Dynamics of short pulse high-intensity laser irradiated surface structures:

Particle-in-Cell simulations, grazing incidence reflectometry and surface scattering

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SBP-SFX Instrument,
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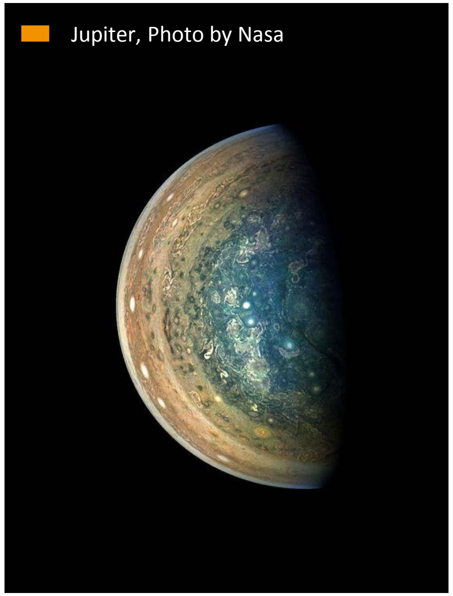
Outline

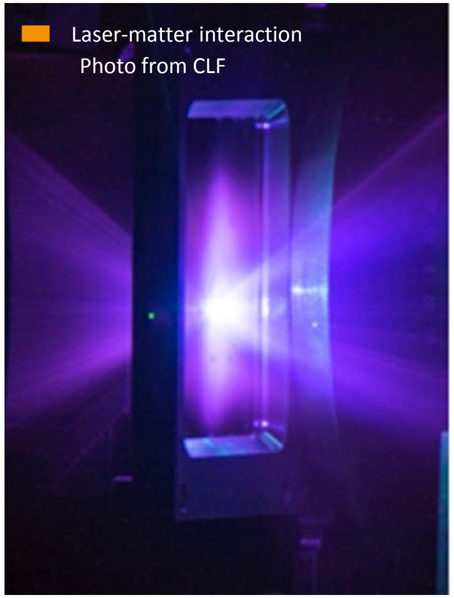
- Introduction: Warm Dense Matter Physics
- Surface dynamics of solids upon high-intensity laser irradiation
- Probing multilayer surface structure and dynamics by x-ray reflectometry and surface scattering
  - Experimental setup
  - Particle-in-Cell simulation
- Simulation results: electron density and scattering
- Treatment of collisions in Particle-in-Cell Simulations
- Summary and conclusion



Jupiter, Photo by Nasa

Planetary physics

- Earth-like planets, gas giants,
- Layer models, convection, and magnetic field depend on EOS, heat, and charge transport properties



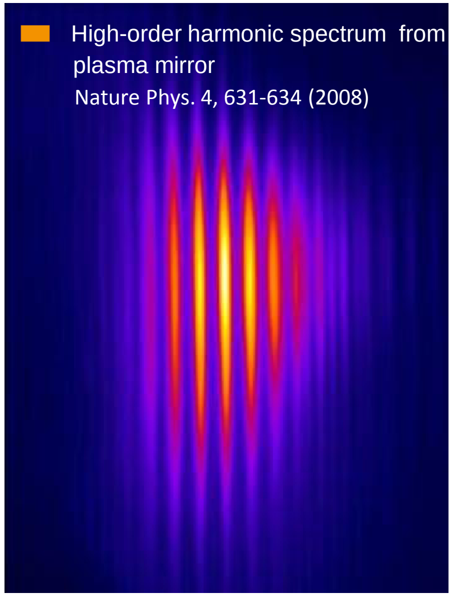
Laser-matter interaction
Photo from CLF

Laser-Matter interactions

- Laser intensity above $10^{14}\ \frac{W}{cm^2}$ irradiation

=> WDM

- Pre-pulse effect for relativistic laser-solid interaction



High-order harmonic spectrum from plasma mirror
Nature Phys. 4, 631-634 (2008)

Plasma optics

- Plasma mirror: temporal contrast improvement
- High-order harmonics: atto-sec XUV

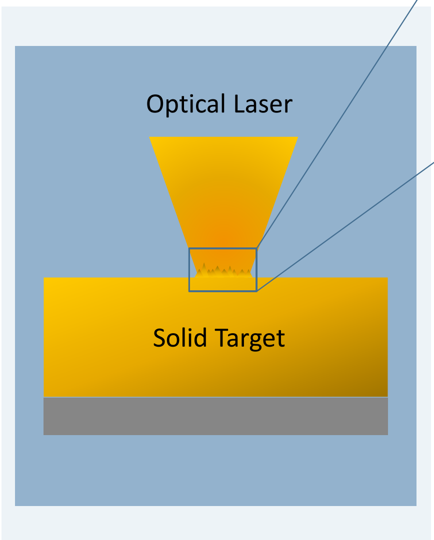
=> Controlling the nano-scale density changes and roughness of surface plasmas is crucial

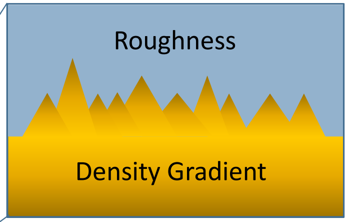
Warm Dense Matter (WDM)

- ~1 – 10x solid density
- 0.1 - 100 eV temperature
- Electrons partially degenerated
- Ions moderately coupled.

Near surface dynamics upon laser-solid interactions

Studying the nanoscale dynamics of high-intensity laser-irradiated solid-density plasma surface by x-ray reflectometry (XRR) and grazing-incidence x-ray diffraction.





Density gradient and roughness:

laser absorption, reflection, electron divergence, E and B-field,…

Optical probe (shadowgraph, reflectometry, …)

- Sensitive to the critical density (~1/100 solid density)
- Limited spatial resolution to > µm
- Limited S/N ratio due to other radiations

X-ray probe (reflectometry, grazing-incidence scattering) **This talk**

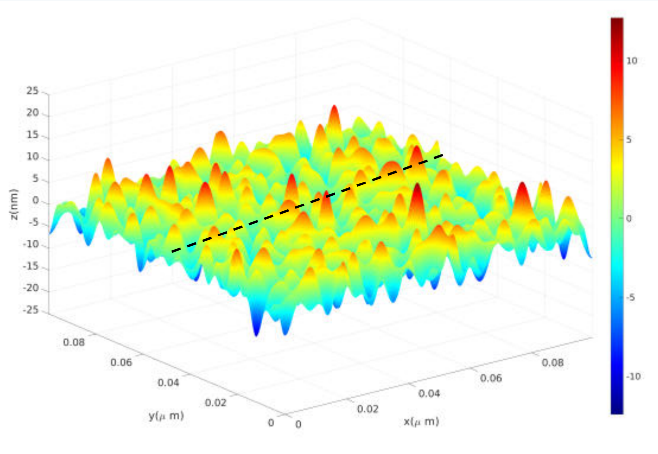
- Sensitive to the solid density
- Nanometer resolution
- XFEL: high number of photons (high S/N), fs duration

Experimental techniques

- High-density
- Sub-µm structure
- Time dependent (fs – ns)

Grazing Incidence X-ray Diffraction (GIXD)

Sensitive to structural in-plane correlations and tells us about characteristics and dynamics of the surface



