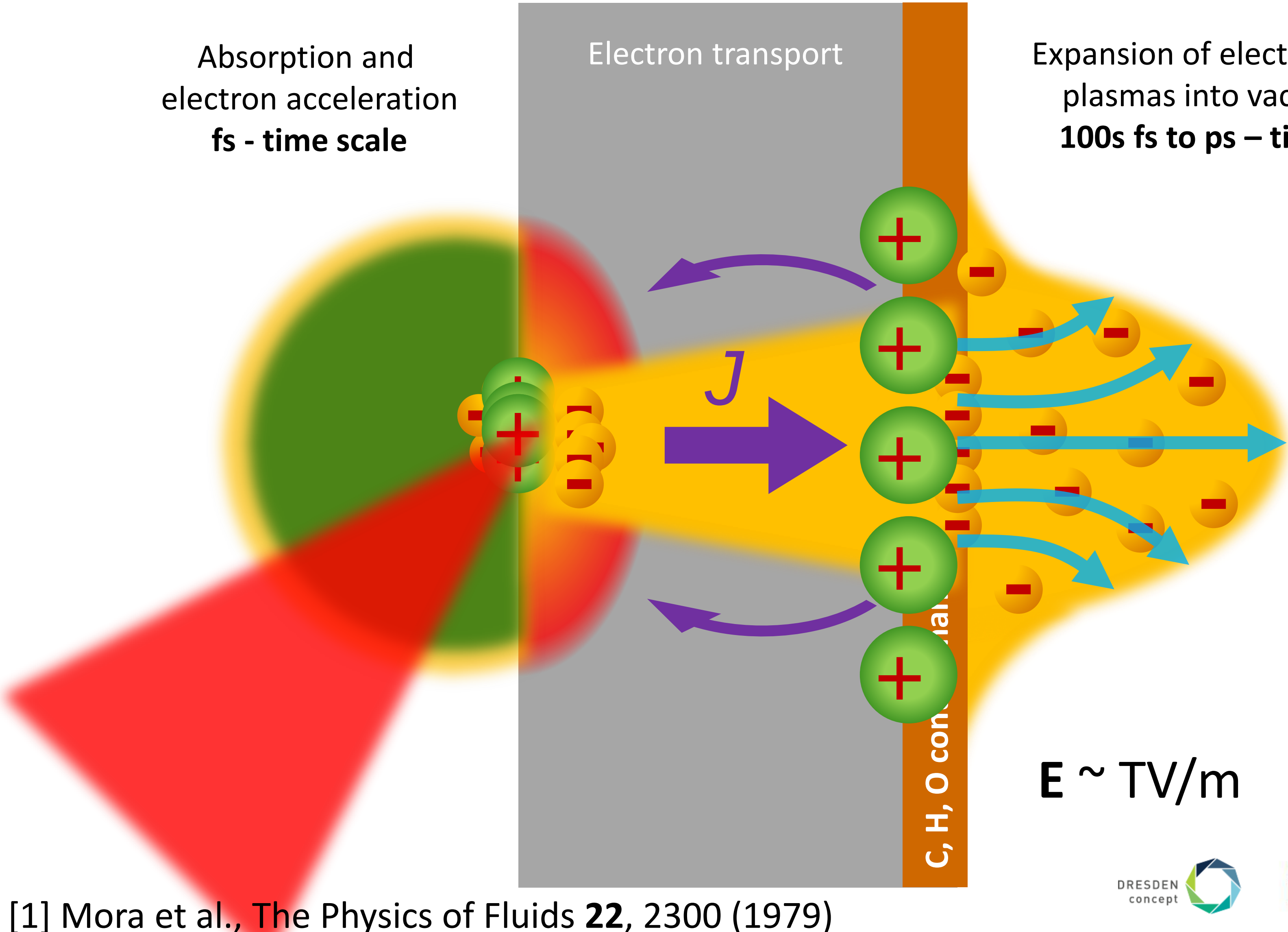
Target normal sheath acceleration (TNSA): ion acceleration

Absorption and
electron acceleration
fs - time scale



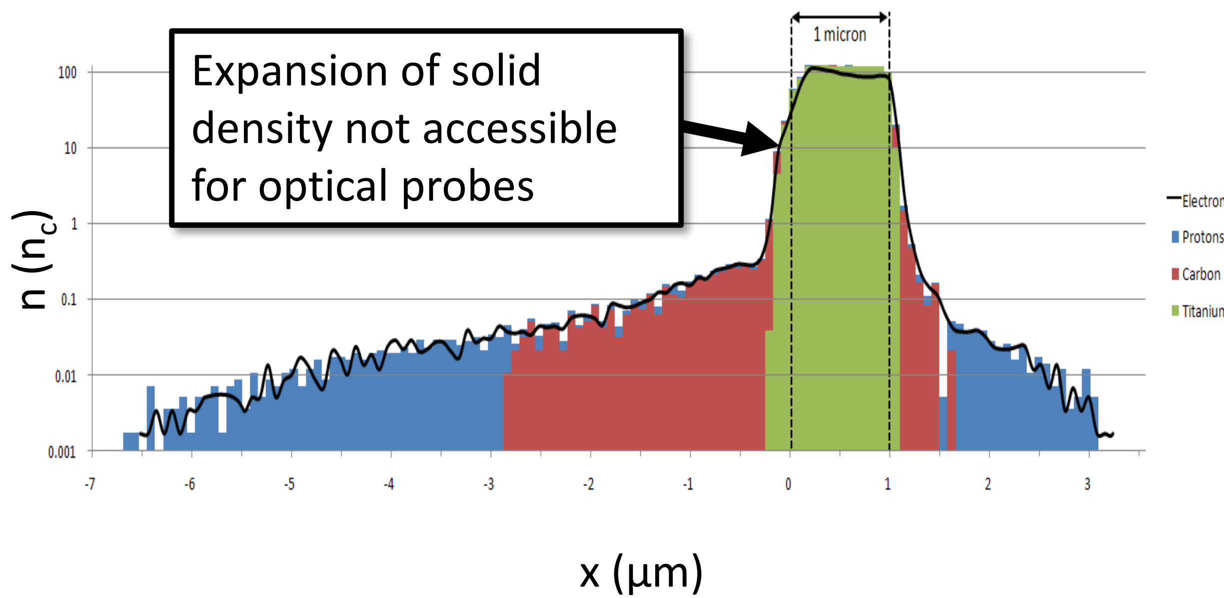
Expansion of electron-proton
plasmas into vacuum [1]
100s fs to ps – time scale

E ~ TV/m

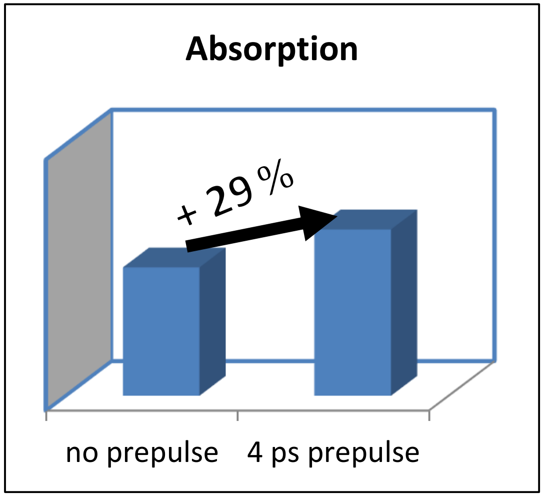
[1] Mora et al., The Physics of Fluids **22**, 2300 (1979)

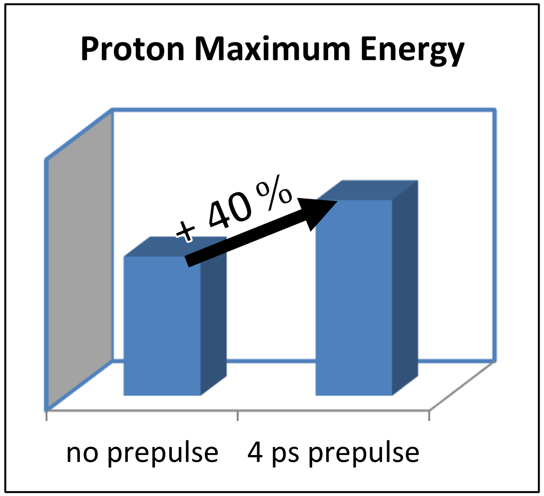
Example 1: prepulse plasma expansion

preplasma after 3ps irradiation with 10^{17} W/cm²:

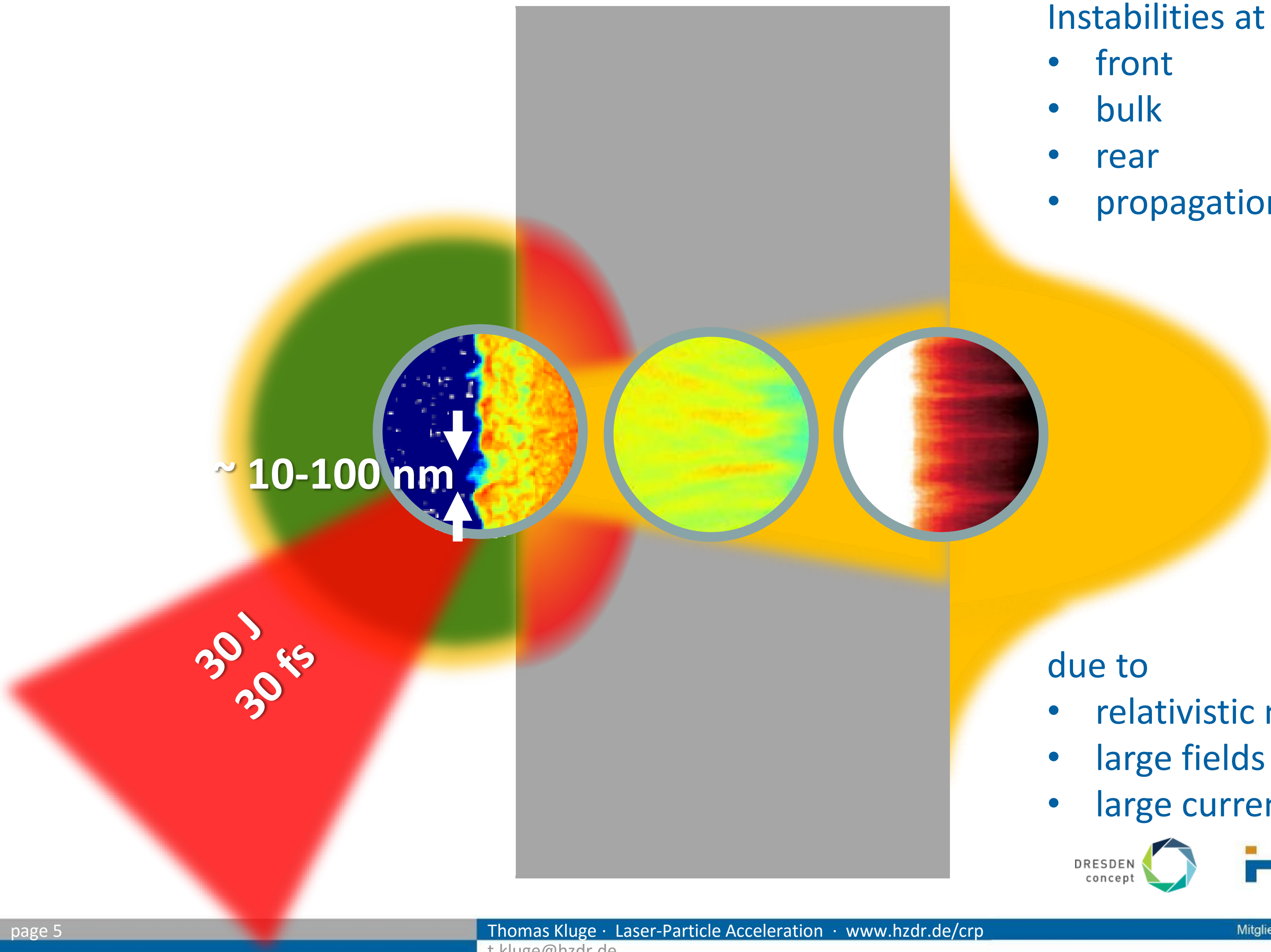


more details next talk by **M. Garten**





Example 2: non-linear processes



Instabilities at

- front
- bulk
- rear
- propagation to detector

due to

- relativistic motion
- large fields
- large currents

Complex plasma dynamics in relativistic laser – solid interaction

- **uncertain initial conditions**
- **complex transport dynamics**

⟷

Indirect and incomplete diagnostics

Existing diagnostics:

