

Entire simulation groups at the University of Helsinki





[http://vlt.ornl.gov/research/20 10119_highlight_doerner.pdf] [For a review see: K. Nordlund, C. Björkas, T. Ahlgren, , A. Lasa, and A. E. Sand, Multiscale modelling of plasma-wall interactions in fusion reactor conditions, J. Phys. D: Appl. Phys. 47, rdund, Departm. 224018 (2014), Invited paper for Special Issue on Fundamentals of plasma-surface interactions].



Kai Nordlund, Department of Physics, University of Helsinki

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iai Nordlund, Department of Physics, Univer [A. Lasa, S. K. Tähtinen and K. Nordlund, EPL 105, 25002 (2014)]



Old results on Be sputtering Sputtering of initially pure Be by D



[C. Björkas, K. Vörtler, K. Nordlund, D. Nishijima, and R. Doerner, New J. Phys. 11, 123017 (2009)]

Kai Nordlund, University of Helsink

Old results on Be sputtering D irradiation of initially pure Be

- At low energies a large fraction of Be is eroded as BeD molecules
 - Chemical sputtering!

7 eV!

- This fraction decreases with ion energy
- This collaboration came out of a previous IAEA meeting with Doerner!



rsity of He



Results on Be sputtering by D **Data collection**

- Since 2012 we have been carrying out a systematic data collection effort for Be sputtering by D as a function of ion energy, sample temperature and sample composition for ERO parametrization
- Data on sputtering yields of both Be total and Be in BeDx molecules, reflection
- Cumulative and non-cumulative runs
- Data for pure Be cells and mixed Be-30% D cells formed from the cumulative runs
 - Non-cumulative runs done for more accurate data collection

Since this is a meeting of the Data group, I put in the following all the D -> Be data collected - even though some of them do not really give new physics insights.





Old results on Be sputtering Sputtering of initially pure Be by D



expansion Lower surface binding energy D⁺ energy (eV)

[C. Björkas et al, Plas na Physics and Controlled Fusion 55, 074004 (2012)]



Results on Be sputtering by D Flux dependence

- We find some flux dependence even for the very high MD fluxes
- Reason: for highest fluxes defective structure does not have time to relax



Results on Be sputtering by D

D on Be cumulative run results: BeD_n molecular sputtering yield







33

32

250



1*BeD2

3*BeD2



Results on Be sputtering by D D on Be results: Discussion

- General overall conclusions of trends in data:
- Sputtering yield of both Be and BeD_n increase with increasing temperature
- Sputtering yields of both Be and BeD_n increase from 20 to roughly 100 eV, after that roughly constant (within current statistics)
- (At least in our potentials) Be sputters as Be, BeD and BeD₂, but the last one is likely very unstable

[E. Safi, A. Lasa, C. Björkas and K. Nordlund, to be published (2015] Kai Nordlund, University of Helsinki



BeW alloy formation Be irradiation of W surfaces

We examined the Be sticking coefficient as a function of incoming ion angle We constructed a geometrical model considering scattering and shadowing that allowed understanding the angle dependence a = d - 2hR

on 54, 083001 (2014)] [A. Lasa, K. Heinola, and K. Nordlund, Nuclear Fus

Mixed D, Be bombardment of W Surface structures formed: overview

We also examined the mixed D, Be bombardment of W



[A. Lasa, K. Heinola, and K. Nordlund, Nuclear



Mixed D. Be bombardment of W Surface structures formed: 33 % Be, 50 eV

b: Formed after high Be fraction (33% Be) 50 eV bombardment



BeW alloy formation Be irradiation of W surfaces





Mixed D, Be bombardment of W Surface structures formed: 10 % Be, 10 eV



Mixed D, Be bombardment of W Surface structures formed: 10 % Be, 100 eV

e: Amorphous W surface layer at 10% Be, 100 eV





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Mixed D, Be bombardment of W D implantation profiles

- D is implanted in the growing mixed layer:
- Higher D implantation than for D only -> pure W or pure Be!



Nordlund, University of Helsinki [A. Lasa, K. Heinola, and K. Nordlund, Nuclear Fusi'on (2014), submitted for publication.



Mixed D, Be bombardment of W Comparison of MD and BCA

- BCA [SDTrimSp by Klaus Schmidt] describes well the Be erosion above 50 eV, not below it (chemical effects)
- BCA does not describe well the D reflection (one energy point can be fixed but not all)



Outlook

- D -> Be: Non-cumulative runs with decreasing D concentration for increasing T being run: should match JET conditions with outgassing better.
- Data to be published
- Be-He potential to be made
- D chemical sputtering of AI:
 AI H potential does exist [Apostolos and Mishin, Phys.
 - Rev. B 82, 144115 (2010)]





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Mixed D, Be bombardment of W W erosion by Be

The Be also causes W sputtering (at energies where pure D irradiation would not)



Conclusions

- MD can be extremely useful for obtaining qualitative understanding of what is going on!
 - And this is most important in science!
- It can also be used to collect lots of data, but one has to be careful about reliability...
 - Definitely more reliably than BCA in low-energy regime anyway
 - Use at least 2 different potentials to get some idea of reliability

Kai Nordlund, University of Helsinki

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Be-O potential?? Challenge...