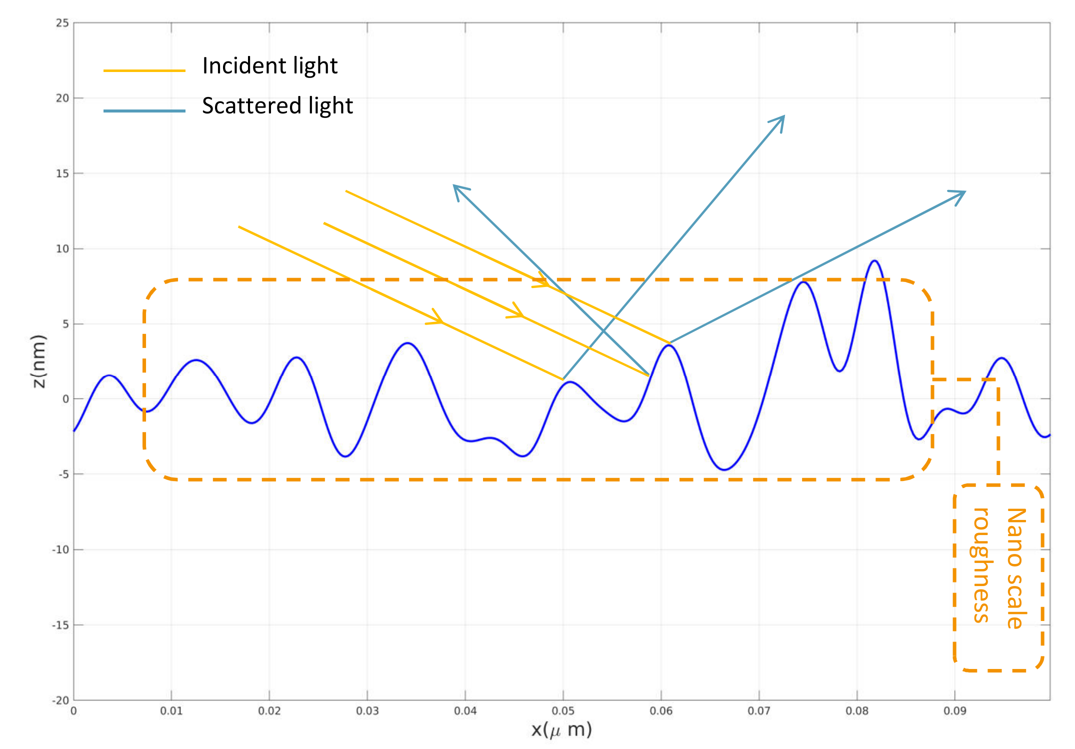


Fig. 1. X-ray diffraction from nano scale roughness

X-ray reflectivity from bulk is sensitive to the nm roughness and longitudinal density gradient at the surface

- Total external reflection angle, or "critical angle" (hard x-ray regime: $\alpha_c < 1°$)
- Small angle = small penetration depth (~10 nm) -> surface sensitive
- Reflectivity drops quickly above critical angle α_c

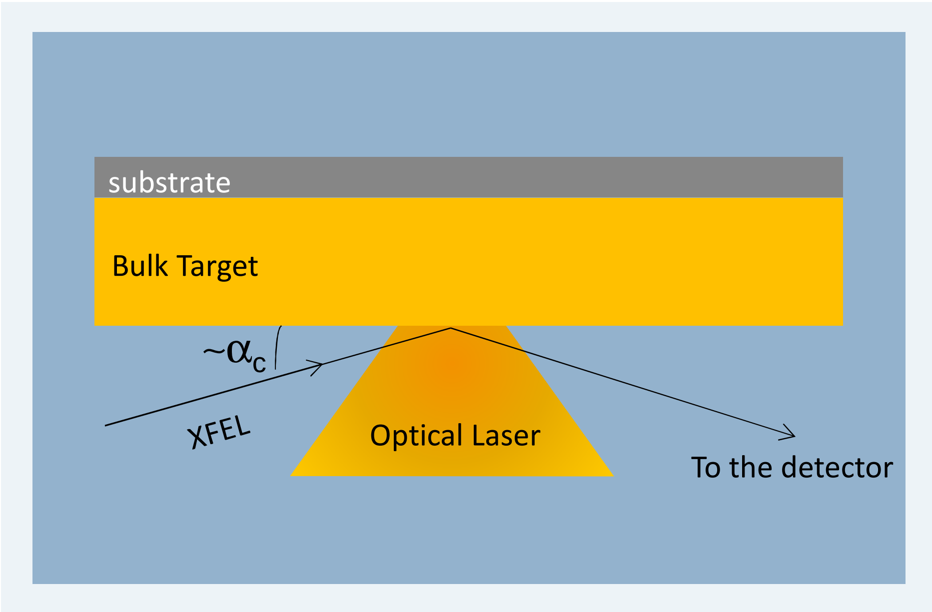
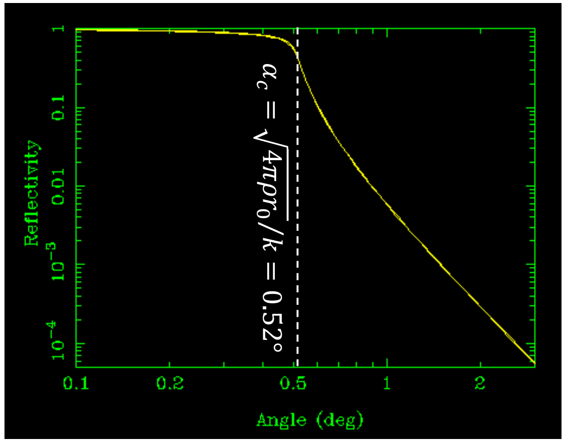


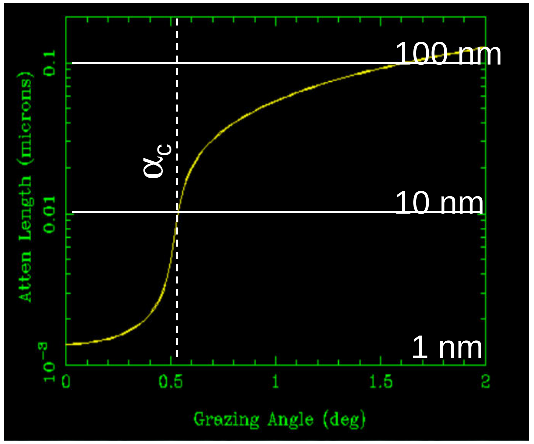
Fig. 2. A schematic of a bulk target setup