Proton radiography	> ps, indirect
Phase contrast imaging	~micron + only underdense for IR
Reflectometry	only surface
Harmonic measurement	only surface, indirect
K-alpha/ self emission	> ps, > micron
	integration of signal over line of sight

Motivation for advanced probes

Complex plasma dynamics in relativistic laser – solid interaction
- **uncertain initial conditions**
- **complex transport dynamics**

⟷

Indirect and incomplete diagnostics

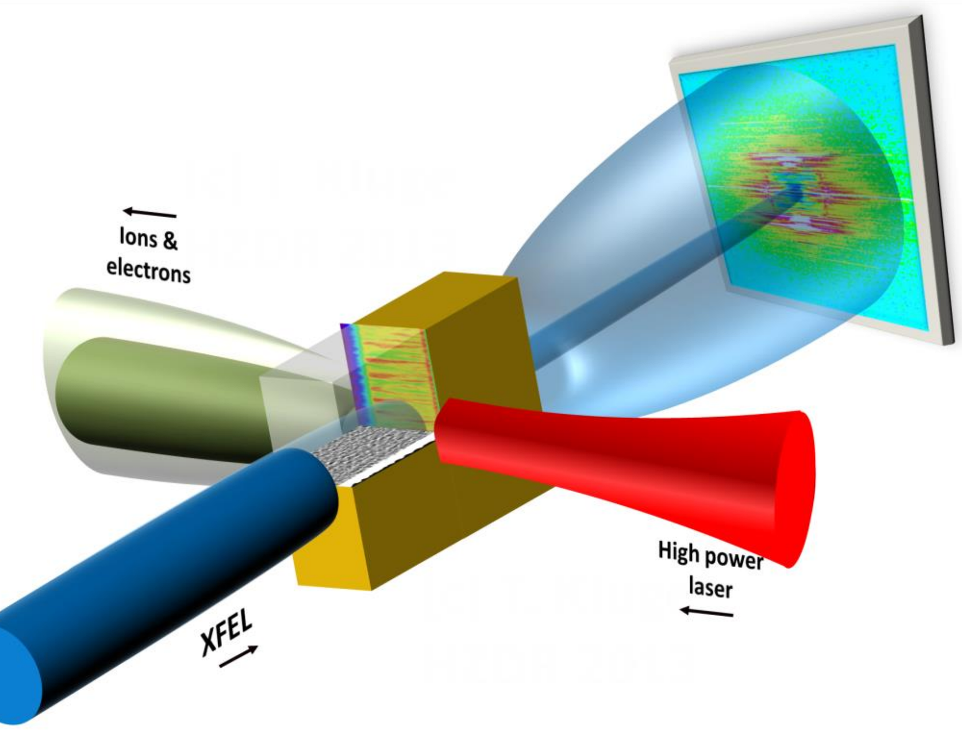
⟷

Limited predictive capabilities of simulations

Simulations in this presentation done with PICLS [1]
- Dispersion-free Maxwell solver: Directional Splitting
- 4th order particle pusher
- Binary collissions
- Ionization: ADK, Thomas-Fermi, SAHA, collissional

[1] J. Comput. Phys. **227**, 6846 (2008)

- Penetration through plasma, with high brightness
- Ultra short duration (down to 2 fs and below)
- Narrow bandwidth (few eV)



1 **SAXS** Small Angle Xray Scattering

density modulation imaging: hole-boring, hydro-expansion, shocks, surface harmonics, filamentation channels

2 **RCXD** Resonant Coherent Xray Diffraction

ionization dynamics, plasma temperature, electronic structure/ excitation

XPCS Xray photon correlation spectroscopy

disorder, melt, plasma temporal evolution

Faraday rotation

internal fields (interfaces, filaments)

XRTS

T_i, T_e, n_e (Z^*)

Phys. Plasmas **21**, 033110 (2014)

[1] J. Comput. Phys. **227**, 6846 (2008)

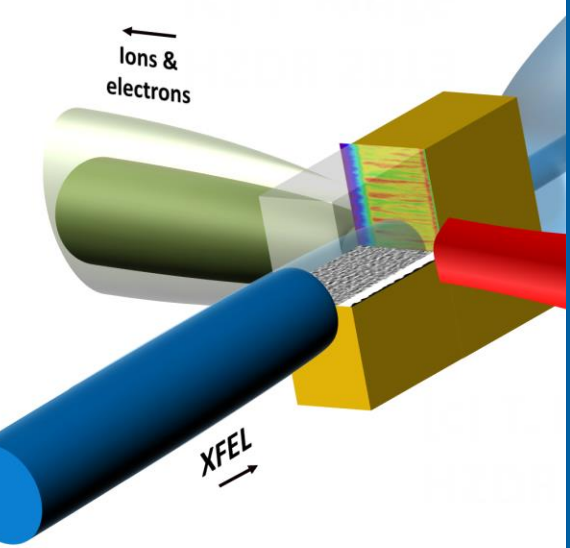
1 | SAXS Small Angle Xray Scattering

- electron – electron, ion – ion correlations
- plasma expansion, filaments, hole boring, HHG

1 | SAXS Small Angle Xray Scattering

...aging: hole-boring,

... geometry



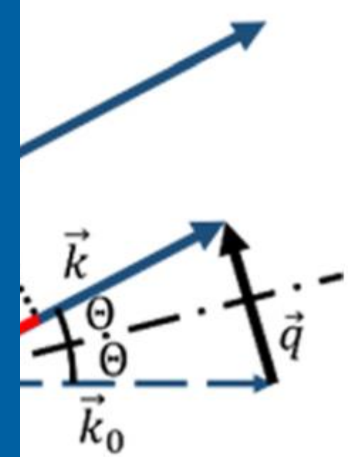
Scattering on

- electrons (Thomson scattering)
- ions (photoionization)

$$I(q) \propto FT\left|n_e(\vec{r}) + \sum n_Q(\vec{r}) f_Q\right|^2$$

n_Q: density of ions with Q bound electrons

f_Q: effective form factor $\langle Q + i\sigma_{ph}/r_e^2 \rangle$



$$= -\vec{r}\,\underbrace{\left(\vec{k} - \vec{k}_0\right)}_{\vec{q}}$$

$$I(\vec{q}) = \sum_{\vec{r}} e^{-(\omega t - \vec{r}\,\vec{q})}$$

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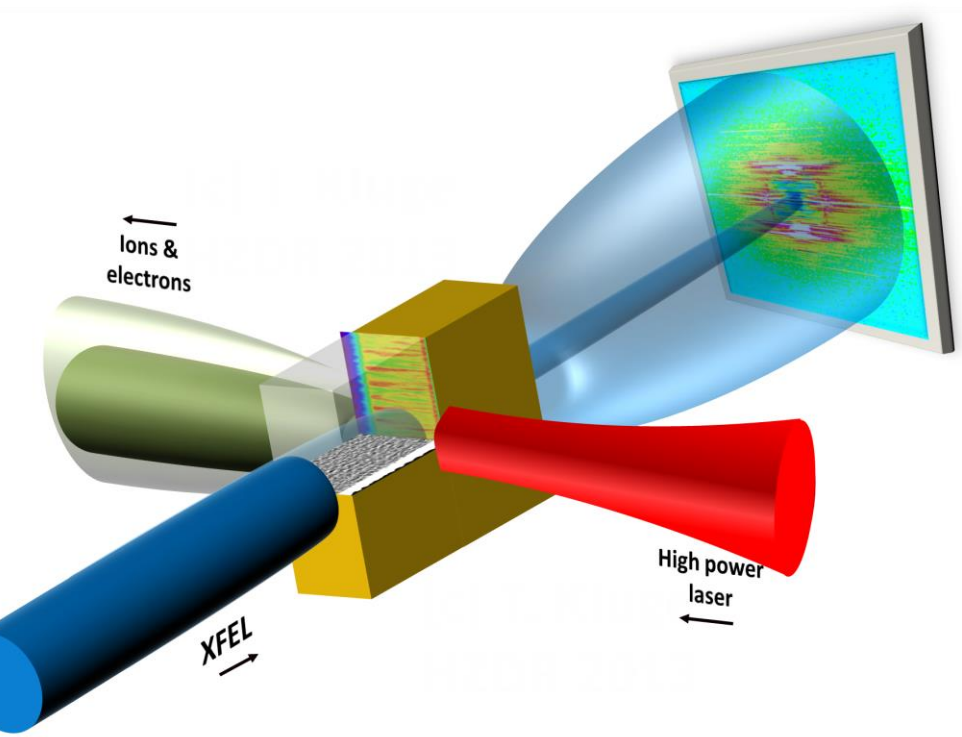
- **<u>plasma expansion</u>, filaments, hole boring, HHG**



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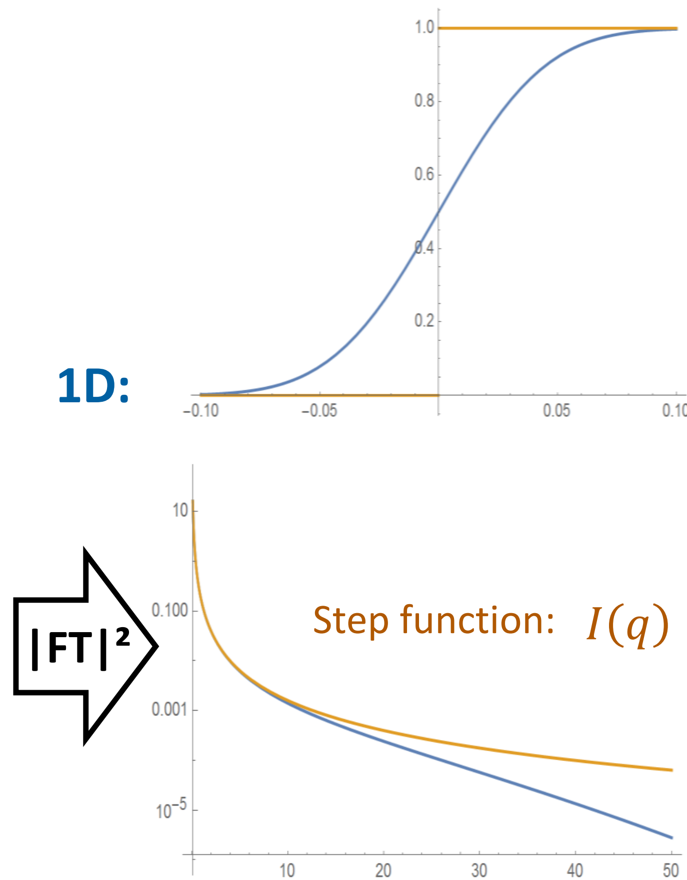

