Atomistic simulations of the deposition, chemical sputtering and blistering of C, W and CW-based divertor materials

Kai Nordlund, Emppu Salonen, Petra Träskelin, Krister Henriksson, Niklas Juslin, Arkady Krasheninnikov and Juhani Keinonen

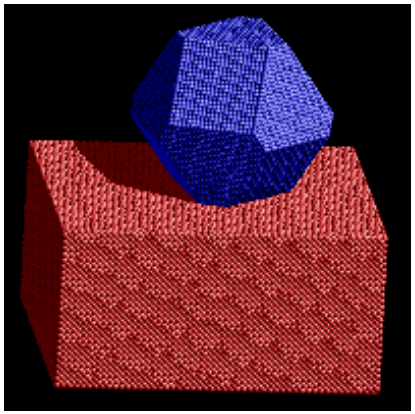
Accelerator Laboratory, University of Helsinki

in contact with

- Chung Wu and Alberto Loarte - Garching
- Manoj Warrier and Ralf Schneider - Greifswald
- Achim von Keudell and Wolfgang Jacob – Bochum/Garching
- Karsten Albe – TU Darmstadt

Research profile

- We use atomistic computer simulations to study radiation effects in interesting systems. Current foci on:
  - Fusion reactor materials
  - Compound semiconductors
  - Carbon nanotubes
  - Nanoclusters



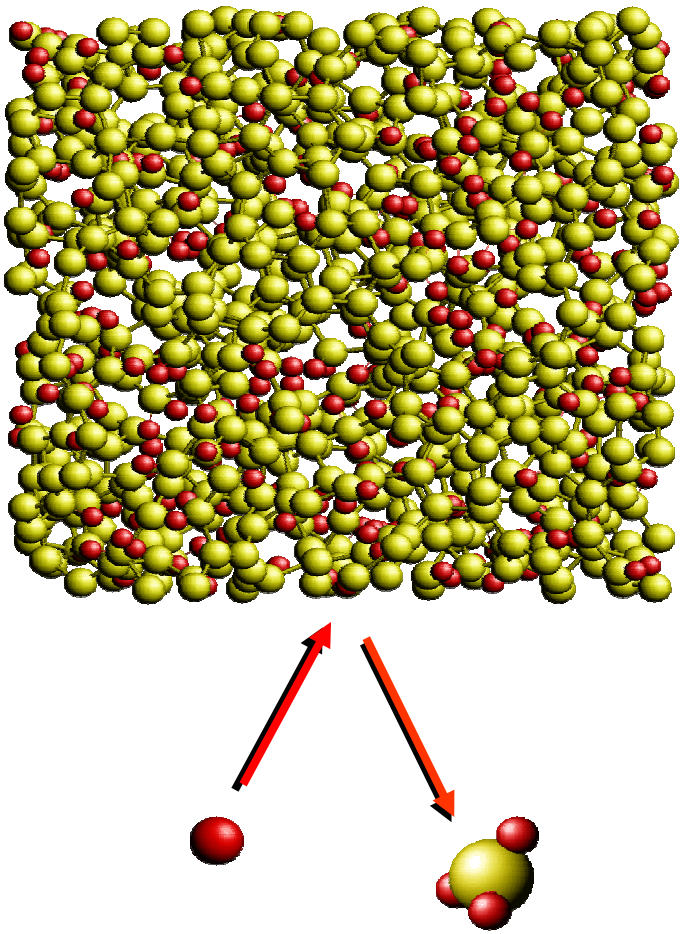
- My group has 10 members, 4 of whom work on fusion reactor problems