Reflection from Tantalum bulk at 8 keV X-ray photon energy

Reflectivity



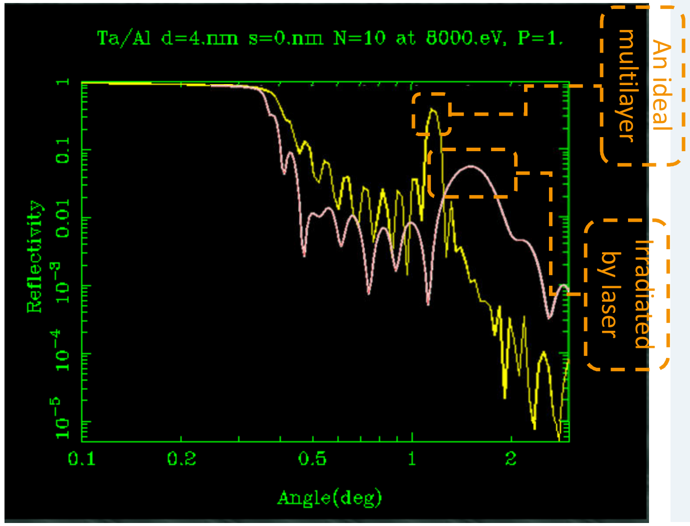
Penetration depth



http://www.cxro.lbl.gov/

X-ray reflection from multilayer samples: in-depth information around the surface

Bragg reflection from multilayers:
Scattering comes from inner layers
➔ **depth information**
Changing the incident angle
➔ **tuning the penetration depth**
Changing the thickness of the multilayer
➔ **tuning the Bragg reflectivity peak**