Step function: $I(q) \propto \dfrac{1}{q^2}$

Error function: $I(q) \propto \dfrac{1}{q^2} e^{-q^2 s^2}$

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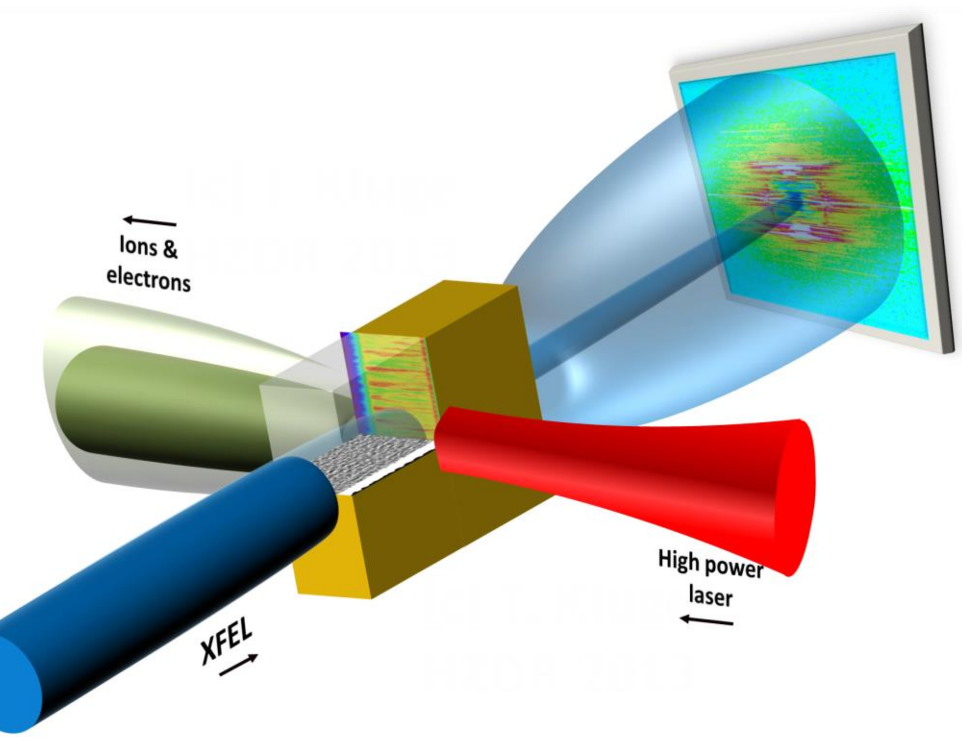

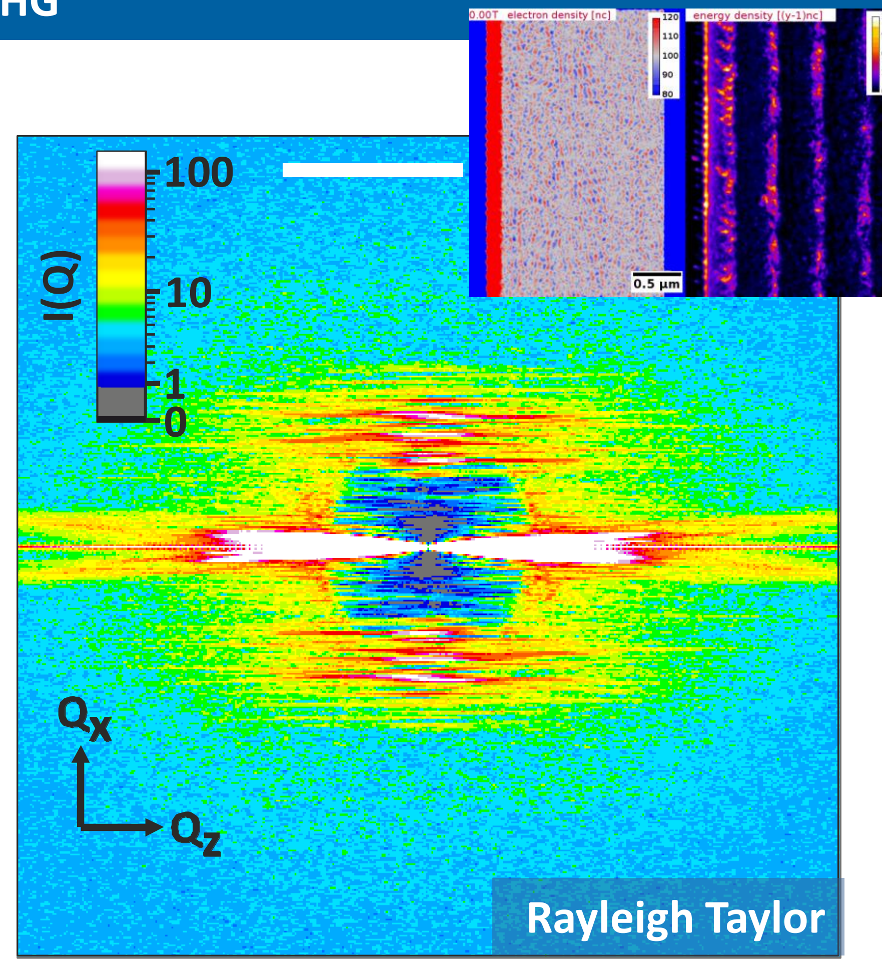

Param.: a_0=10, n=100 n_c, Z/A=**1/2**, **no** preplasma

XFEL 8 keV, 10^{10} phot., focused to 5x5 µm, 6.6 fs

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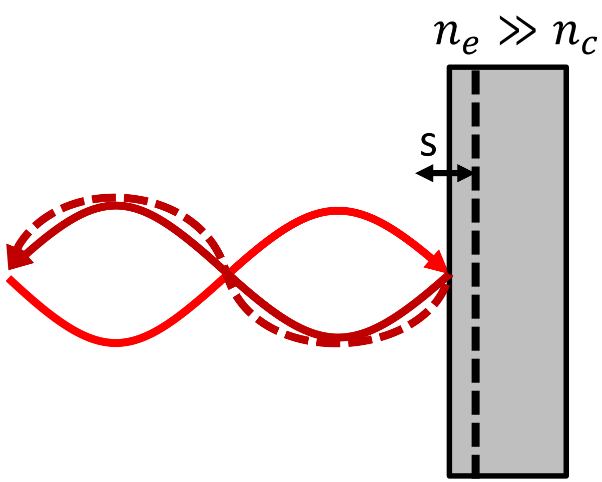
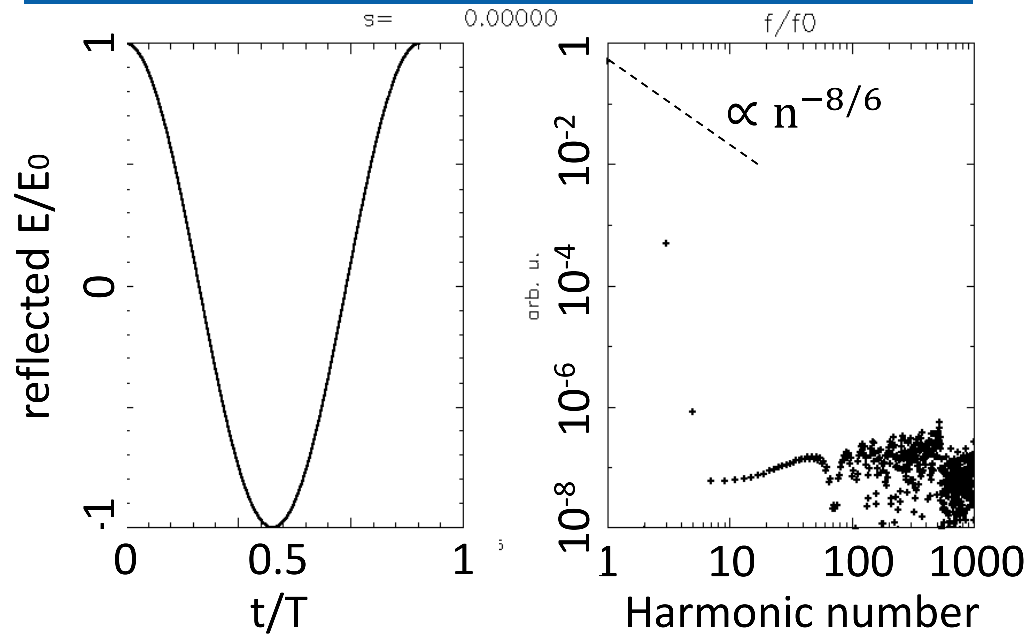


$\omega_M = 2\omega_0$ (s-pol.)



- **Universal** spectrum [1]:
  - power law for $n < 3\gamma_S^3$
  - exponential roll-off for higher harmonics
- Detailed harmonic spectrum depends on detailed surface oscillation

[1] S. Gordienko et al., Phys. Rev. Lett. **94** (2005)
T. Baeva et al., Phys. Rev. E **14**, 2006.

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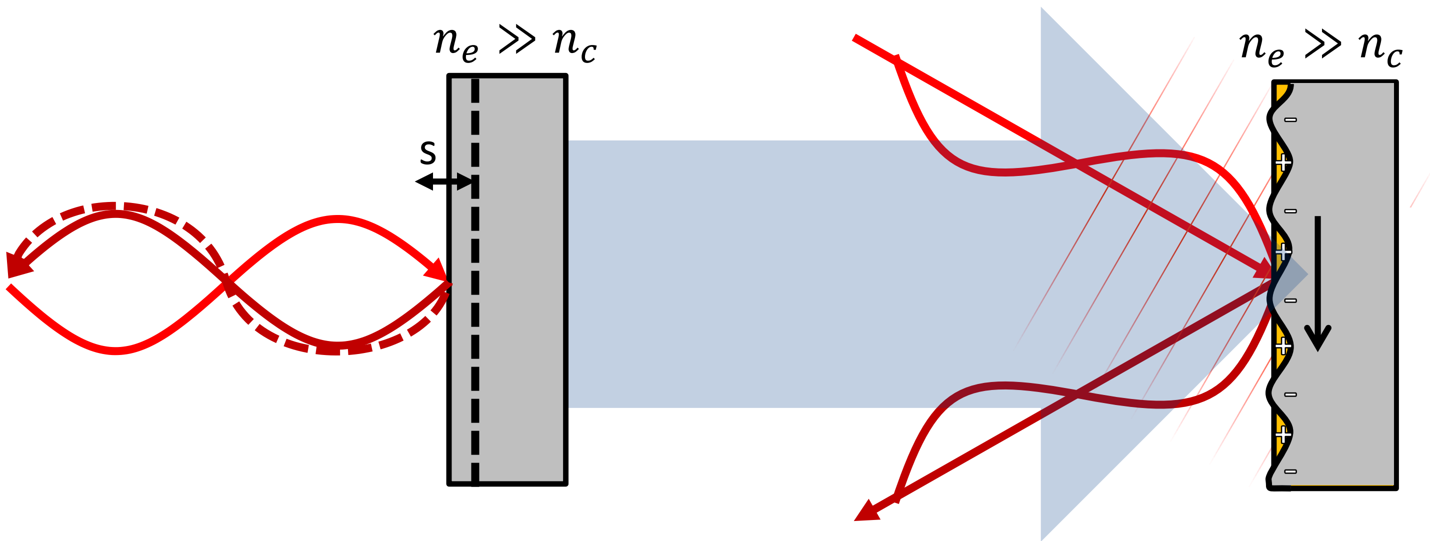