Contents

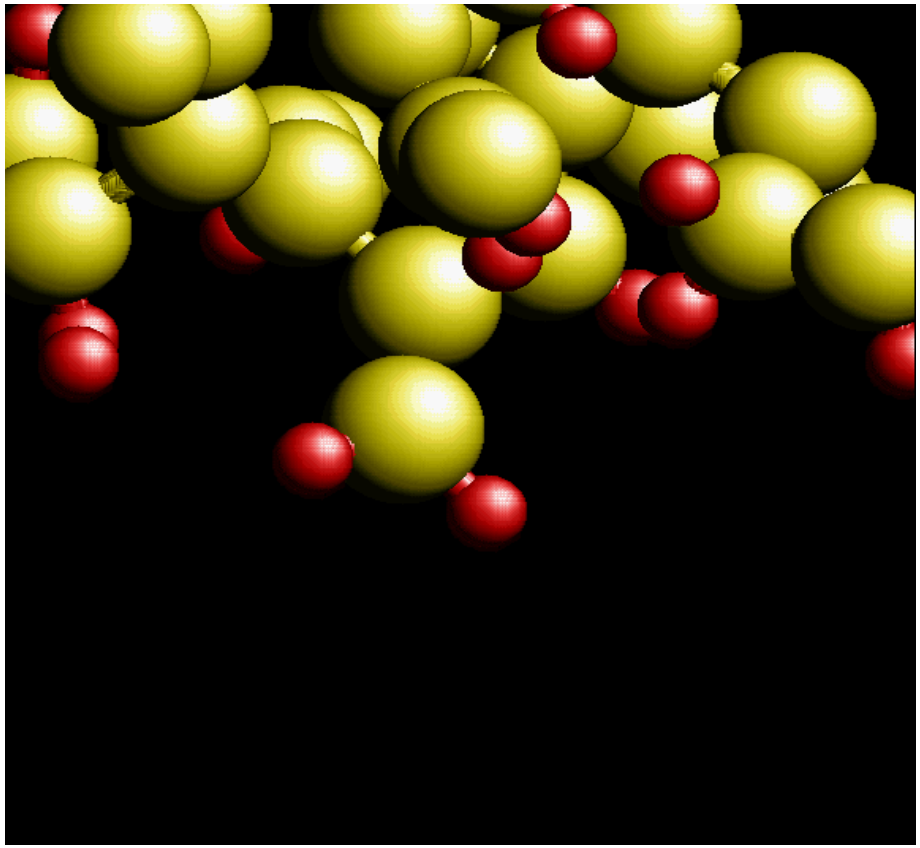
- Low-E H, D and T bombardment of a-C:H
  - Swift chemical sputtering
- Sticking of CH_x species on C surfaces
- Blistering of W by incoming H and He ions
- Low-E D bombardment of WC