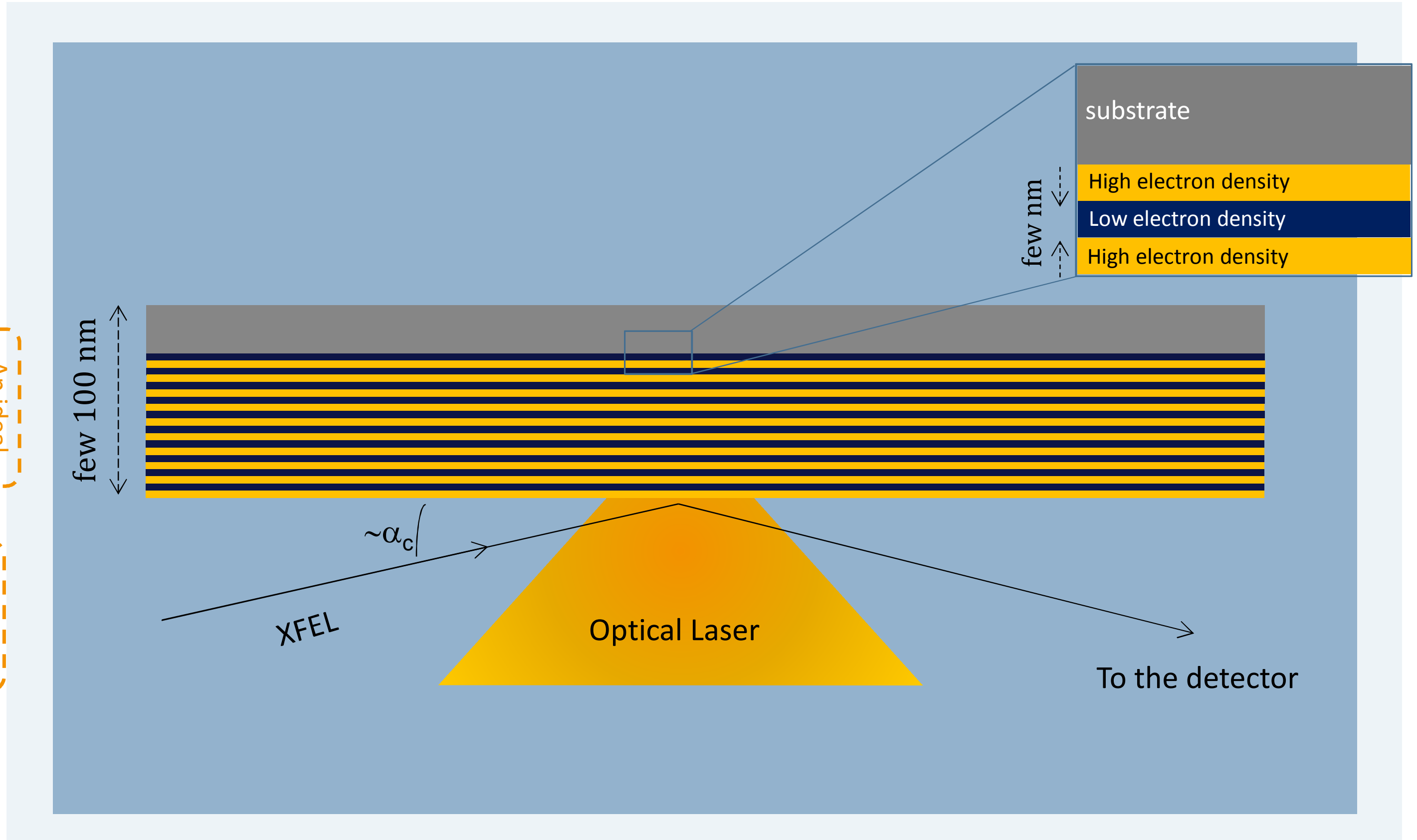


Fig. 3. A schematic of multilayer target setup

Experimental Setup

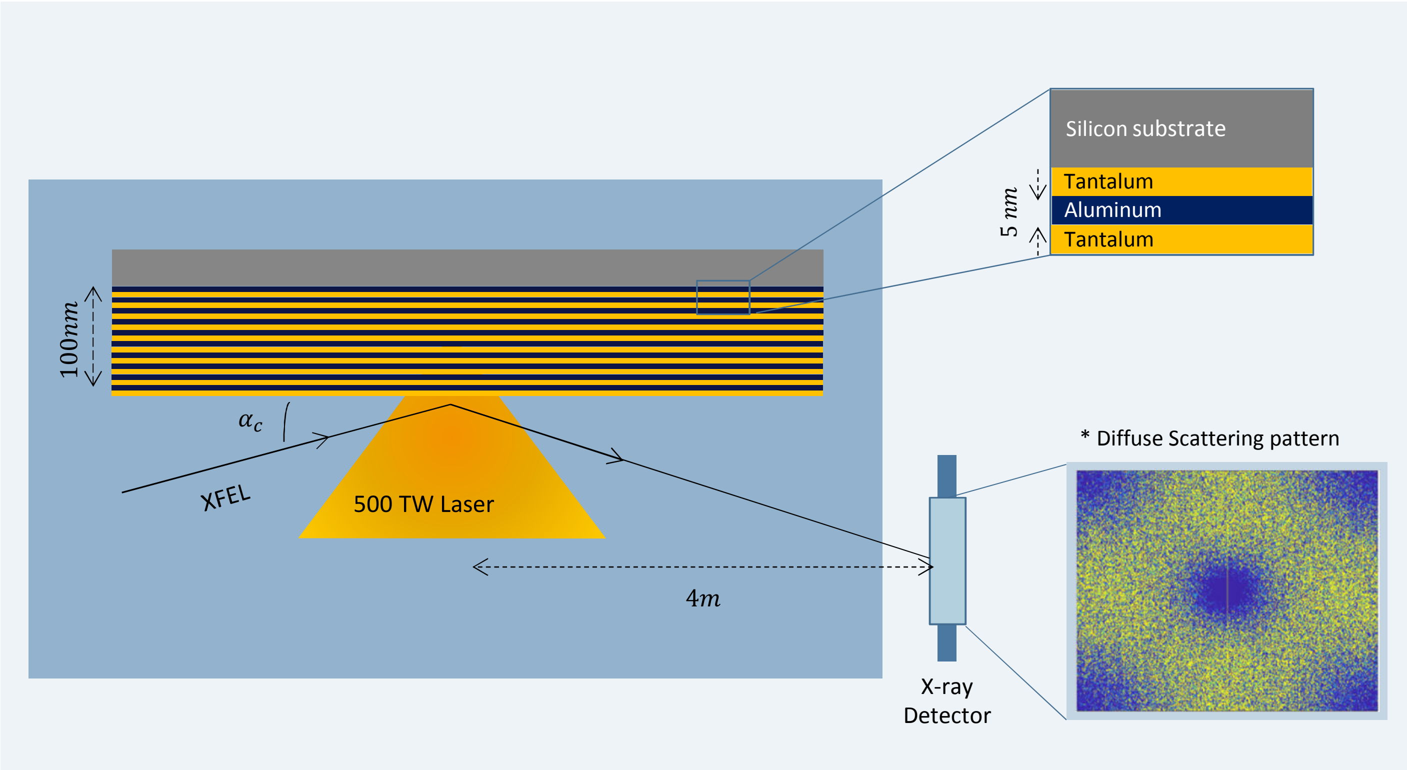


Fig. 6. A schematic of experimental setup

- The target is a 10 times reps of Ta-Al double-layers
- Thickness of each layer is 5 nm
- Optical laser pulse Parameters:
  - Intensity: 10^{14} $to 10^{16}$ $\frac{W}{cm^2}$
  - Wavelength: 0.8 μm $(Ti{:}sapphire)$
  - Duration: 50 fs FWHM
  - Focus: 500 μmFWHM
- XFEL Parameters:
  - Photon energy: $8keV$
  - Focus: ~ 3.0 μm
  - Duration ~ 10 fs FWHM

*Diffuse scattering pattern from PIC simulation (Christian Gutt)

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Particle-in-Cell Simulations

- The PIC algorithm is a particle-mesh method
- Data in PIC simulation are divided in two domain
  - Grid data (charge and current densities, fields,…)
  - Finite particles data (position, momentum, mass, charge,…)

PIC simulation issues in WDM regime

- Ionization dynamics
- Electron-Ion collision frequency
  - Absorption
  - Electron energy transfer
  - Plasma conductivity
- Invalidity of heat conduction models at steep temperature gradients

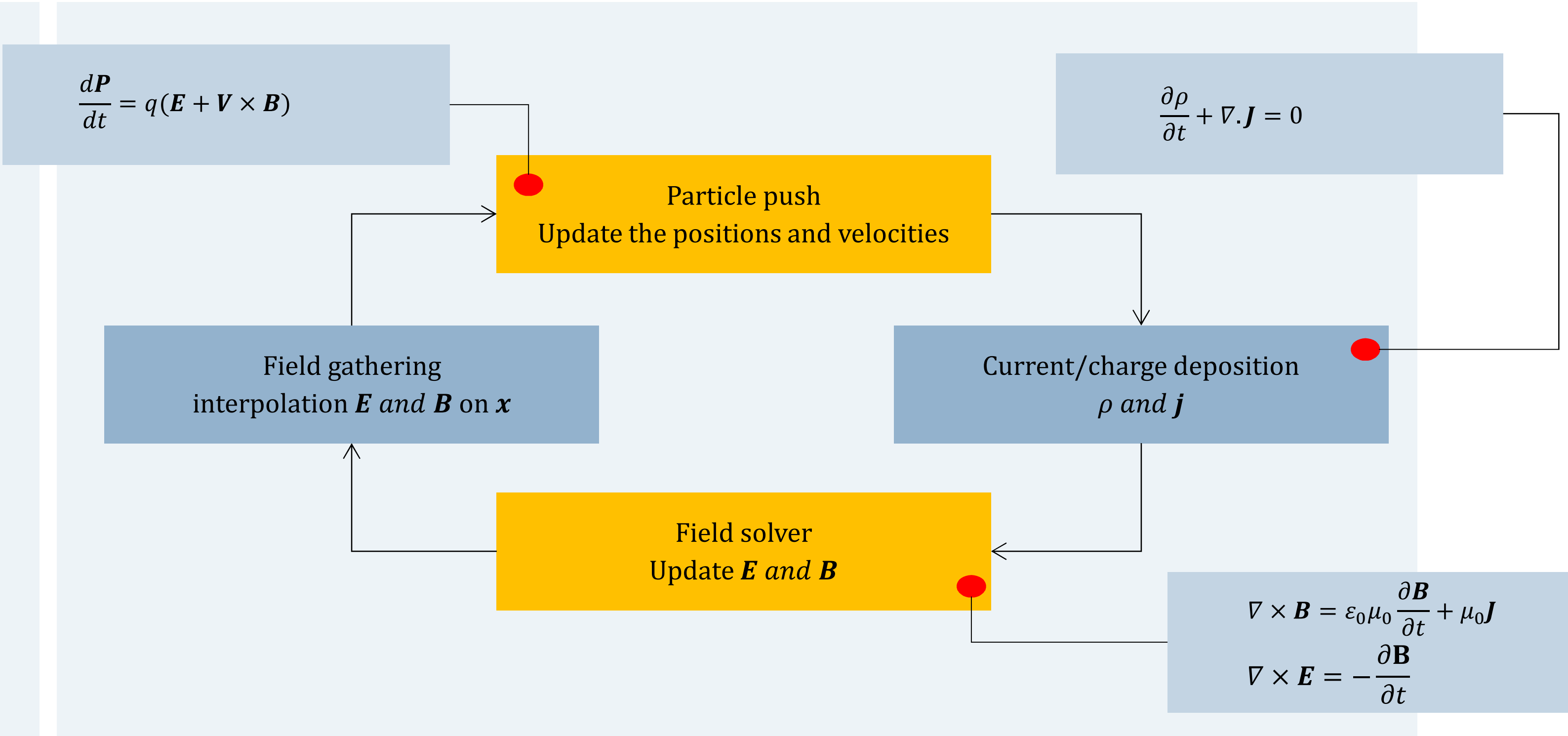

Fig. 7. The explicit PIC cycle, advancing the simulation with one time step

Particle-in-Cell Simulations Setup

- Simulations: **PIConGPU** (developed and maintained by **Helmholtz-Zentrum Dresden-Rossendorf (HZDR)**)

M. Busmann et al. Proc. SC'13 (2013)

- The target is a 10 times reps of Ta-Al (Ta-Si) double-layers
- Layers thickness in 5 nm
- Si bulk 20 nm
- It includes ionization
- Without collision
- Simulation Box Parameters
  - Sim. box Dimension: $1.0\ \mu m\ \times 2.0\ \mu m$,
  - Cells' Dimensions: $5.0\ \mathring{A}\ \times 5.0\ \mathring{A}$
  - Target Dimensions: $120\ nm\ \times 2\ \mu m$
- Pulse Parameters
  - Intensity: $1.\times 10^{16}\ \frac{W}{cm^2}$
  - Profile: Plane wave
  - Wavelength: $0.8\ \mu m$
  - Duration: $50\ fs$
  - Spot size: $5\ \mu m$

