MOD/1 fusion devices

Summary

This week’s MOD/1 fusion devices agenda

Detailed charge exchange neutral distribution modelling for the ITER main wall — *Sven Wiesen*
CR-2, Vienna International Centre — 15:45 - 16:15

Impact of H, D, T and D-T Hydrogenic Isotopes on Detachment in JET ITER-like Wall Low-Confinement Mode Plasmas
Mathias Groth

Effects of surface roughness on W sputtering — *Christian Cupak*
CR-2, Vienna International Centre — 10:15 - 10:45

Computational study of tungsten surface sputtering under various conditions — *Dr. Fredric Granberg*
CR-2, Vienna International Centre — 10:45 - 11:15

Modelling of Reflection and Sputtering properties from structured and crystalline surfaces: Old and new insights
Udo von Toussaint

Global tungsten erosion and impurity migration modeling for the DEMO with the ERO2.0 code — *Christoph Baumann*
CR-2, Vienna International Centre — 14:00 - 14:30

Detailed charge exchange neutral distribution modelling for the ITER main wall (S. Wiesen)

- Neutral particle energy and angular distributions $f(E, \cos\alpha)$ collected on diagnostic surfaces for ITER reference SOLPS-ITER plasmas with manually extended grid up to FW (A. Khan et al)

- **Result: detailed distributions give 2-3 larger D → W sputter yields $\langle Y(E, cos\,\alpha)\rangle$ compared to standard estimates $Y(\langle E\rangle)$, depends on far-SOL assumptions or H/L-mode, $\cos\alpha$-dependence gives a factor 2,**
  H-mode: main contribution from tail of distribution

- Next Step: Ne → W calculation, and compare relevance to D → W

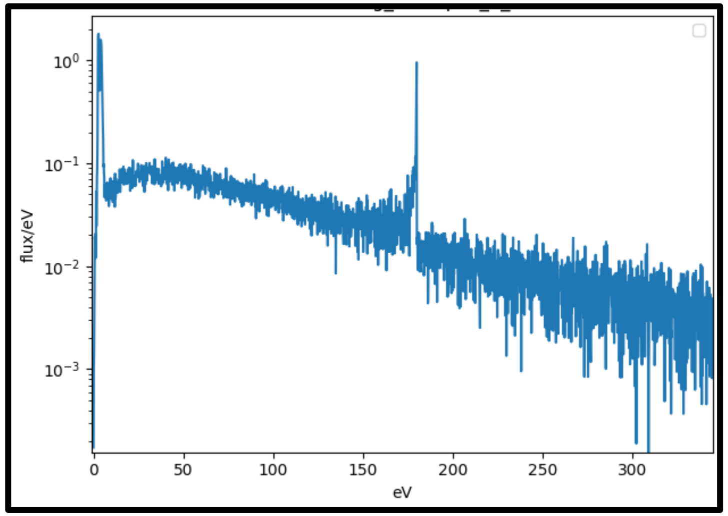
- SOLPS-ITER with wide-grid option should provide a better picture (IO task to provide data)

- Also: JET post-processing with EIRENE on-going (M. Groth et al), DEMO (Wiesen, Brenzke FZJ), ITER (FZJ)

- So far only uncorrelated energy and angular distributions collected
  → extension to multi-variate distribution functions possible $f = f\big(E, cos(\alpha)\big)$
  → requires longer EIRENE run-times for improved statistics and requires large memory
  → data compression through MaxEnt regularization

- Only polar angles are collected (toroidally symmetric)
  → extension to full 3D possible (e.g. post-processing EMC3 plasma-backgrounds)

Further points of discussion (S. Wiesen)



- Q: neutral spectrum also for impurities
  A: yes, possible

- Q: 2nd peak in ITER spectra credible?
  (not seen in DEMO case)

- Q: Exp. validation, detectors?
  Action: revise what is done (e.g DIIID/proposal existed, AUG)