low-E H bombardment of a-C:H

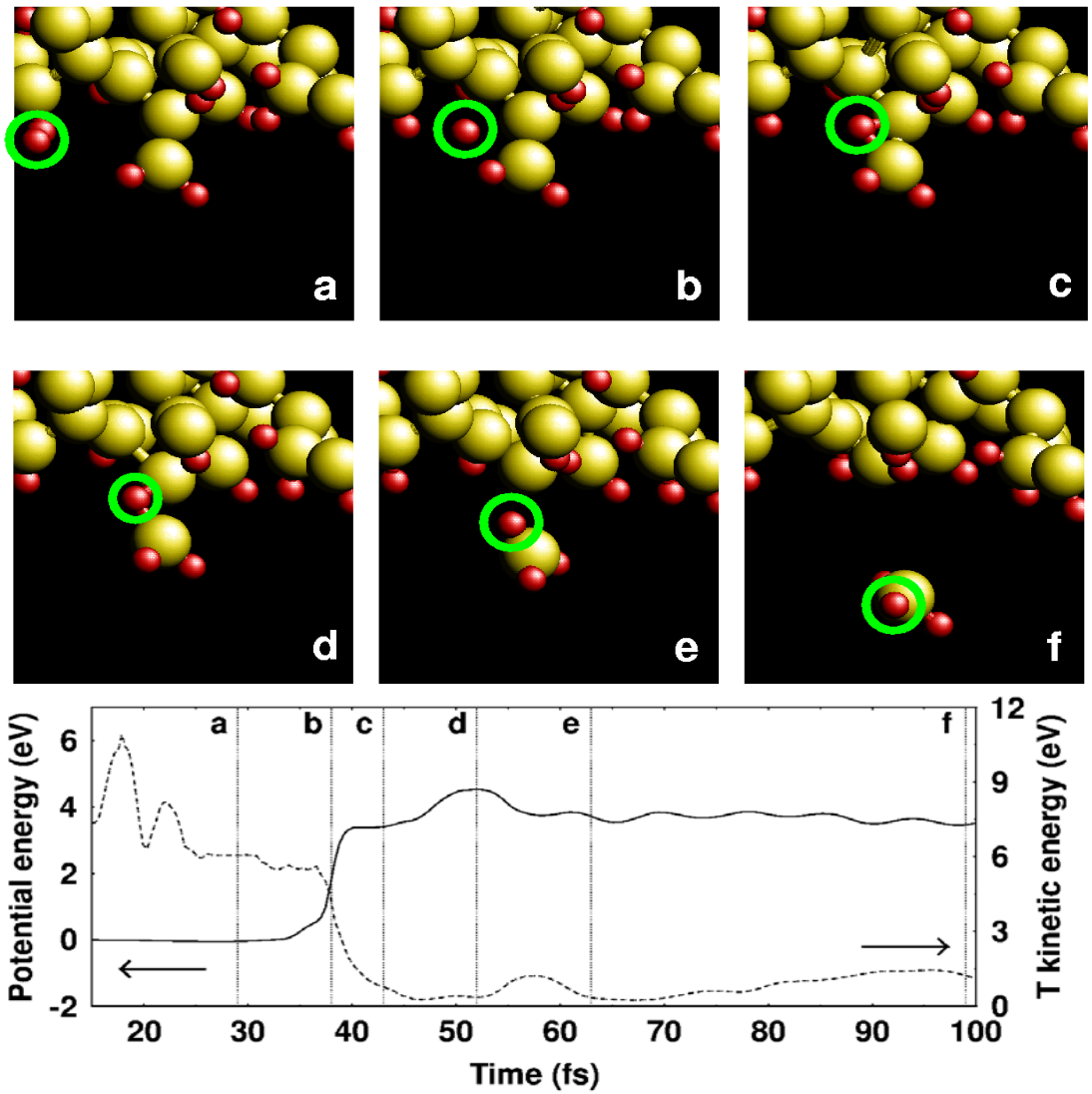
- We first create a model of surface amorphous hydrogenated carbon (a-C:H)
  - H/C ~ 0.4, sp^2 bonds 70 % of all
- Then H/D/T ion created above the surface, kinetic energy and impact angle assigned
  - H energy 1 – 35 eV
  - Sputtered C species counted to get sputtering yield
  - Classical and quantum mechanical (TB) MD methods used



Main result: swift chemical sputtering



- The hydrogen ion enters the region between two atoms and raises the energy by a few eV, more than the strength of the bond!

