Self-consistent modelling of particle-reflection-distributions of rough surfaces

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ABSTRACT

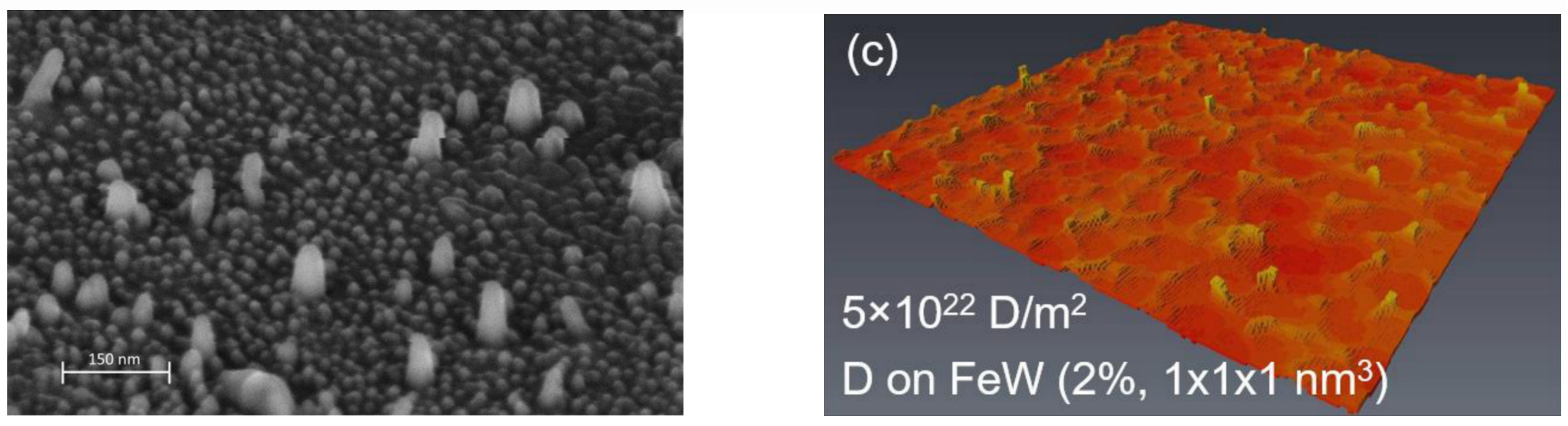
- Modelling of Plasma-Wall-Interactions (PWI) depends on distributions describing the angle- and energy distribution of particles scattered at first wall $R(\rho,\theta,E|E_0,\varphi_0,\theta_0,S)$
- Most PWI codes (like SOLPS, EIRENE) rely on extensive tables based on reflection simulations (e.g. by SDTrimSP-1D) or analytical formulae – however, both approaches assume an atomistically flat (smooth) surface
- Rough surfaces which are formed under particle impact typically display **a very different particle distribution** compared to smooth surfaces [1] – also the differences are much larger compared to the effects on sputter yields
- Roughening almost unavoidable e.g. due to preferential sputtering, crystal-orientation dependent sputtering, precipitates, thermal cycling [2]
- The effects of roughening on the reflection distributions have been investigated using W- and W-Fe-surfaces of different morphology with molecular dynamics (LAMMPS) and within the binary collision approximation (BCA) by SDTrimSP-2D