- Q: validity of separable distribution functions for E and cos alpha
  → could be combined into f(E,cos alpha) non separable, requires more memory and comp. time (signal-to-noise ratio)

Impact of H, D, T and D-T Hydrogenic Isotopes on Detachment in JET ITER-like Wall Low-Confinement Mode Plasmas (M. Groth)

- T, D and DT plasmas are more strongly detached than H plasmas, same detachment onset density, but lower DL ⇒ narrower detachment window ⊖
- 40% higher divertor densities ⊕ and broader SOL density profiles at the LFS midplane for T and DT than for H and D ⊖

⇒ EDGE2D-EIRENE qualitatively explains higher divertor densities in T plasmas by 3x longer ionisation mean free path of H than T atoms

⊖ Predicted divertor conds. highly sensitive on imposed LFS midpl. conds.: div. densities generally underpredicted in high-rec. and detached conds.

⇒ Revisit simulations, also for ion-molecular reaction rates**, Ly-α opacity***

Further questions (M. Groth)

- Inclusion of surface effects in molecule recycling ⇒ full or reduced data from Molecular Dynamics calculations

⇒ Generally:

  - Comparison of energy and angular distributions of recycling H and H2, and their isotopes/isotopologues, between TRIM and MD
  - Surface binding energy for ion impact energies < 10 eV, for W and C

- For Ly-α, comparison of 0D escape factors, pre-run photon transport (e.g., Hoshino et al., CPP 2016), post-processing CRETIN (Scott, J. Quant. Spec. Rad. Transfer 2001) and non-linear gas-photon transports (e.g., Kotov, Wiesen → Chandra et al., PSI 2024)

- Treatment/separation of $D^+ + D_2$ charge exchange and momentum transfer

Further points of discussion (M. Groth)

- C: reflection of particles (H vs T), in reality: 3D problem

- Q: What surf model to be used, TRIM sufficient (valid only for high energies)? MD?
  Action on WG: launch calculations for low energies (e.g MD) coord by IAEA?

- Q: surface reflections for photons, CHERAB (good wrt geometry), physics questionable?
  C: surface composition matters (redeposition as f(t)); old Eksaeva work; employ Bayesian methods,..

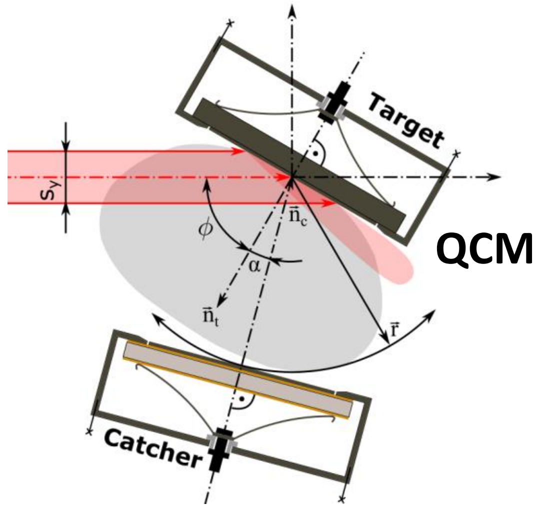
- Q: molecules, preferential vibrational state, isotope change? Again: avoid C, better W
  C: vibrational info not to be retrieved from JET, better: linear devices (diagnostics), comparing W with other (e.g MAGNUM-PSI, reactor conditions), focus on Carbon

- C: A&M model: remove AMJUEL, use CRM iteration (e.g COLRAD) inside EIRENE/SOLPS, computational times? Maybe OK with MPI parallelisation → **action on TSVV-5**

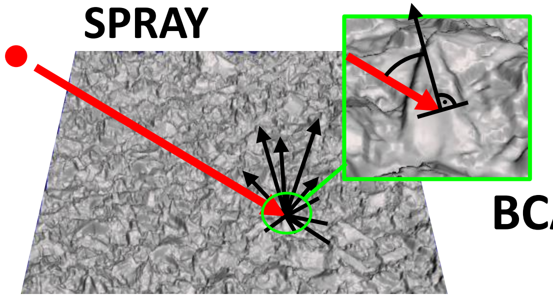
Effects of surface roughness on W sputtering