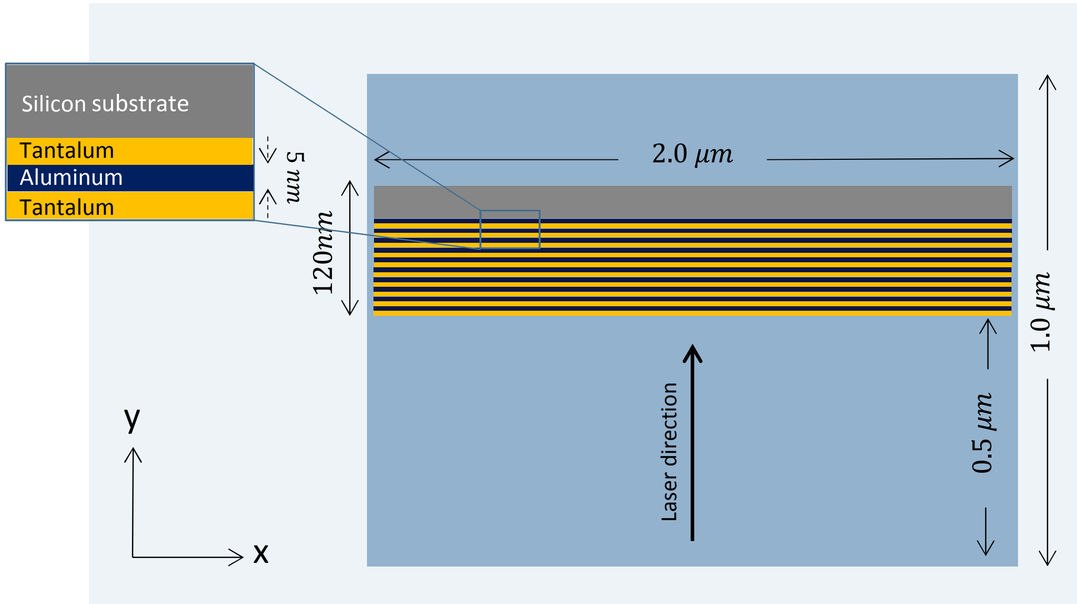

Fig. 8. A schematic of simulation setup

Free, Bound, and total Electron Density (Ta-Al)

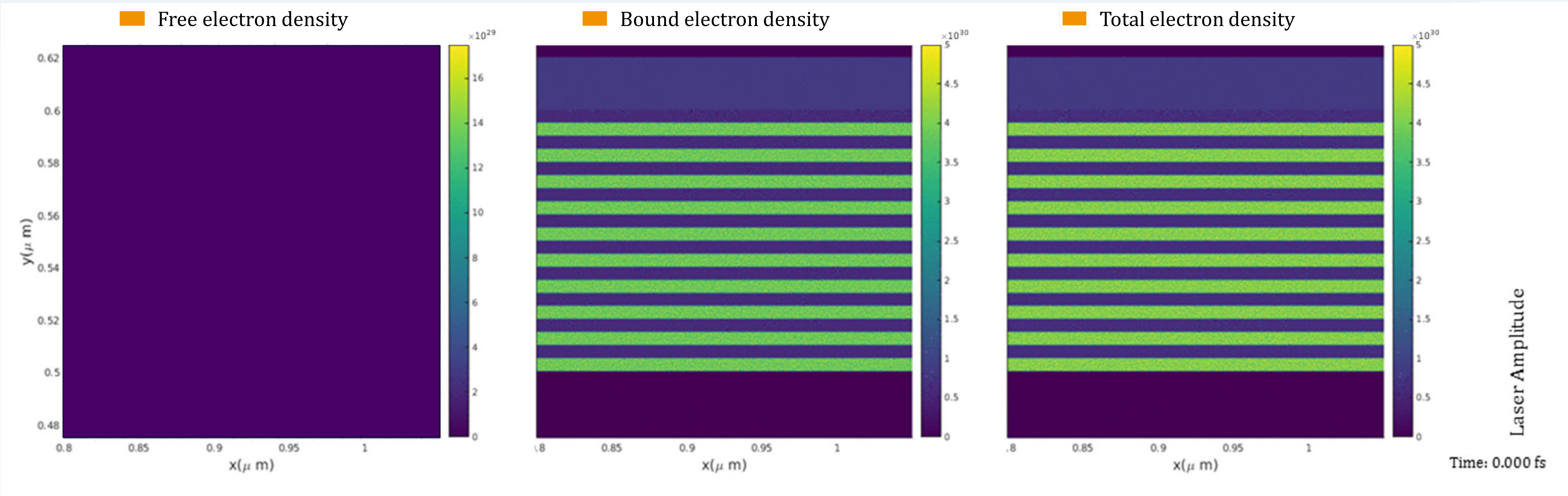

Fig. 9. 2D animated maps of free, bound, and total electron density evolution

Free, Bound, and total Electron Density (Ta-Al)

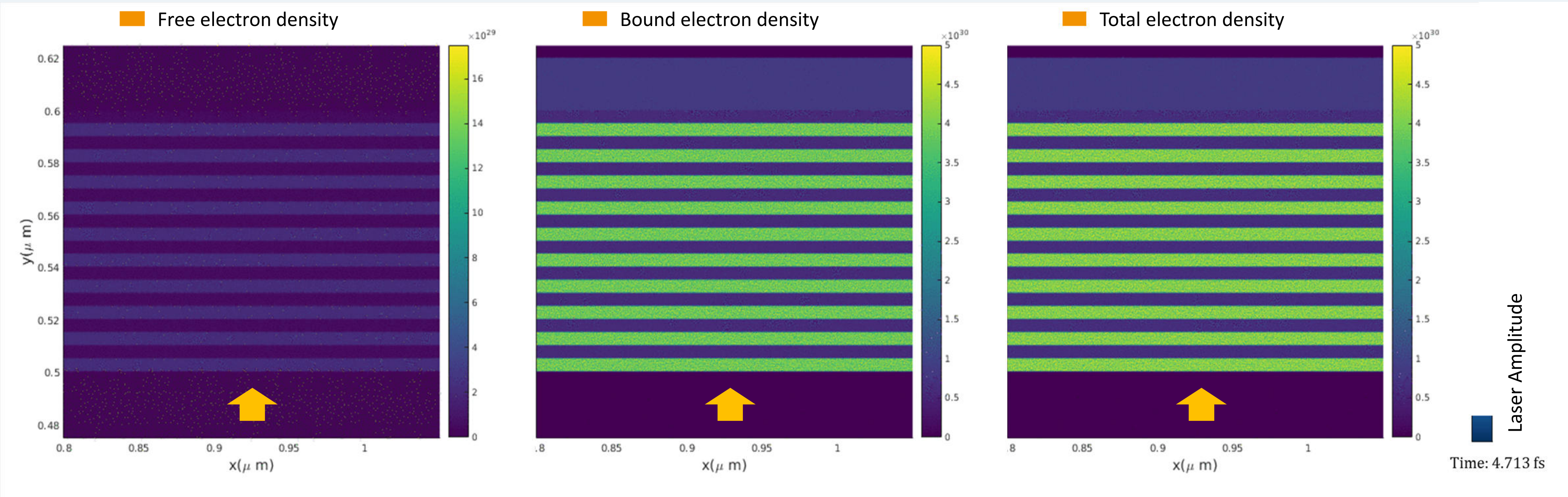

Fig. 9. 2D animated maps of free, bound, and total electron density evolution

X-ray Specular Reflection

Via density dependent index of refraction

Christian Gutt et al.