MODELLING APPROACH

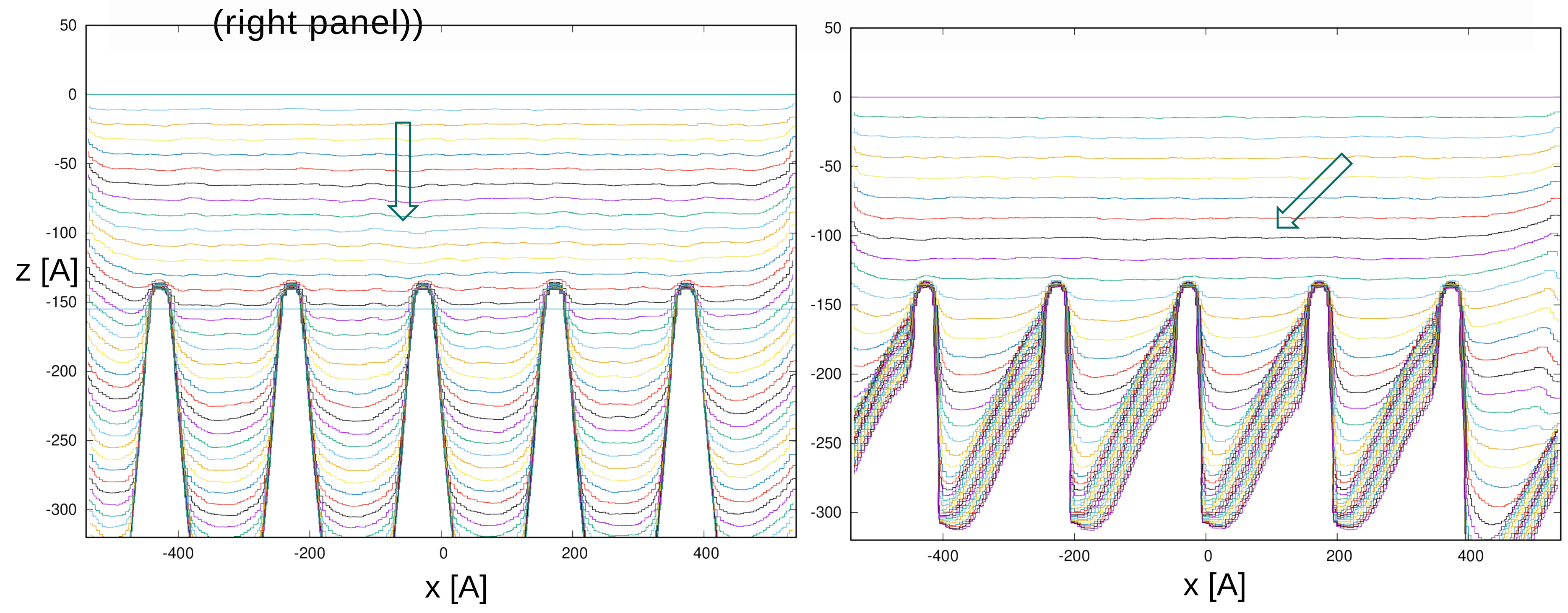
- Dynamic surface evolution under ion-irradiation has been modelled using SDTrimSP-2D (version 2.06)
- Determination of reflection distributions at various fluence steps keeping the surface unchanged (static mode)
- Molecular dynamic simulations are performed with LAMMPS using the Tersoff-type potential by Juslin [3] for the WH-system
- SDTrimSP 7.00 for BCA-type simulations using a W-bcc-lattice at 700 K
- Data compression using **hemi-spherical** harmonic basis functions Y^m_l [4] for $R(\rho,\theta|E_i, E_0,\varphi_0,\theta_0,S)$ followed by a Chebyshev-series for the individual $Y^m_l(E_i)$ as function of E_i

DYNAMIC SURFACE EVOLUTION

- Example of EUROFER and surrogate (2%W in Fe) [5] under ion-irradiation with 200 eV D left: SEM-image right: simulation with SDrimSP-3D



- Focus on simplified model-system with 2d-periodic structure (Fe with embedded tungsten pillars) : surface erosion under 200 eV D bombardment for two different angles (perpendicular impact (θ =0 deg) (left panel) and θ=45 deg (right panel))