- **Universal** spectrum [1]:
  - power law for $n < 3\gamma_S^3$
  - exponential roll-off for higher harmonics
- Detailed harmonic spectrum depends on detailed surface oscillation
- Temporal oscillation **structure transforms into spatial surface modulations** for oblique incidence

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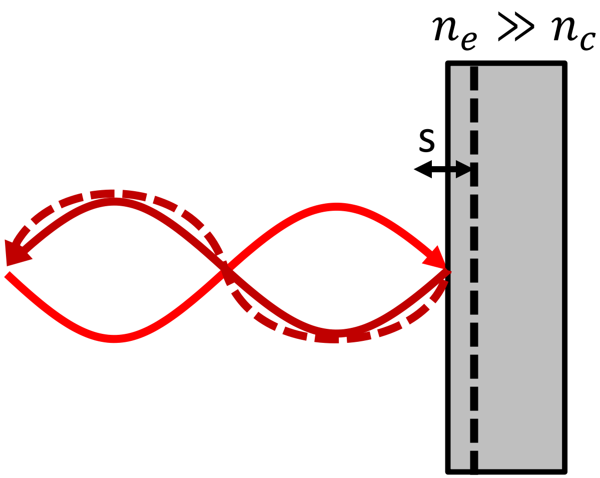
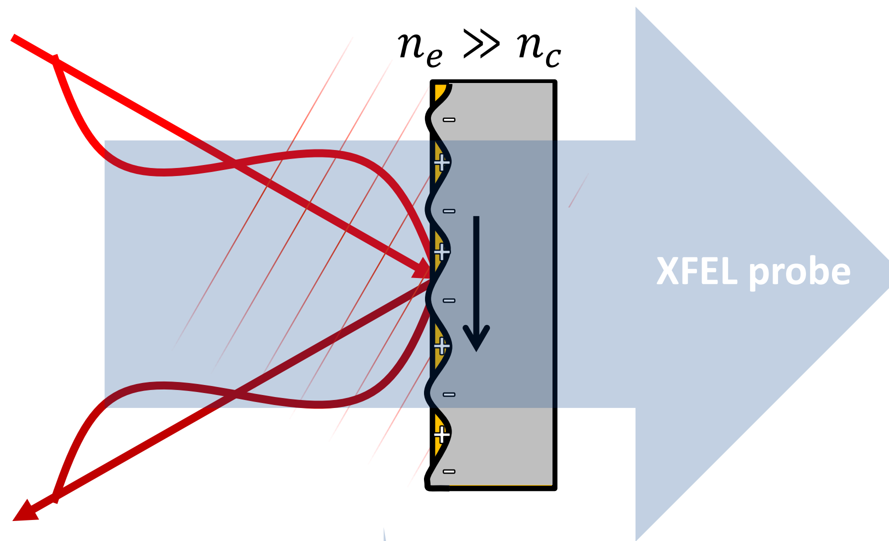
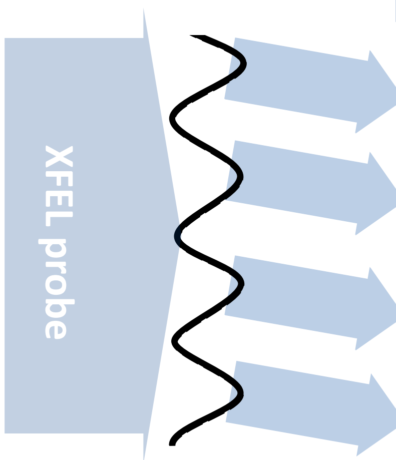




„Atto-SAXS“

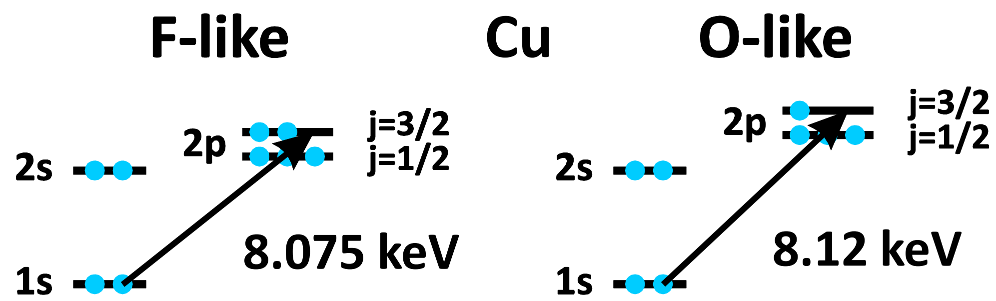


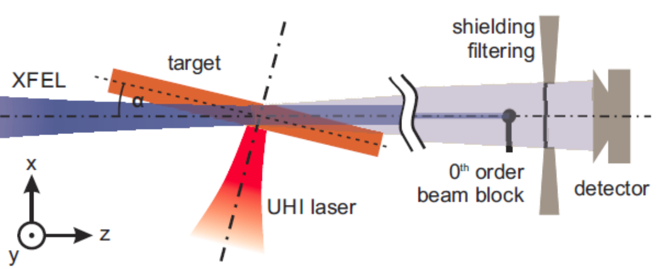
scattering:
scattering always in **same direction,** smearing by movement only **during feature passage**

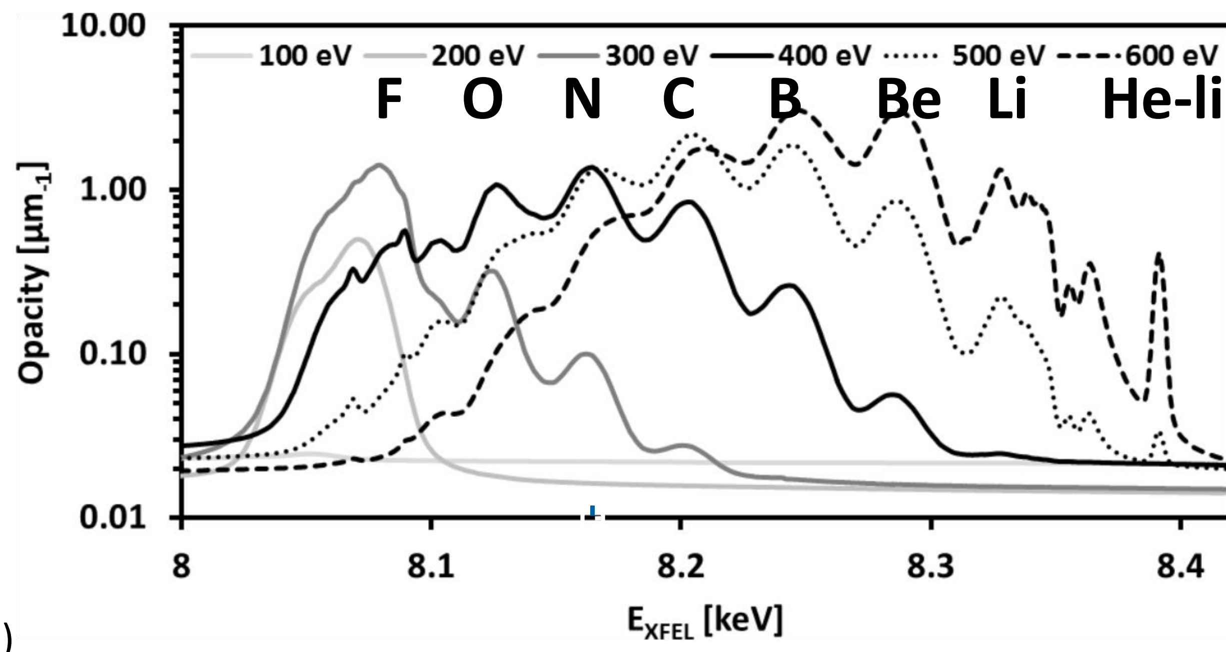
2 | RXCD Resonant Coherent Diffraction

- bound-bound resonances dramatically increase scattering cross section
- SAXS on ions
- elemental + charge state specificity

Similar to Anomalous Diffraction/ XANES
C. Song et al., PRL 100, 025504 (2008)
S.-K. Son, H. N. Chapman, R. Santra PRL 107 218102 (2011)
but here bound-bound resonances to enable charge state/electronic configuration sensitive diffraction







FLYCHK (H.-K. Chung et al. HEDP 2005)

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but here bound-b

enable charge state

configuration sensit

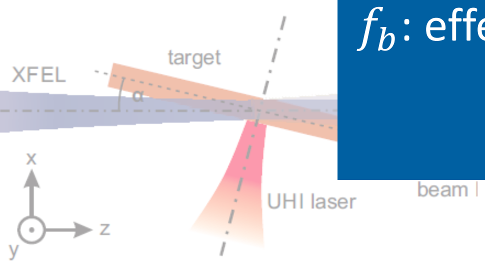
F-like Cu O-like

keV

$$I(q) \propto FT\left|n_e(\vec{r}) + \sum n_Q(\vec{r}) f_Q + \sum n_b(\vec{r}) f_b\right|^2$$

n_b: density of ions with b bound electrons in the transition core shells

f_b: effective form factor for bound-bound transitions



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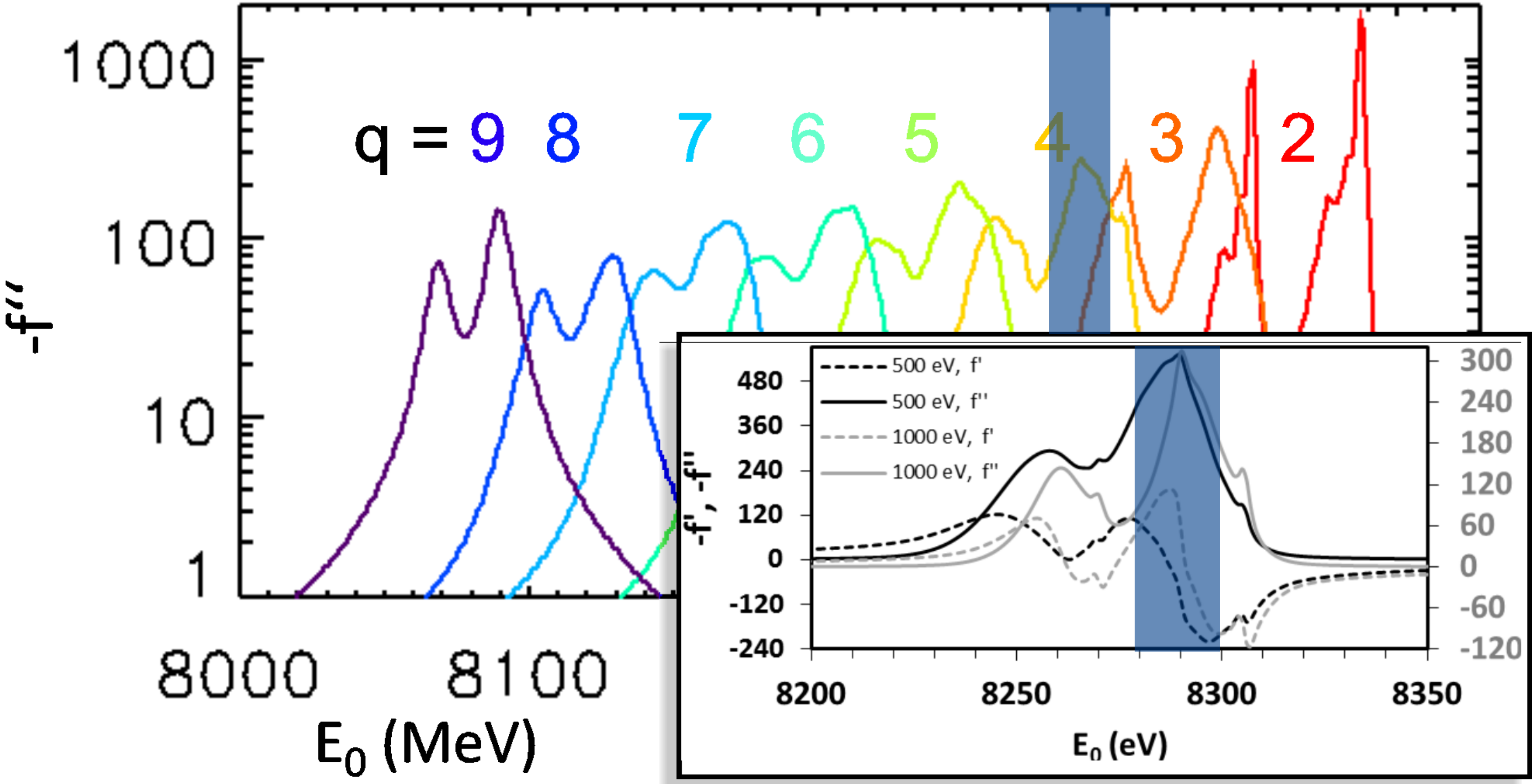
2 | RXCD Resonant Coherent Diffraction