Fusion@ÖAW
Vienna, Austria

QCM and SPRAY



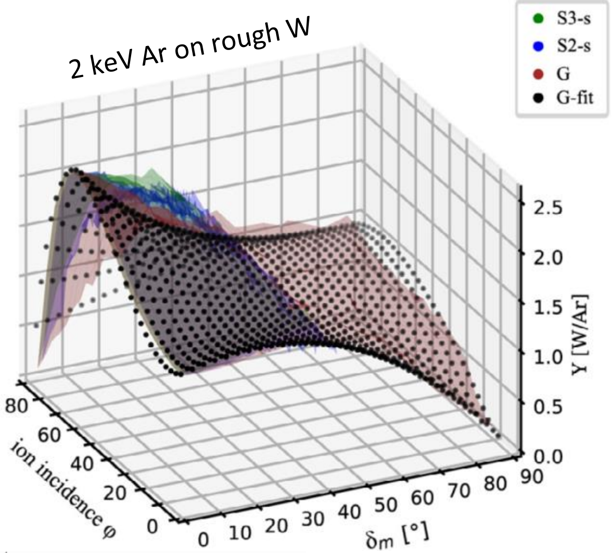
SPRAY

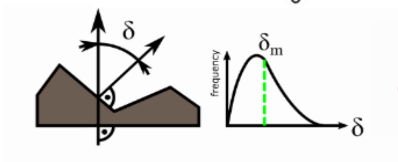


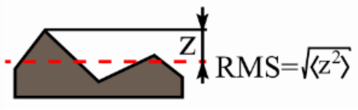
BCA

Raytracing

Sputtering of rough surfaces





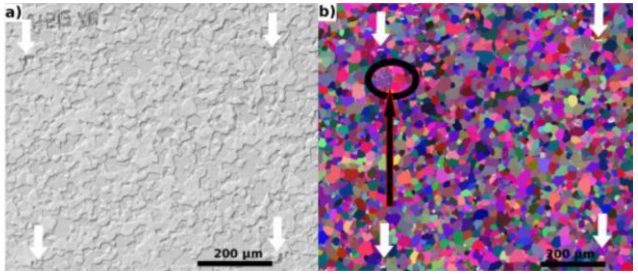


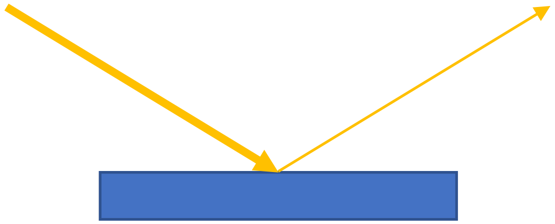
δ_m

RMS

Outlook and potentials

SPRAY for topography + crystal texture





Light reflection to assess δ_m during dynamic erosion

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Cupak et al., Appl. Surf. Sci. 570, 2021, 101924
Szabo et al., Surf. Interfaces 30, 2022, 151204
A. Lopez-Cazalilla & C. Cupak et al., Phys. Rev. Mater. 6, 2022, 075402

PhD Thesis C. Cupak (2023) https://doi.org/10.34726/hss.2023.76544
He et al., ACM SIGGRAPH Comput. Graph. 25 (1991) 175-186
J. Brötzner et al., Nucl. Mater. Energy; 37 (2023), 101507

Further points of discussion (Ch Cupak)

- C: what is changed is the effective yield (as result of roughness change); one can use ERO2.0 to test, but so far only reduced models

- **Necessary: measuring roughness w.r.t grain size orientation in reactor, high fluence + redeposition expts, impact on yields? (action)**