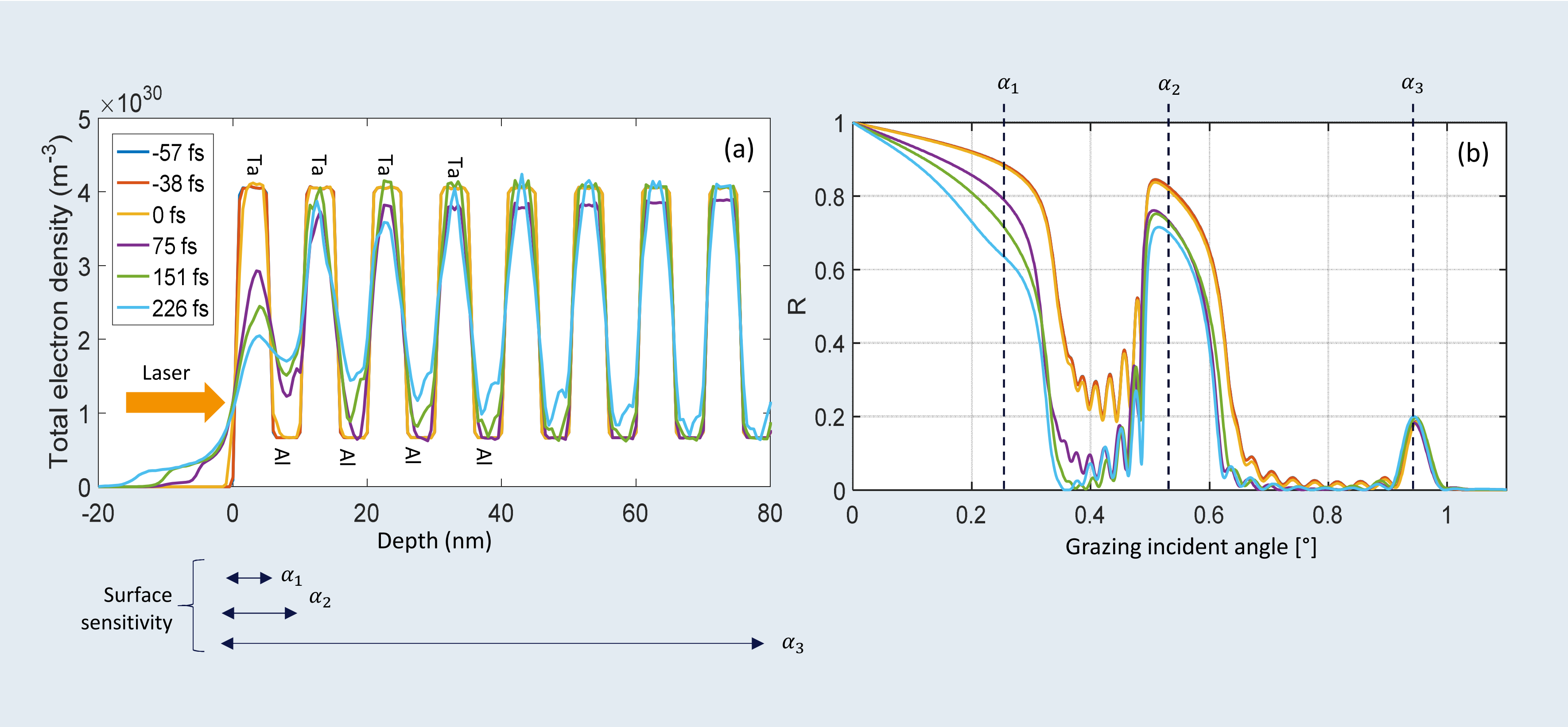

Fig. 10. (a) Total (bound + free) electron density map along the sample depth direction, calculated by Collisionless particle in-cell simulation. (b) Corresponding reflectivity curve at 8 Kev photon energy.

Off-specular Diffuse Scattering

done by Prof. Dr. Christian Gutt's group, Department of Physics, University of Siegen

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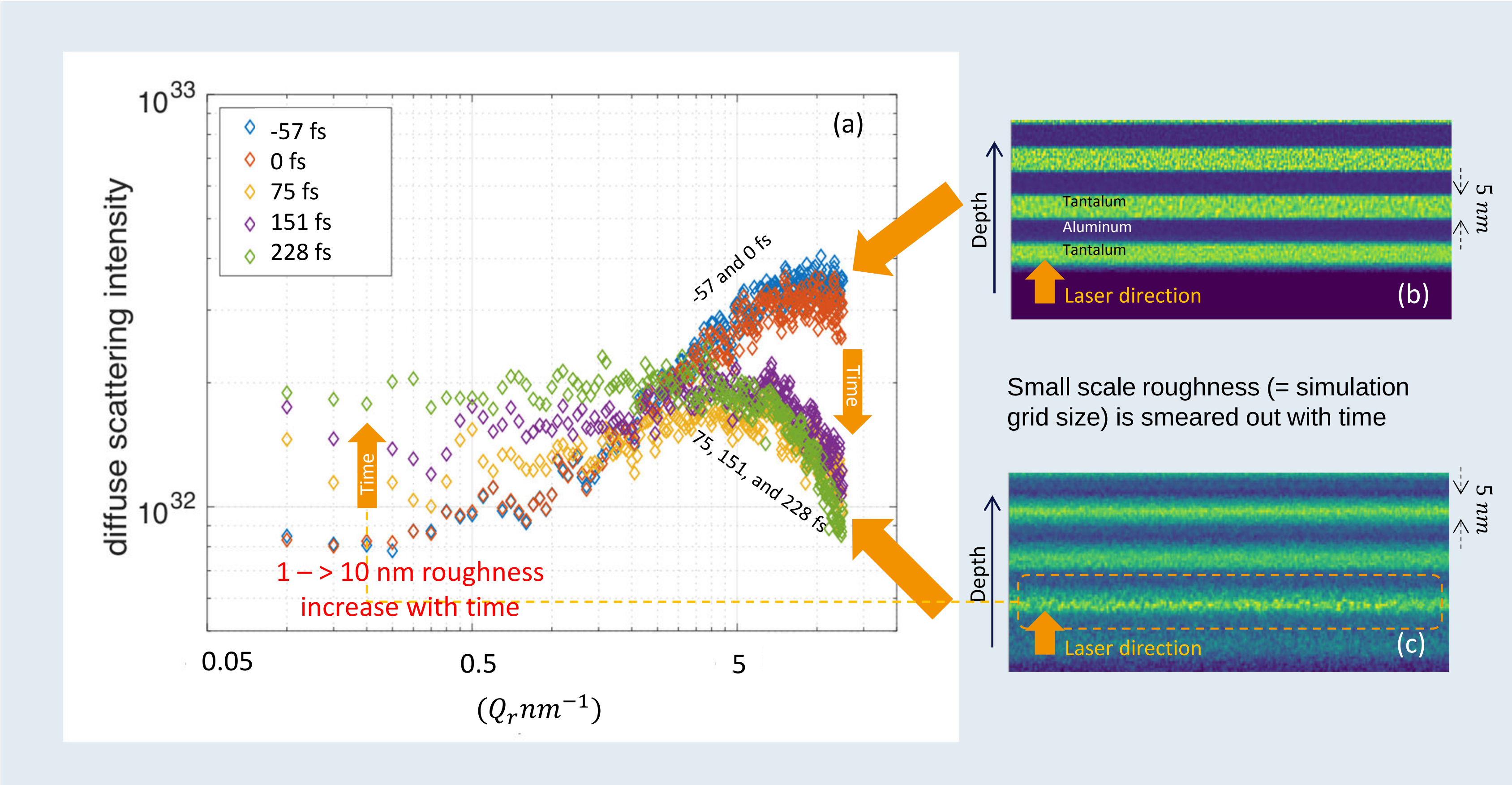


Fig. 11. (a) diffuse scattering intensity for different time delays (0 fs corresponds to the laser intensity peak) as a function of wave vector transfer parallel to the sample plane. (b) and (c) Real space 2D density (PIConGPU calculation).