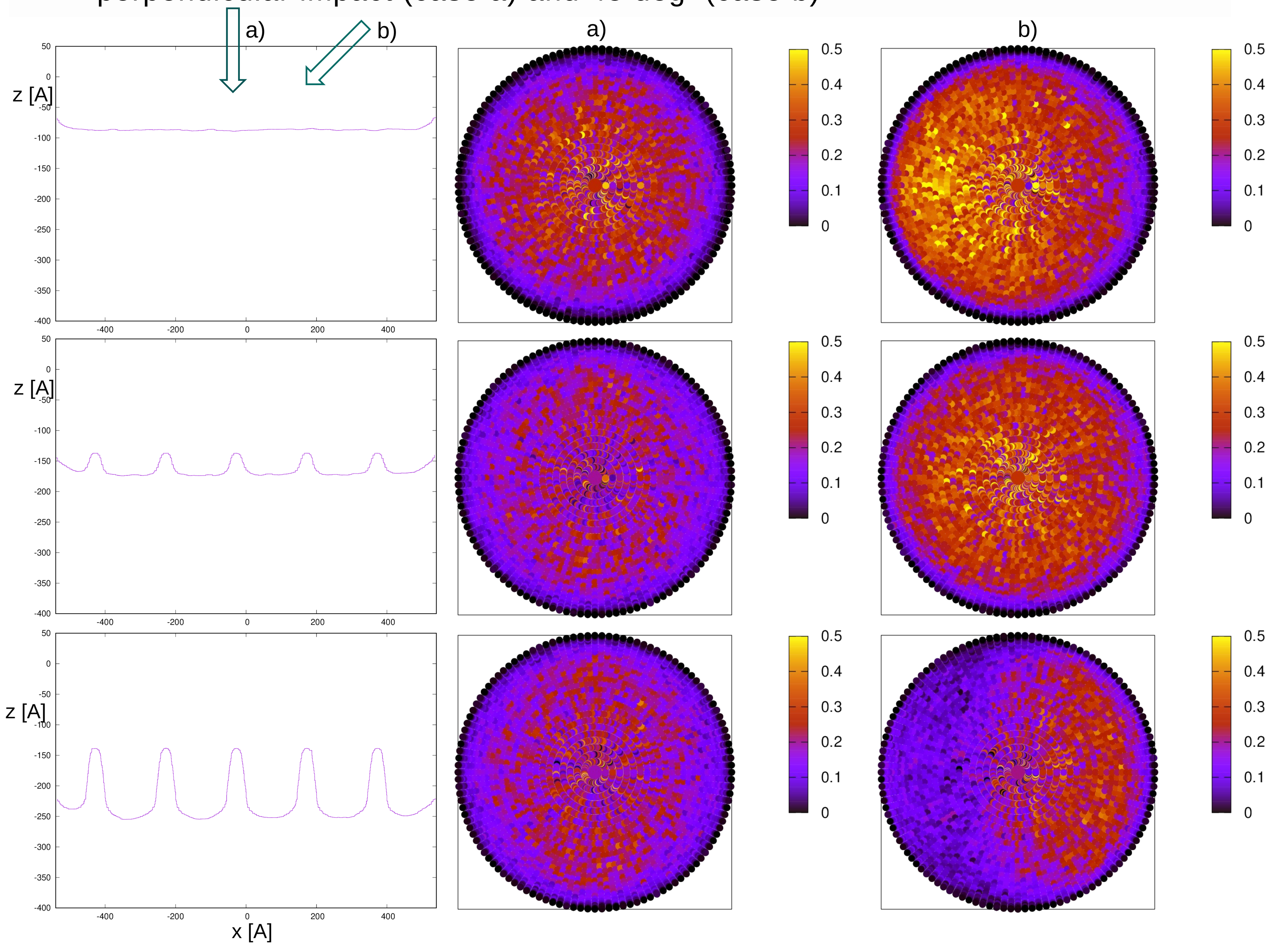


CONCLUSION

- Reflection properties of surfaces are much *stronger affected* by surface morphologies (ie. roughness) than sputter yields
- A robust result is the **strong attenuation** of the often assumed specular (forward) reflection of non-perpendicular impinging particles – typically most pronounced for the reflected particles with the highest energies. In some structures even **backward-reflection** may become **dominant** : consequences on PWI-modelling results need to be assessed
- Effect is present in amorphous and crystalline samples
- Efficient tabulation of data (particle-reflection distribution function $R(\rho,\theta,E|E_0,(\varphi_0),\theta_0,S)$) for PWI-codes appears feasible using a suitable orthogonal basis-function system
- Dynamically evolving 3-d morphologies are feasible - but computationally still **very** heavy : put focus on reference surfaces?