- C: Steady state in reactor expected (contrary to nowadays devices),
  Q: does a model for saturated phase exist?
  A: dynamic sims can be done, incl smoothing/roughening (non-linear), more complicated with impurities, inclusion of B-field (sheath physics, etc)

- Q: Description of roughness → 2D FFT, and then projection on lower dimensionality
  Q: Impact of thermal conductivities, T-gradients?
  Q: also: boron might complicate things

Computational study of tungsten surface sputtering under various conditions (F. Granberg) part 1/2

- Flat surface sputtering simulations:
  - Low index surface results are within the previous experimental values
  - Random surface simulations agree with experiments on polycrystals in outgoing angle distributions very well
  - Effect of channelling could be seen in reflection yields
  - Atomistic features drastically affects the sputtering yields
    - Ledges can increase the sputtering yield by orders of magnitude
  - The random surface sputtering yield was different from all low index surfaces as well as their average
    - Needed for polycrystalline studies/applications

Computational study of tungsten surface sputtering under various conditions (F. Granberg) part 2/2

- Effect of surface features:
  - The pillar height is drastically affecting the sputtering yield
  - Reaches the “reference” value at about 3 : 1 height to separation distance ratio
  - The “fuzz” surfaces shows a lowering of the sputtering yield
  - Hills are sputtered differently under different incoming angles
  - The amorphous surface behaves differently from all other crystalline surfaces, due to lack of linear-collision-sequences
- Cumulative impacts necessary for comparison to experiments
- Deuterium saturation affects the sputtering
  - More simulations are needed
- Lattice deuterium sputters even though (almost) no W is sputtering

Further points of discussion (F. Granberg)

- Q: what is the amplitude/size of roughness A: ~ < nm (ie will not impact optical params)
- Q: no W-D released in MD, why → A depends on potential used
- Q: So far comparisons with SRIM, why not making comparison with modern code SDTrimSP A: community uses a lot SRIM still, but comparison w/ other codes possible
- C:Polycrystalline surfaces also doable by randomising surfaces
- Q: T effect at target (up to 1000 degC), any effect? A: probably not, some results show even the opposite, some T-dep seen but not for W, C: impact energues ~eV, Tsurf ~ meV, so nothing strong expected
- C: MD seen as "ground-truth", but strong dependence on assumed potentials
  → **Action: assessment of potential validity reqd**, to avoid "fishy" results.
- C: Also: MD as method also depends on the person doing it
  → **Action: provide best-practices or standard set of observables**
- C: IAEA DB exists for potentials, should include errors/UQ
- Q: what are the most relevant params (e.g. roughness) → turning / transfer into a yield
  A: roughness 2D FFT (RMS no physical relevance)
  C: depends also on initial conditions, possibility to correct "dynamical" erosion yields?

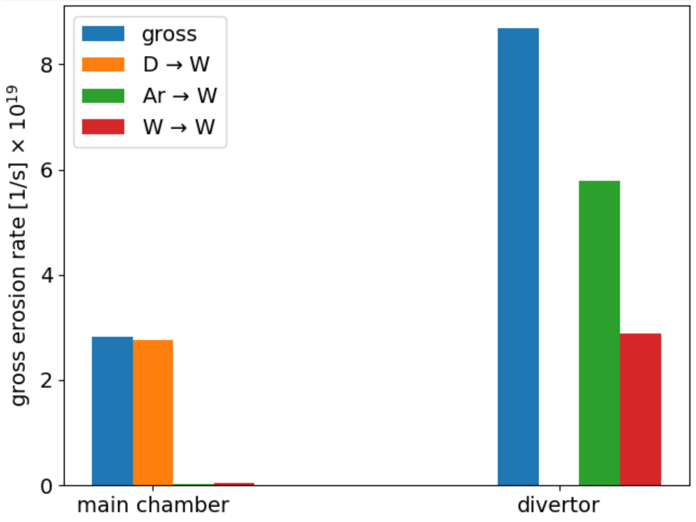
Modelling of Reflection and Sputtering properties from structured and crystalline surfaces: Old and new insights (U. v. Toussaint)