- need to compute the ion scattering factors: SCFLY
- opacity → select only transition of specific number of e- in 1s, 2s and 2p, average over all configurations, normalize to ion abundance → f'' (imaginary part of f)



2 | RXCD Resonant Coherent Diffraction

- **need to compute the ion scattering factors:**
- **opacity → select only transition of specific number of e- in 1s, 2s and 2p, average over all configurations, normalize to ion abundance → f“ (imaginary part of f)**

n_b,f'_b and f''_b are averaged quantities over all ions with different electron configurations and are therefore temperature dependent (and temperature history!)

→ in principle for each pixel in the PIC simulation, individual SCFLY-runs, including full time history, is needed

$$\frac{2048\times 2048\times \mathbf{10\ min}}{60\times 24\times 365\ \mathrm{min/yr}} \approx 100\ CPU\ yrs.!$$

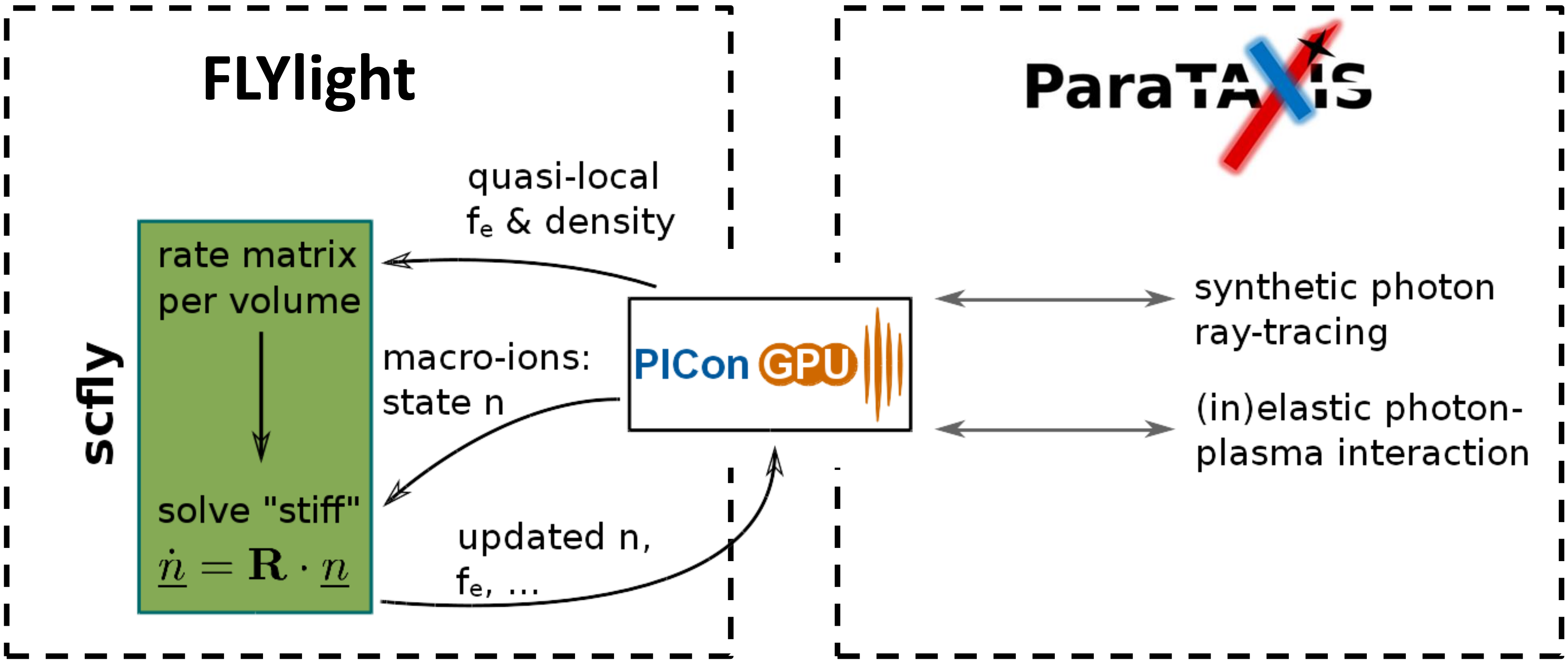
→ For now we use lookup tables and average time history
→ General features and order of magnitude estimate

→ work in progress: atomic physics self constistently in PIC: **FLYlite**

Implementing Non-LTE Rate Equations of SCFLY

Collisional Ionization Methods in PIConGPU

Slide courtesy A. Huebl



List of processes:

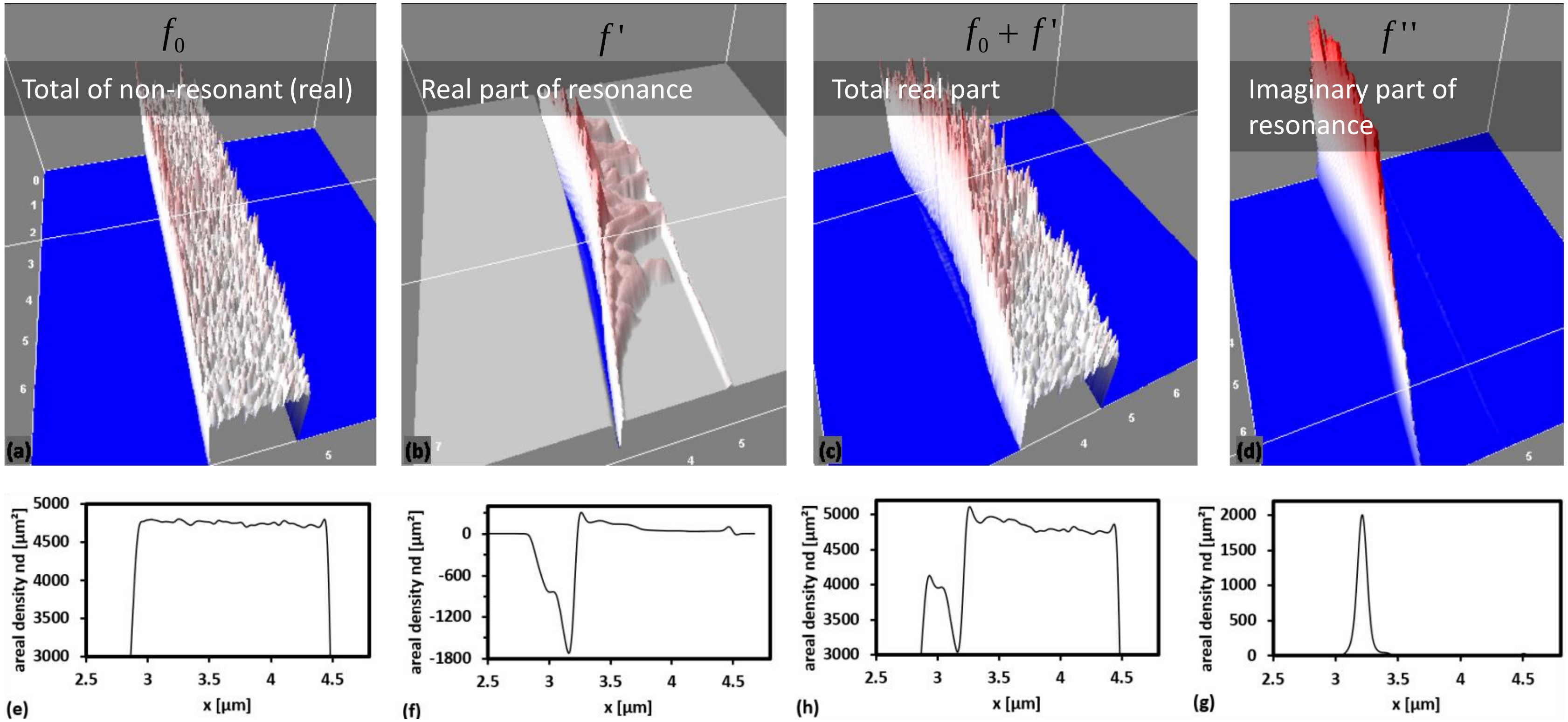
- collisional excitation & deexcitation
- collisional ionization & recombination
- autoionization
- electron capture
- radiative recombination
- radiative pumping
  - spontaneous emission