Binary Collision Model (BMD) in Particle-in-Cell Simulation

treating non-thermal distributions

➔ **modeling ultra-intense laser-plasma interactions (Spitzer Collision rate).**

low temperature plasmas the

➔ **Spitzer rate diverges**

➔ **dephasing**

➔ **exaggeration of randomized motion of the heated species.**

Incorporation of collision rates beyond Spitzer subject to current investigations.

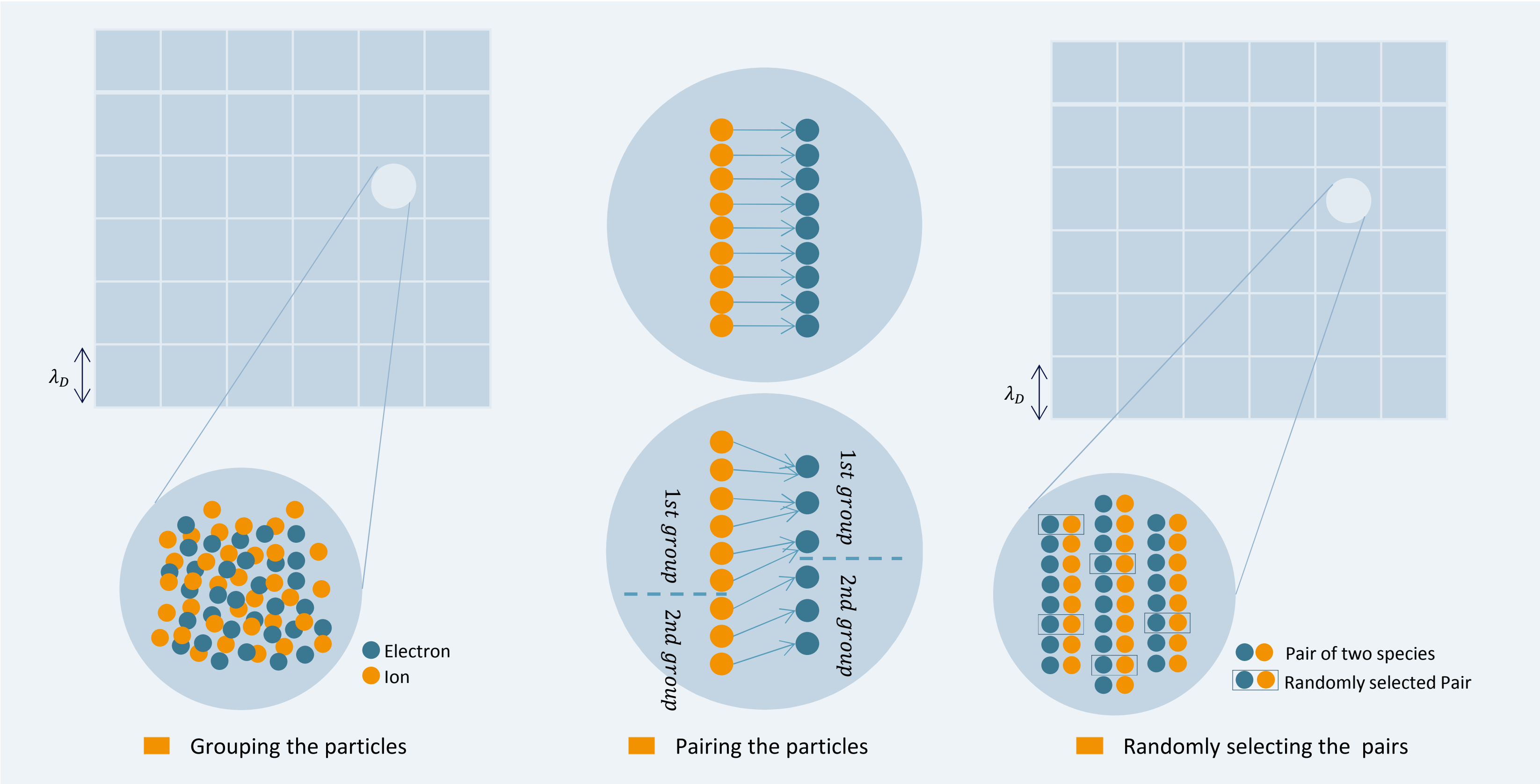
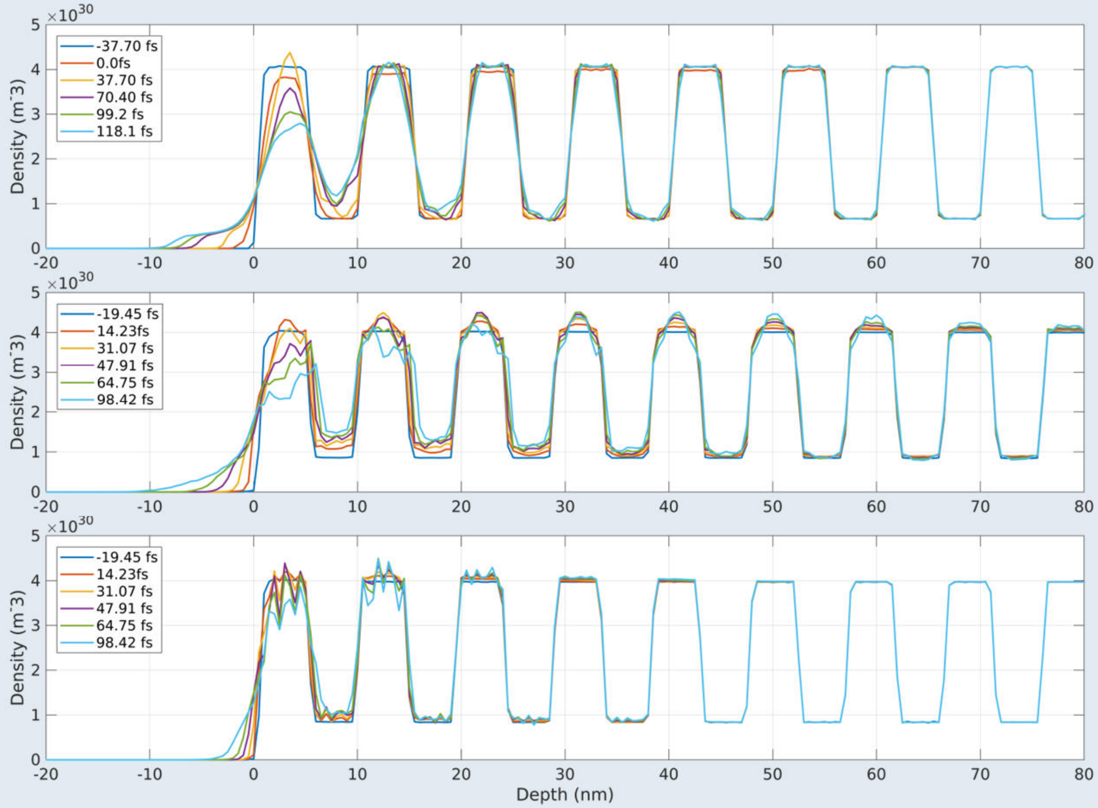