- Validated 3D SDTrimSP for static and dynamic targets, production ready;
  The same for crystal SDTrimSP in 1D
- Discrepancies between different MD potentials exceed difference results between SDTrimSP and MD
  → comparison method for many-body MD potentials urgently needed
- UQ for any of the data used in codes necessary (not existing at the moment)
  Action

Further points of discussion (U. v. Toussaint)

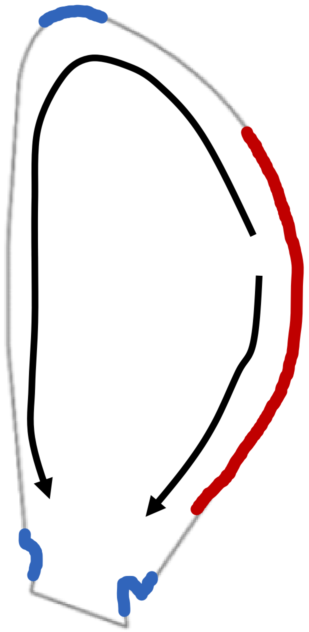
- C: reflection of particles (other direction that impact angle) also seen in expts, also for sputtered species (good!)
- C: Limits for amorphous layers do not exist, for crystal phase limit is lattice unit
- C: Reactors, inclusion of B-field (ERO does it) required
  A: one can include gyro-motion but some issues (in 1D), maybe in 3D it would work
- C: MD still required as SDTrim has no molecules included
- Q: thin layers on top (e.g. B) increased sputtering rate?
  A: 1D problem, can be done quickly **(Action)**
- C: As for SRIM, GUI exists also for SDTrimSP

Global tungsten erosion and impurity migration modeling for the DEMO with the ERO2.0 code (Ch. Baumann)



Key results for preliminary PWI-DEMO modelling

- W main chamber erosion dominated by CXN at low-field side
- W divertor erosion dominated by Ar ions and W self-sputtering
  → relative contribution: ~ 2/3 by Ar, ~ 1/3 by W
- strong W transport from main chamber into divertor due to long ionization mean free paths
- main deposition locations:
  - inner and outer divertor above strike lines up to shoulders
  - remote areas above outer divertor
  - top of the machine (upper X-point)
- large uncertainty in modelling due to large separation between plasma grid and wall



Global tungsten erosion and impurity migration modeling for the DEMO with the ERO2.0 code (Ch. Baumann)

Tungsten data needs

- ERO2.0 is a 3D code for PWI and impurity migration studies, which needs various W-related input data

PWI part:	Impurity migration part:

- sputtering and reflection coefficients for various W-target combinations (H isotopes, He ash, B, seeding species)
 	
- now, mainly SDTrimSP input (internal data generation possible), but MD data required to improve data especially for low impact energies
	- atomic rate coefficients needed in range determined by background
	  - ionization rate coefficient (density dependence)
	  - recombination rate coefficient (entire density range)
	
	- relevance of non-resonant W charge exchange with H isotopes?

- when talking about full-W devices, one should not forget about boron data!

Further points of discussion (Ch. Baumann)

- C: assumption of T at wall 2eV in DEMO different than assumption in ITER (10eV), revision required with wide-grid option in SOLPS (for both ITER and DEMO) **(action)**

- Q: What is the highest expected W charge state
  A: assume state prominent close at spx

- Q: angular distribution of sputtered particles?
  A: can be implemented in ERO

- Q: Data compression to avoid large matrices
  A: yes, possible, but currently not required

- Long discussion about validity of assumed W rates in ERO (recombination, ionization, CX)

General discussion (Friday)

- K. Verhaegh: intermediate solutions to improve standard AMJUEL by CRMs, e.g. look-up tables, e.g. YACORA-data and plug it into EIRENE

- K. Lawson: Additional information from JET on Deuterium Ly-alpha opaxcity could be provided (similar to the Helium work)