H.-K. Chung et al. High Energy Density Physics 1 (2005) 3-12

H.-K. Chung et al. High Energy Density Physics 3 (2007) 57-64

2 | RXCD Resonant Coherent Diffraction

- **calculation of scattering patterns**



$$I(\boldsymbol{k}) \propto H(\boldsymbol{k})H(\boldsymbol{k})^*$$

$$f_q^{\mathrm{res}}(E_0) = f_q'(E_0) + i f_q''(E_0)$$

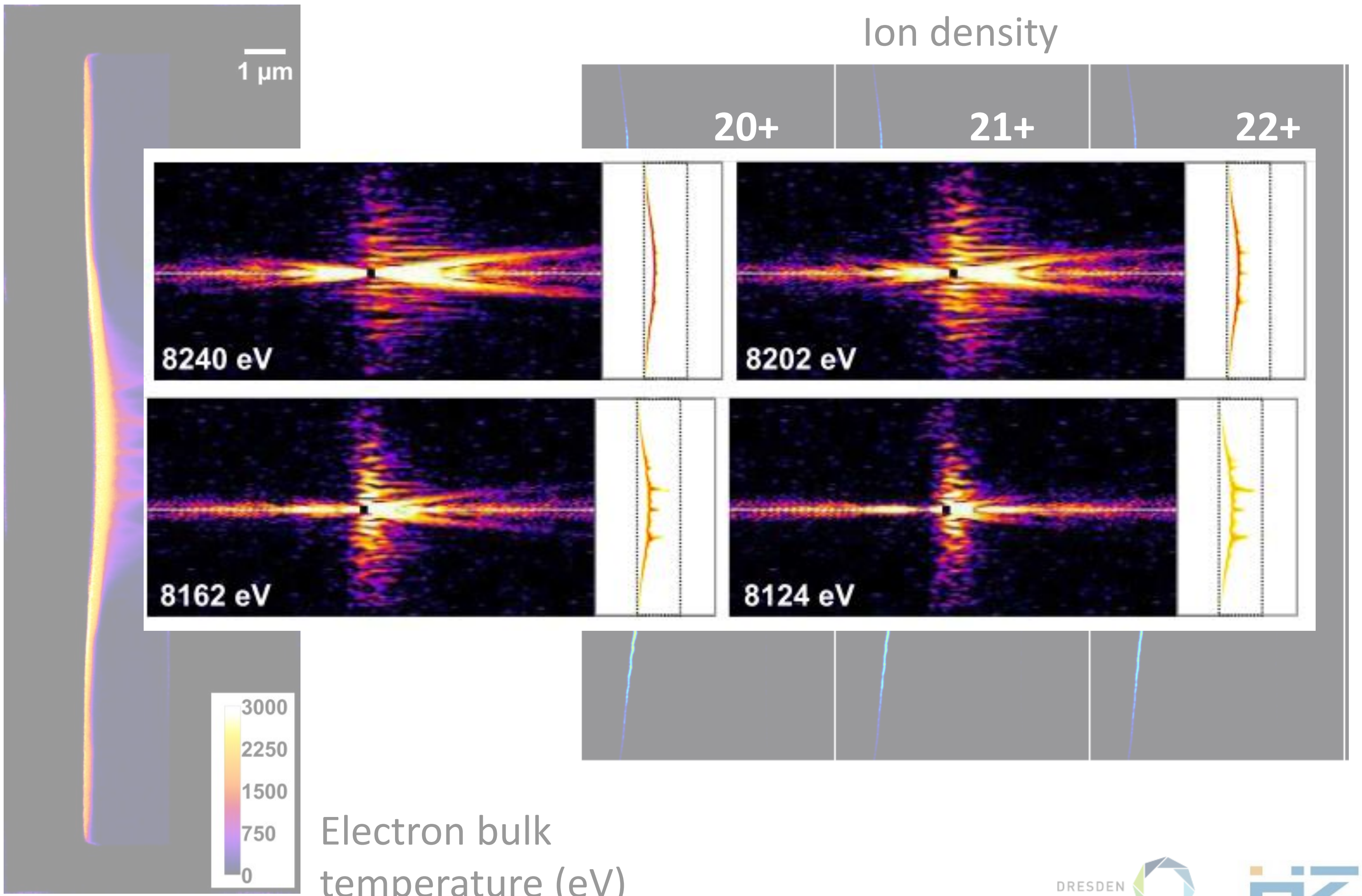
$$H(\boldsymbol{r}) \equiv h^{\mathrm{free}}(\boldsymbol{r}) + h^{\mathrm{bound}}(\boldsymbol{r}) + h^{\mathrm{res}}(\boldsymbol{r})$$

$$= n_e^{\mathrm{free}}(\boldsymbol{r}) + \sum_{Q=0}^{Z-1} (Z-Q)\cdot n_{i,Q}(\boldsymbol{r}) + \sum_{q=1}^{q_u} n_{i,q}(\boldsymbol{r}) f_q^{\mathrm{res}}$$

Simulation: $a_0 = 8.5$, material: Cu, thickness: 2 µm, Thomas – Fermi ionization

2 | RXCD Resonant Coherent Diffraction

- **calculation of scattering patterns**



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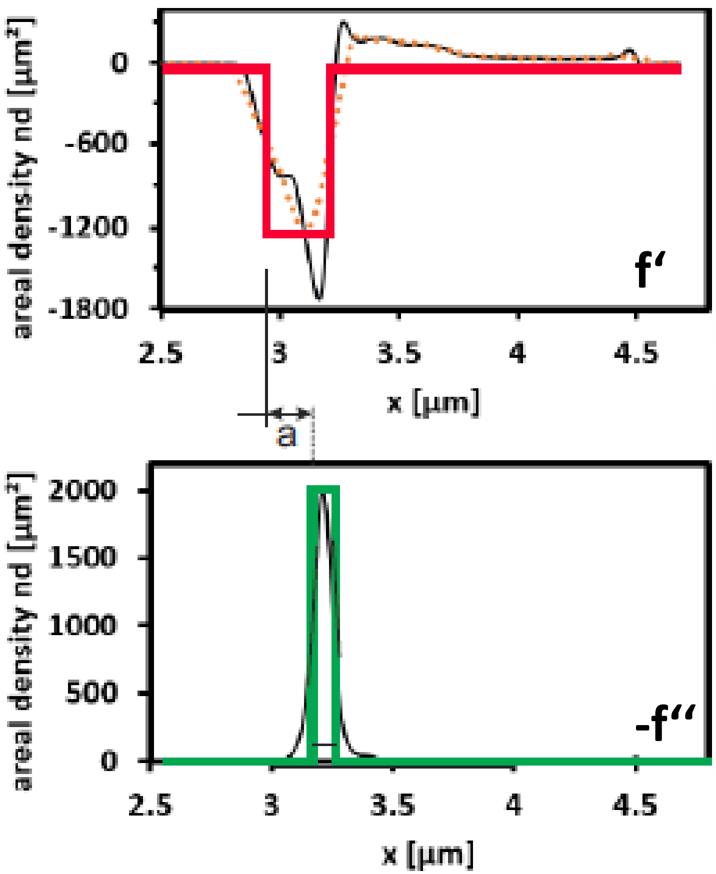
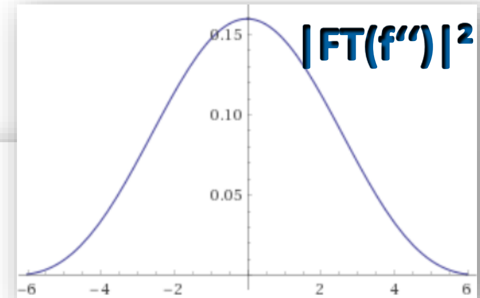
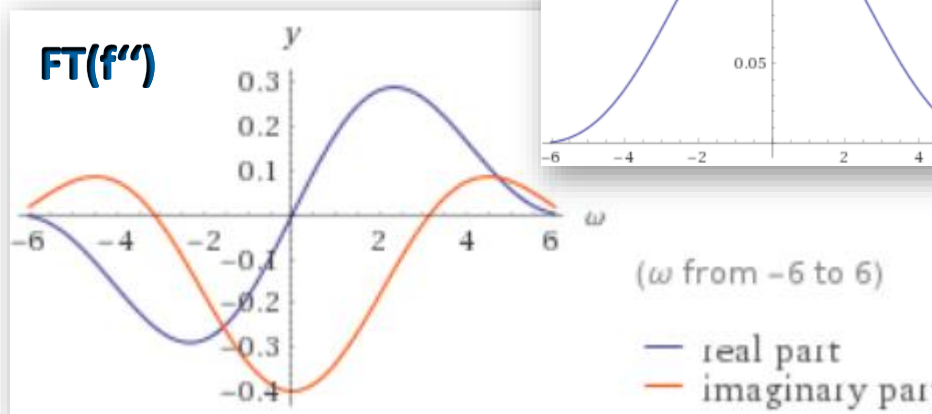
2 | RXCD Resonant Coherent Diffraction

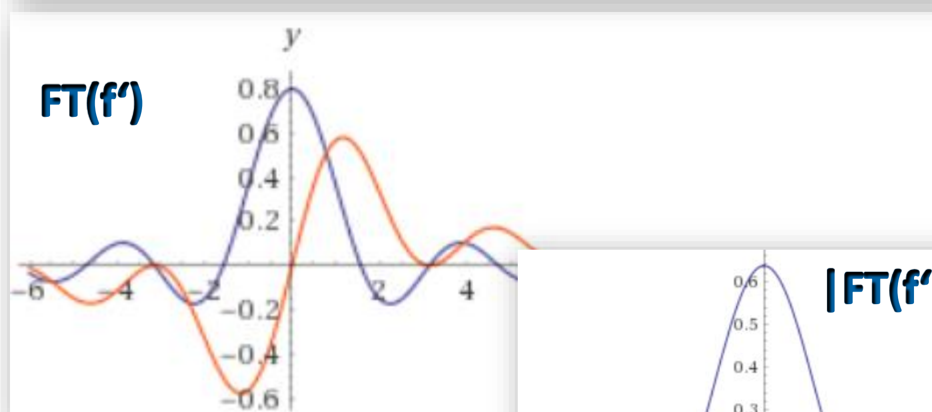
- **calculation of scattering patterns**

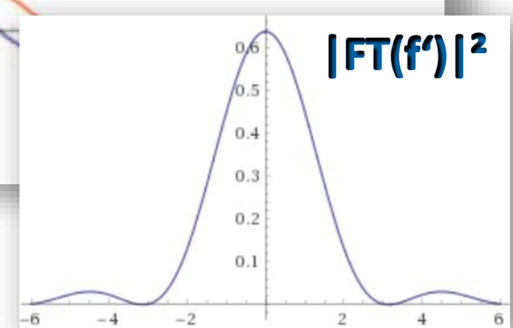
free e- + Kramers Kronig of bound-bound/bound-free
→ real part broader in energy space than imaginary part











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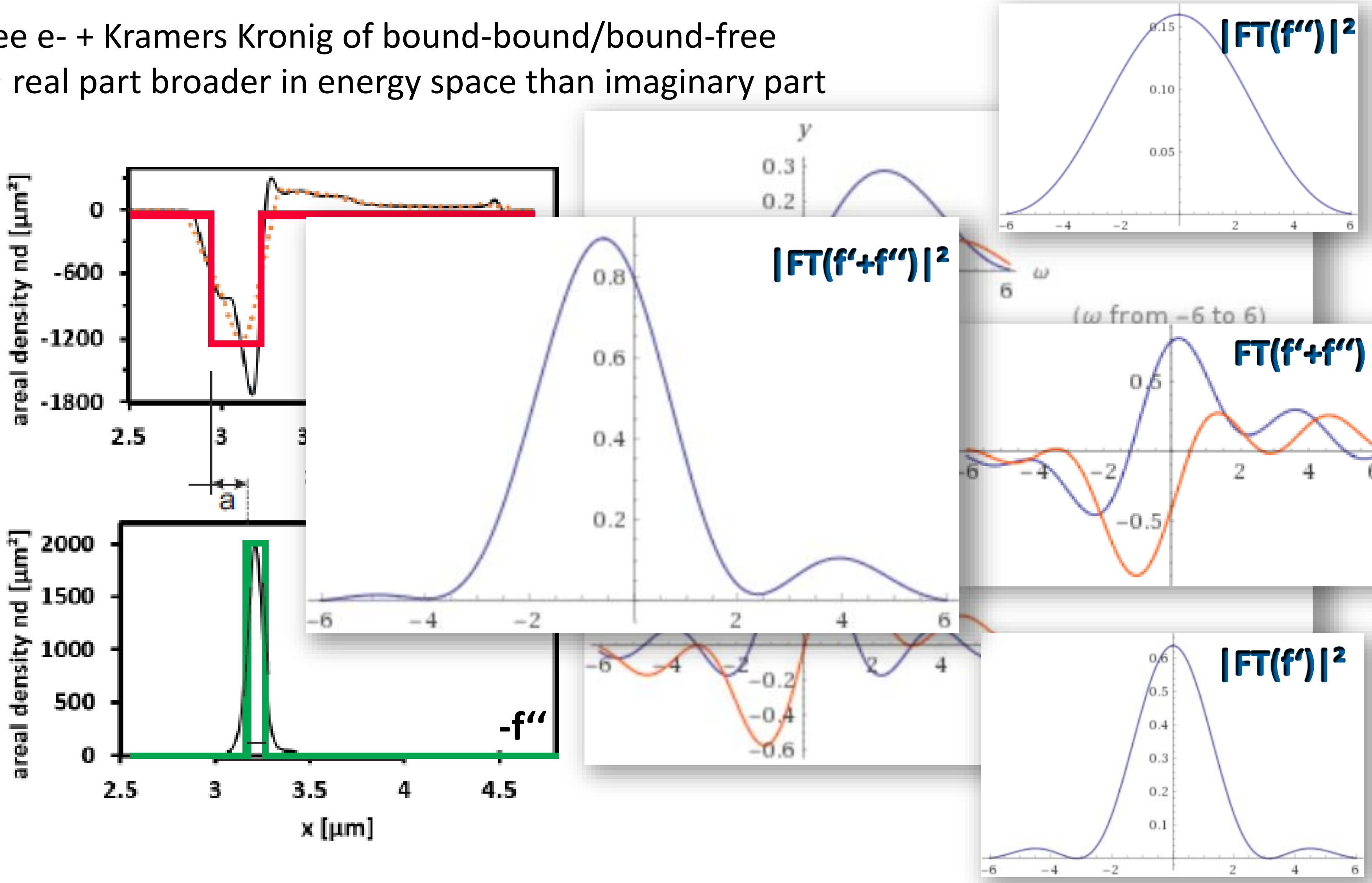
- **calculation of scattering patterns**

free e- + Kramers Kronig of bound-bound/bound-free
→ real part broader in energy space than imaginary part