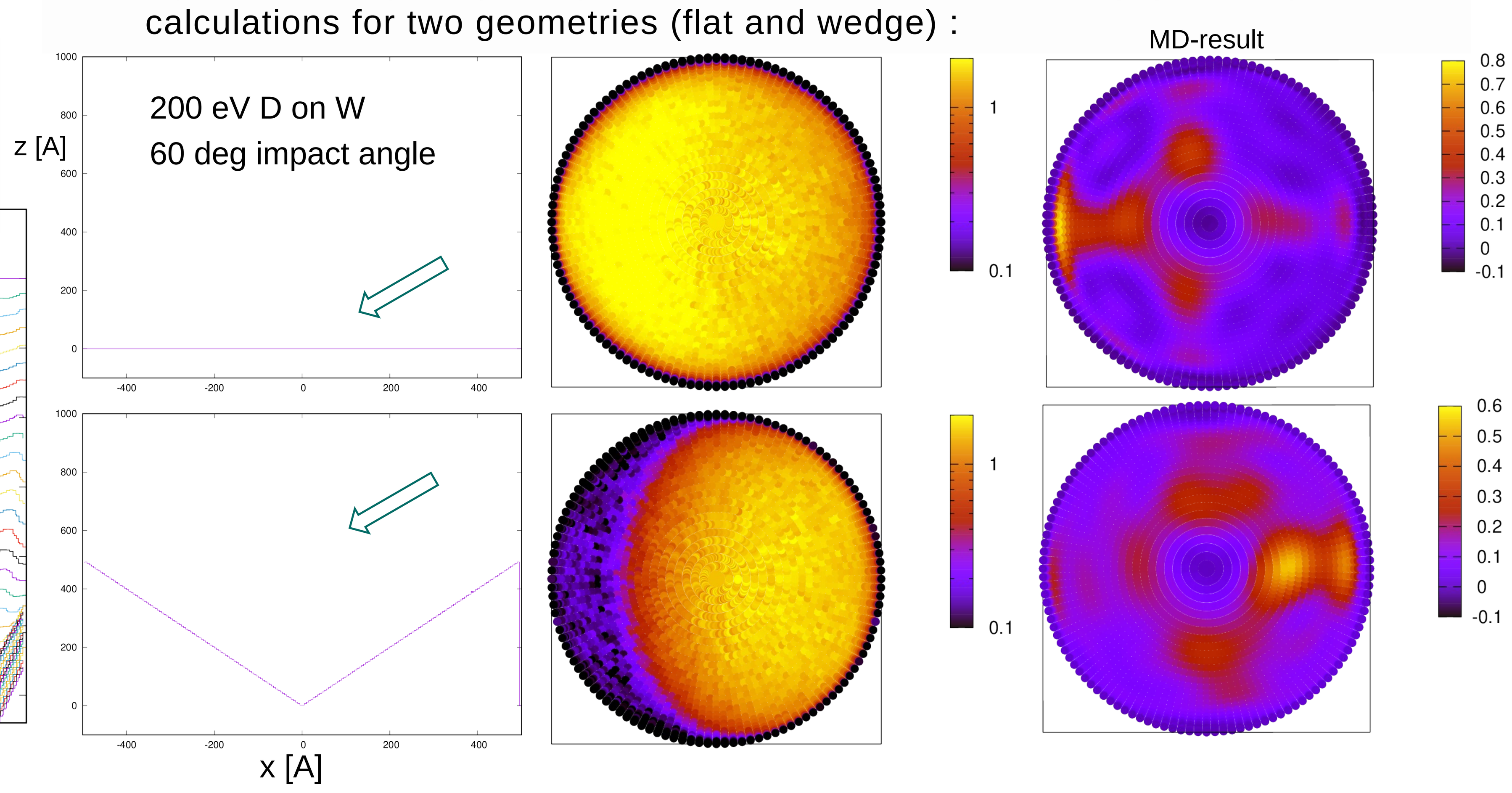
MODELLING RESULTS I

- (φ-θ)-polar plots of reflected particle distributions (φ=[0..360] deg, θ=[0..90] deg), perpendicular impact (case a) and 45 deg (case b)