Fig. 12. A Schematic of the Monte Carlo based method steps to randomly choosing the pairs for suffering the collision

Impact of collisions on density profiles (work in progress)



PIConGPU
Without Collision

PICLS
With Collision

PICLS
Without Collision

Fig. 13. Comparison between PIConGPU result without collision and PICLS with and without collision

Summary and conclusions

- Reflectivity simulations from PIC results reveal experimental points of interest and support in-depth characterization of ionization dynamics, charge transport, and structural changes in multilayer targets
- Results will constrain collision models in PIC simulations of WDM

Acknowledgements

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Christian Gutt

Thanks

Probing bulk WDM by multilayer reflectivity measurement

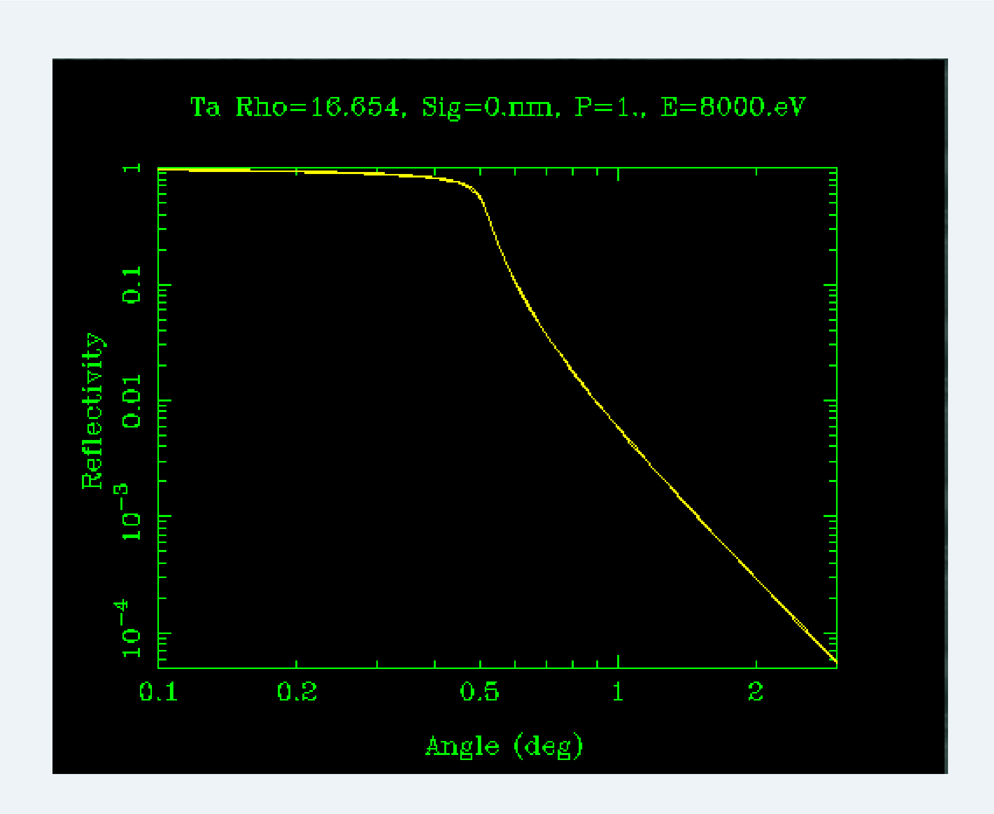

Fig. 4. X-ray reflection from a Tantalum bulk

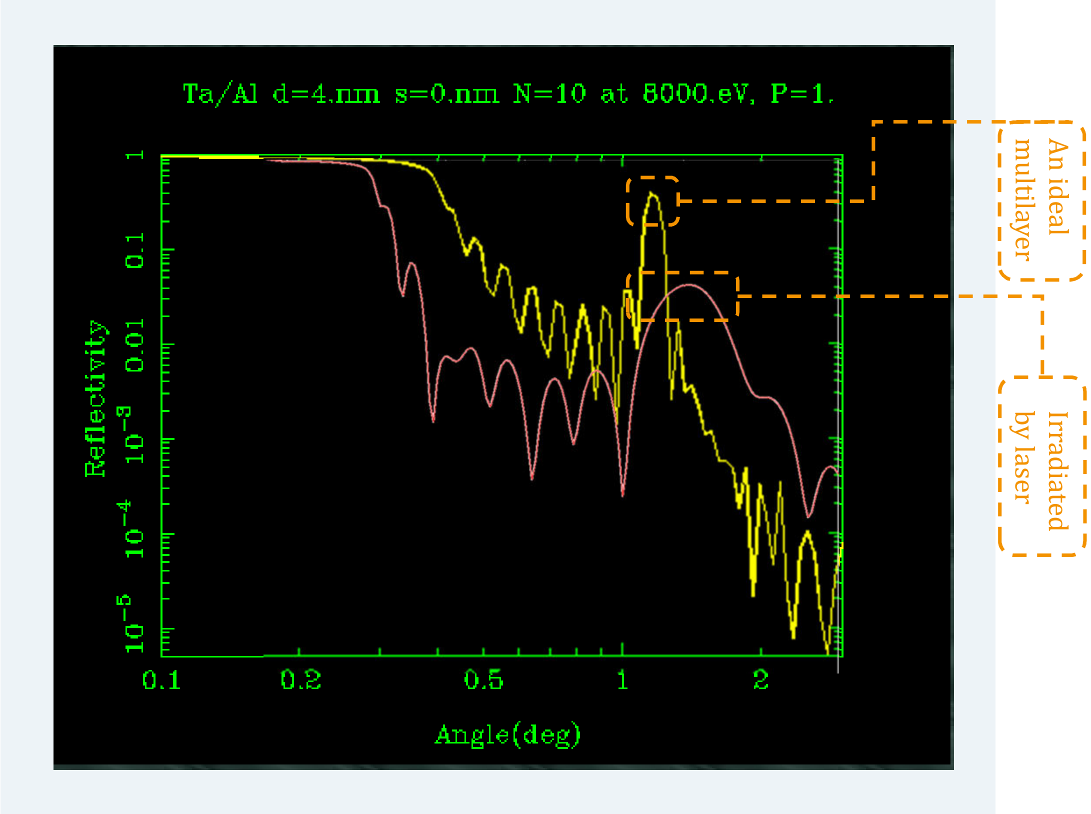

Fig. 5. X-ray reflection from a Tantalum and Aluminium multilayer