2 | **RXCD** Resonant Coherent Diffraction

- **asymmetry in scattering pattern**

free e- + Kramers Kronig of bound-bound/bound-free
→ real part broader in energy space than imaginary part

$$I(q) \propto FT\left|n_e(\vec{r}) + \sum n_Q(\vec{r}) f_Q + \sum n_b(\vec{r}) f_b\right|^2$$

n_b: density of ions with b bound electrons in the transition core shells

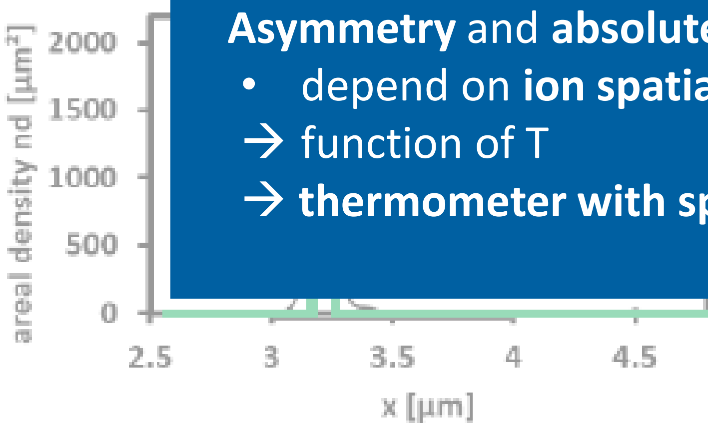
f_b: effective form factor for bound-bound transitions

Asymmetry and **absolute signal level**

- depend on **ion spatial distribution/ configuration**

→ function of T

→ **thermometer with spatial resolution**



SAXS @ UHI lasers:

- sensitive to **few nm** features
  - features can be periodic, less correlated or single
  - → plasma expansion, ripples, two-stream instabilities, hole boring, …
  - probing at solid density
- measure distribution of opacity:
  - ionization structure and spatial „temperature“ distribution
- fast features
  - surface waves/HHG („Atto-SAXS“)
  - pump-probe (**few femtoseconds** XFEL duration)
  - XPCS (XFEL pulse split-and-delay changes of speckle contrast)

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- Motivation for better probes and concept of Small Angle X-ray Scattering
  - Step interfaces
  - Instabilities
  - Higher Harmonics Generation (HHG)
  - resonant scattering (RCXD)
- **Experimental realization**
  - Wires
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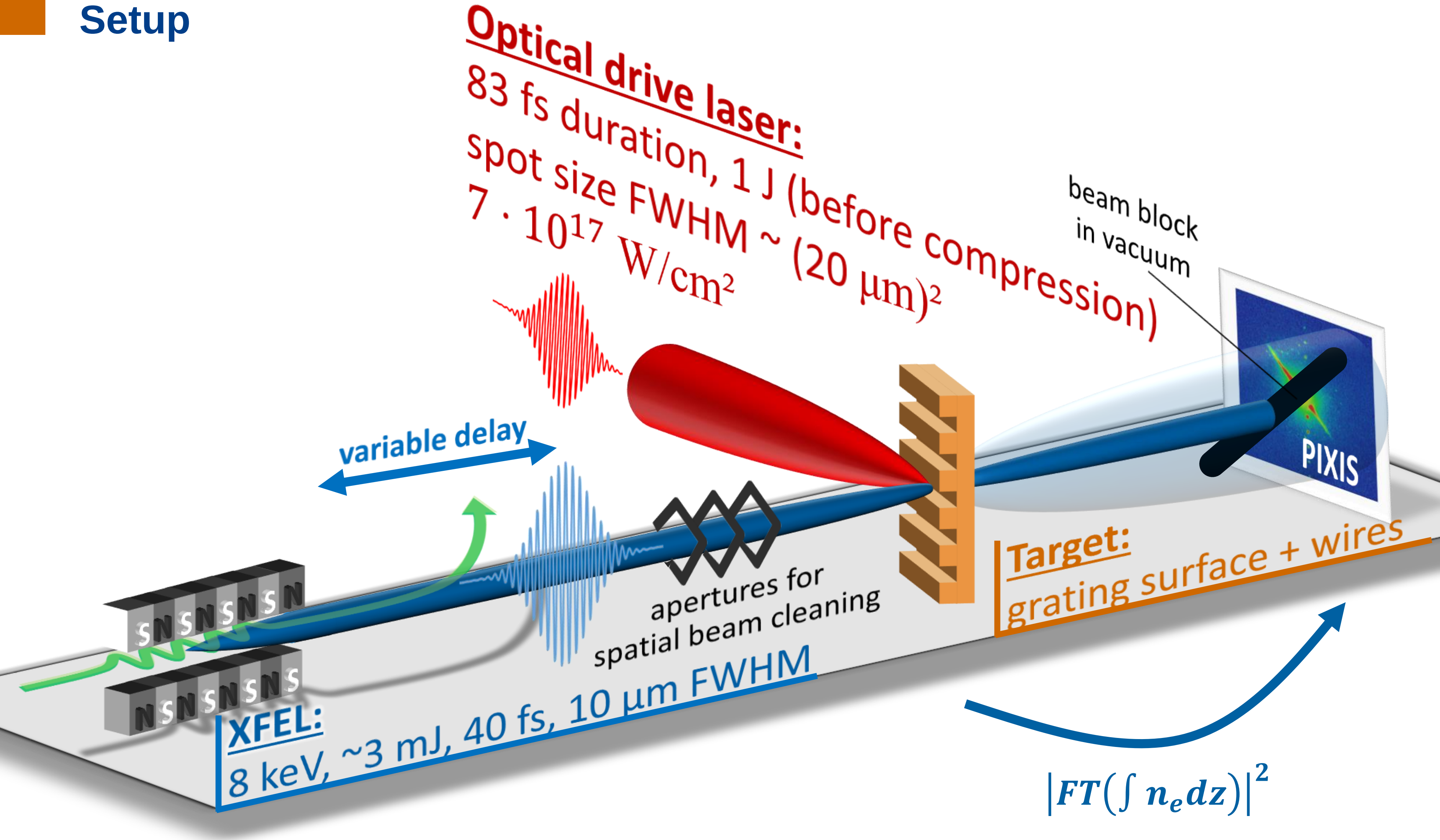
Setup


Optical drive laser:
83 fs duration, 1 J (before compression)
spot size FWHM ~ (20 µm)²
7 · 10¹⁷ W/cm²
beam block
in vacuum
PIXIS
variable delay
S N S N S N S N
N S N S N S N S
apertures for
spatial beam cleaning
Target:
grating surface + wires
XFEL:
8 keV, ~3 mJ, 40 fs, 10 µm FWHM
$|FT(\int n_e dz)|^2$

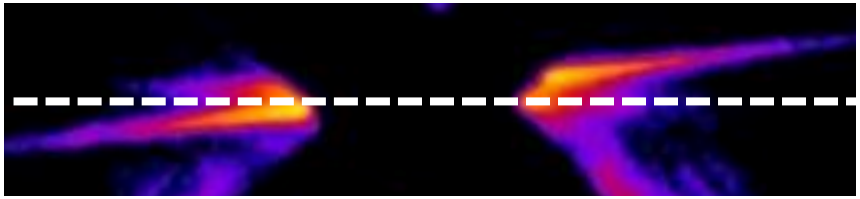
1| Structural changes during laser-solid interaction with a wire

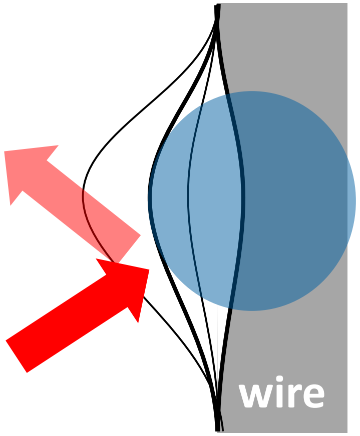
- „holeboring" probed at solid density interface unaccessible to optical probing

un-pumped

XFEL probe 40 ps after optical laser:

Pumped
50%
8.7°
→ 2.8 µm

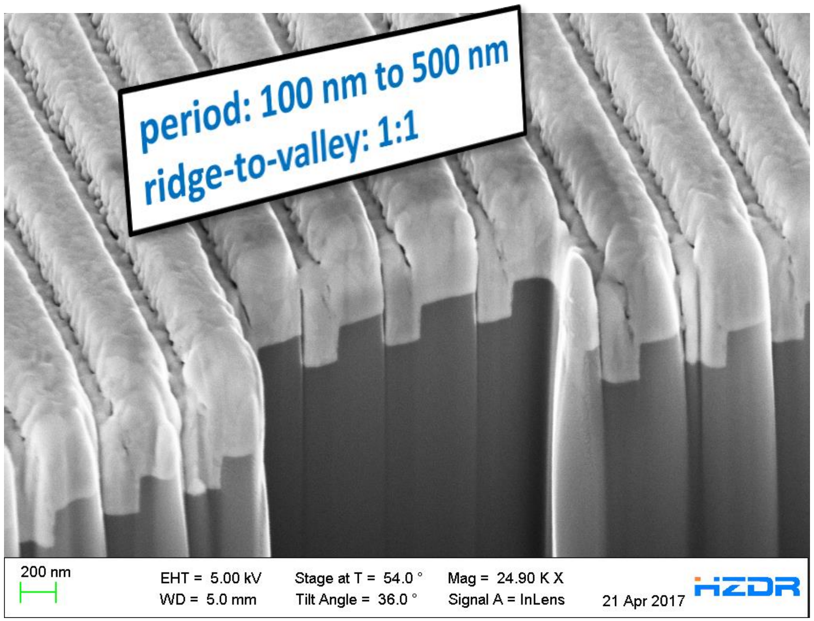


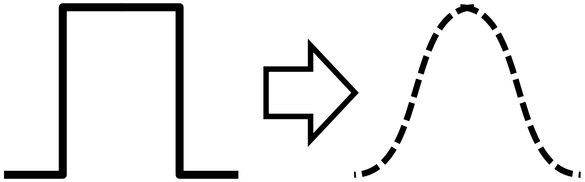


I (W/cm^2)