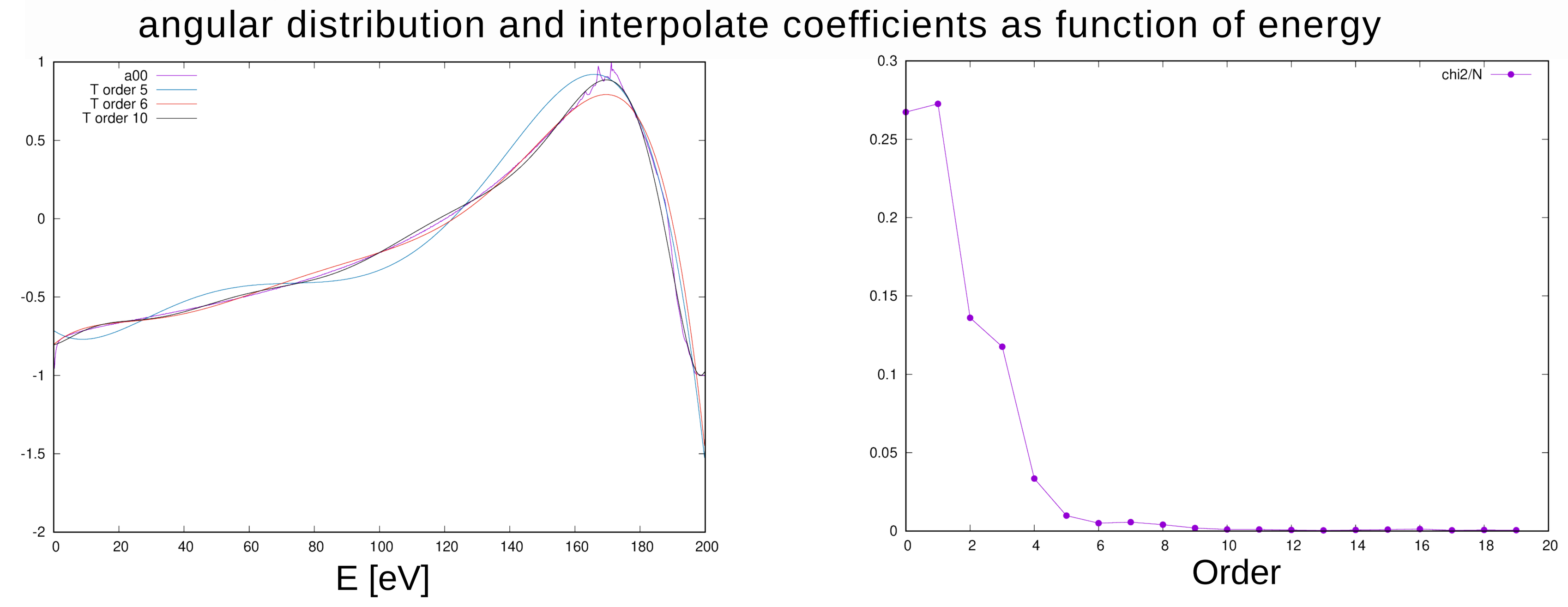
MODELLING RESULTS II

- Comparison of (amorphous) SDTrimSP-simulations with (crystalline) MD-calculations for two geometries (flat and wedge) :

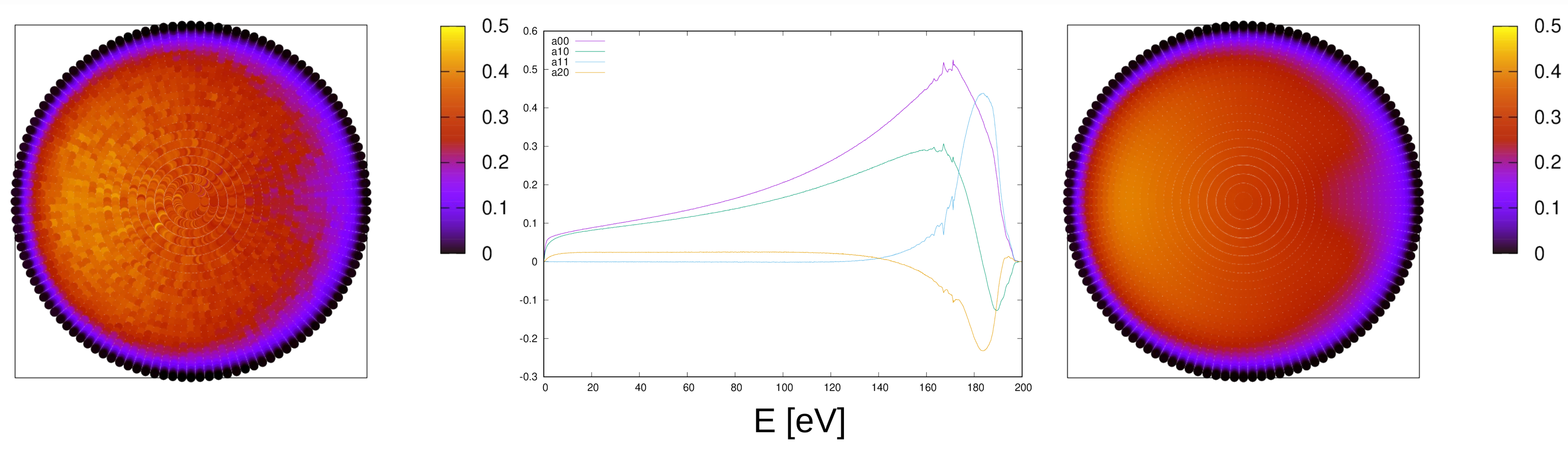


DATA COMPRESSION USING A NEW BASIS SYSTEM

- 3-dimensional distributions are impractical to handle by tables and coarse graining possibilities are limited → use of hemispherical orthonormal basis for angular distribution and interpolate coefficients as function of energy



- Example: reflection of 200 eV D impinging under 45 degrees onto tungsten : angular distribution for D atoms reflected with E_r = 164 eV: particle histogram (left panel), series coefficients of Y-expansion (middle panel), derived density (right panel)



Refs: **[1]** M. Hellwig et al. Cond. Matter 4 (2019) p. 29 **[2]** T.W. Morgan, NF 61(11) (2021) 116045 **[3]** N. Juslin et al., J. Appl. Phys. 98 (2005) 123520 **[4]** P. Gautron et al., Euro Phys Symp Rendering (2004) **[5]** R. Arredondo et al, NME 23 (2020) 100749

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