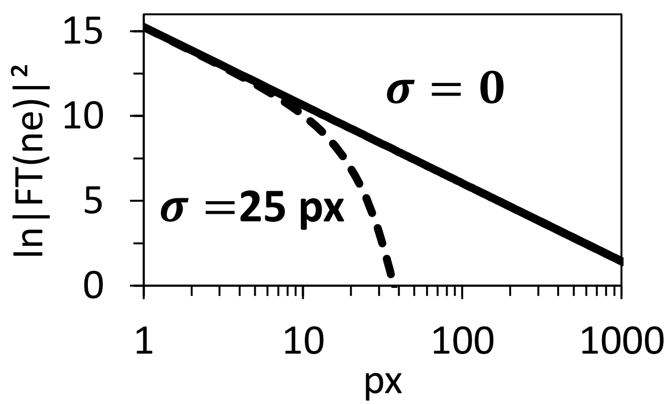
2 | measurement of sharpness with accuracy < nm

- fitting with grating equation and edge function





assuming erf-shape



Grating equation with pitch g, gap width b:

$$I(\varphi) = I_0 \cdot \left(\frac{\sin(\pi \frac{b}{\lambda} \sin\varphi)}{\pi \frac{b}{\lambda} \sin\varphi} \frac{\sin(N\pi \frac{g}{\lambda} \sin\varphi)}{\sin(\pi \frac{g}{\lambda} \sin\varphi)} \right)^2$$

Edge function

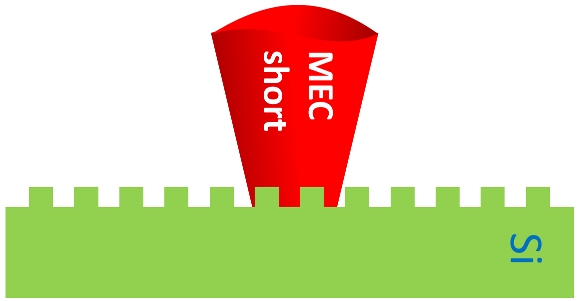
$$I(q) \propto \frac{1}{q^2} e^{-q^2\sigma^2}$$

q... scattering vector

2 | measurement of sharpness with accuracy < nm

- fitting with edge function and grating equation

$$\propto \frac{1}{q^2} e^{-q^2\sigma^2}$$

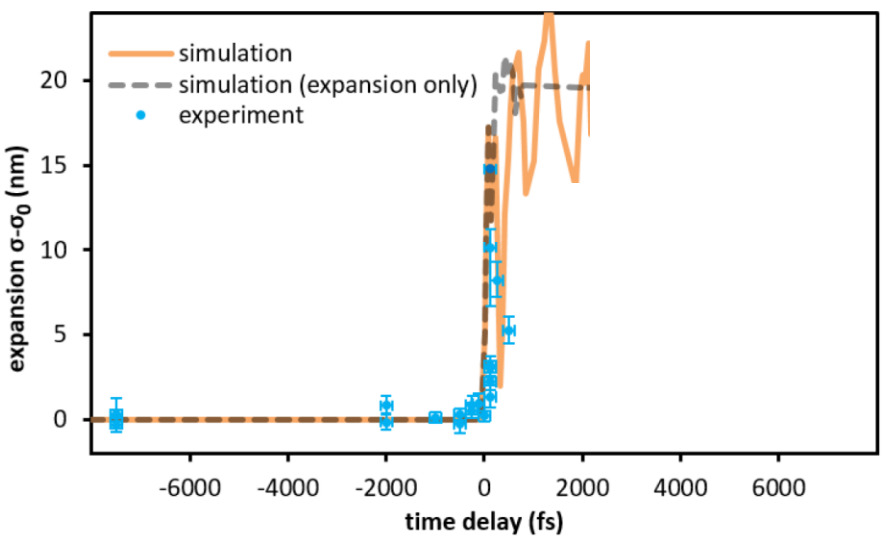


- First direct in-sutu measurement of solid plasma density expansion during **near-relativistic laser intensity**
- Unprecedented resolution (**nm, few fs**)

Kluge et al. „Observation of ultrafast solid-density plasma dynamics using femtosecond X-ray pulses from a free-electron laser" (submitted)

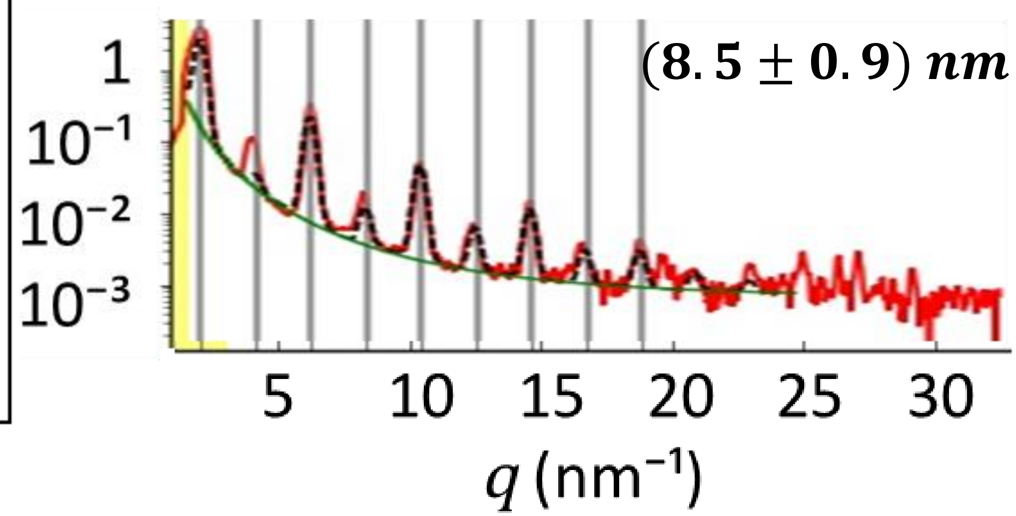
Front side grating

1 J



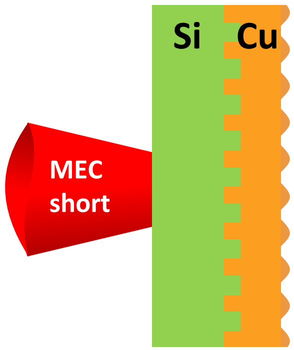
0 fs

un-pumped preshot



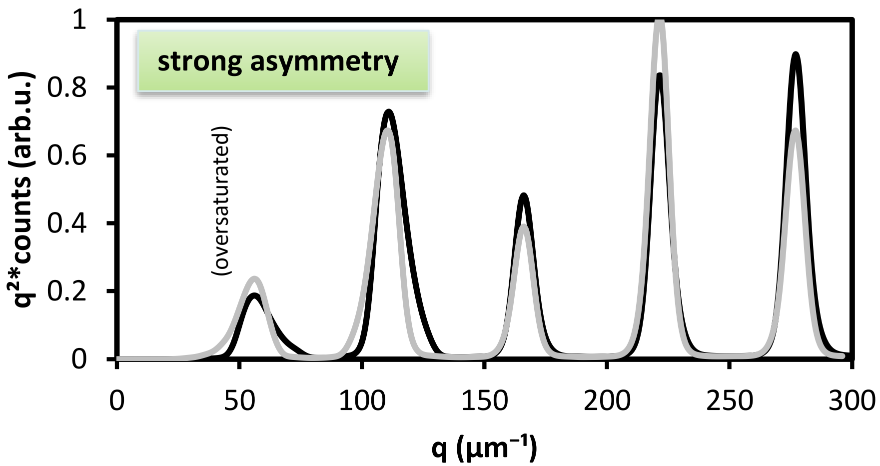
- Upon laser irradiation reduction of signal strength: grating is washed out

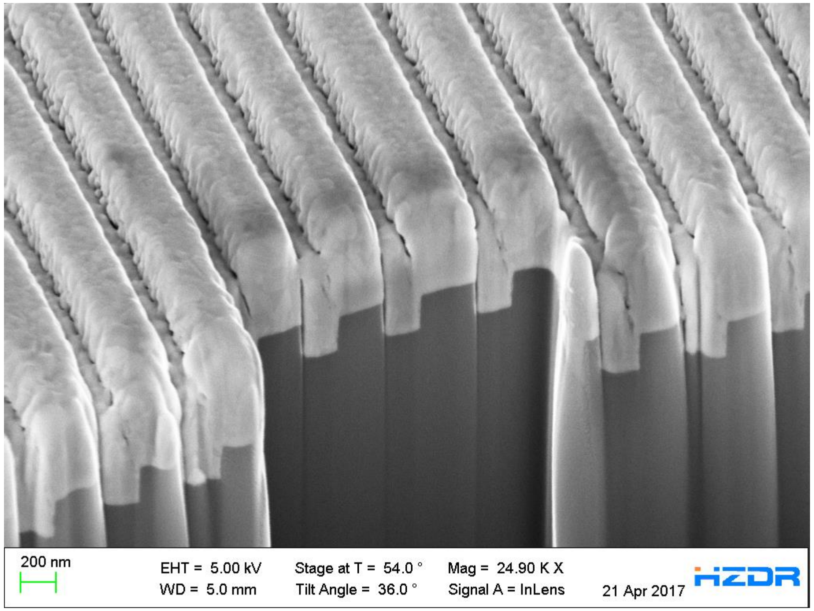
- compound targets
- different distribution of f_1, f_2
- → asymmetry



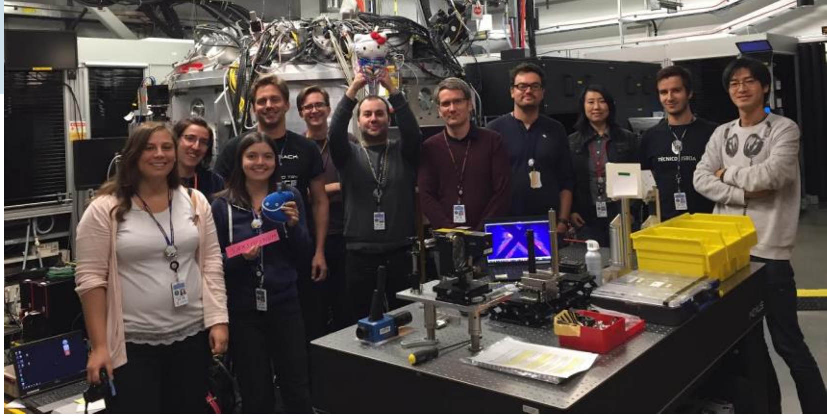
Scattering ∝ $|FT(real + imaginary)|^2$
real: Thomson scattering ∝ $Z_i n_i$
imaginary: bound-bound + bound-free opacity
$\propto (\sigma_{bb,i} + \sigma_{bf,i}) n_i \equiv \tau_i$

Preshots (XFEL only)





LN04: Cross the beams



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Future tasks

- include atomic excitations into PIConGPU: project „FLYlite“
- calculate scattering patterns from PIC: ParaTAXIS
- reconstruct scattering patterns
- put error bars on simulations („predictive simulations“)

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PIConGPU

plasma simulations for the manycore era

OpenSource Development
HZDR (GPL/LGPL)

HELMHOLTZ
ZENTRUM DRESDEN
ROSSENDORF

General Many-Core Algorithms

runs on
GPU, CPU, Power, ARM, Phi, ...

7.2 PFlop/s reported in
ACM Gordon Bell 2013

modular, general purpose,
particle-mesh library

Regular production runs on:
Titan (ORNL), Piz Daint (CSCS)

implements fully-relativistic
3D3V **particle-in-cell** algorithm

ionization, radiation reaction,
QED photon emission,
in situ diagnostics, far-field radiation,
live rendering, interactive simulations,
high-throughput I/O with ADIOS on **openPMD**

simulate **laser-plasma interactions**
for next-gen. *particle accelerators*