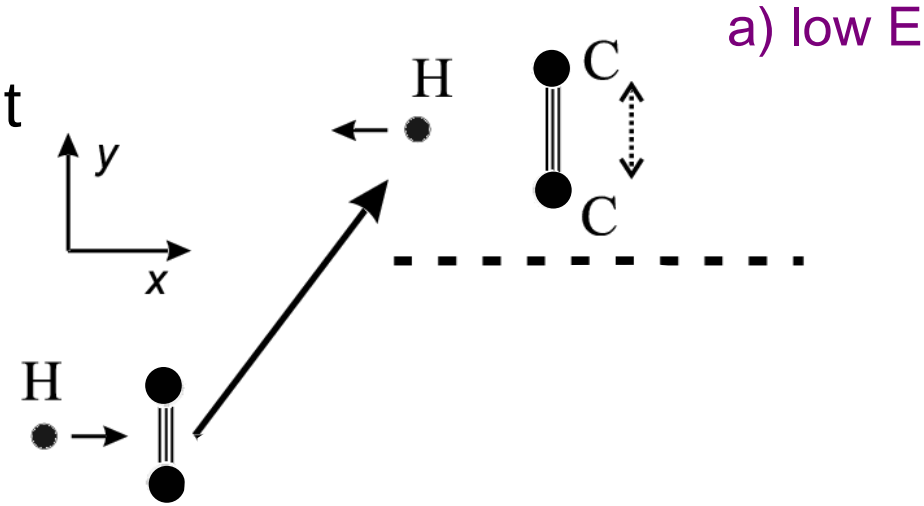


[Salonen, Europhys. Lett. 52 (2000) 504;
Phys. Rev. B 63 (2001) 195415]

Physical insight

- A model system of a single H atom colliding with a C dimer gives insight to the basic mechanism
- Momentum transfer in y direction is

$$p_y = \int_{-\infty}^{\infty} f_y(t, E_{kin}[\mathrm{H}])dt \approx \bar{f}_y \bar{\tau}$$



a) low E: H does not penetrate and is reflected

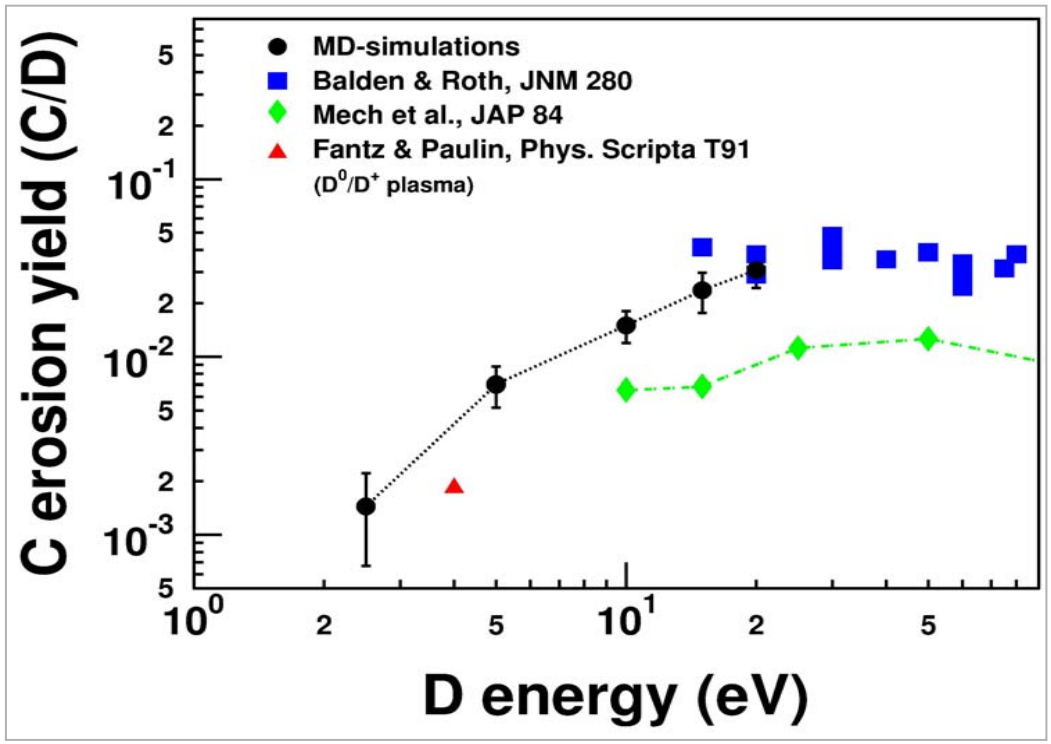
b) medium E: H penetrates slowly => large τ => large p_y => bond breaking occurs

c) high E: H penetrates rapidly => small τ => small p_y => no bond breaking

[Krasheninnikov et al, Contrib. Plasma Phys. 42 (2002) 451]

Comparison to experiments

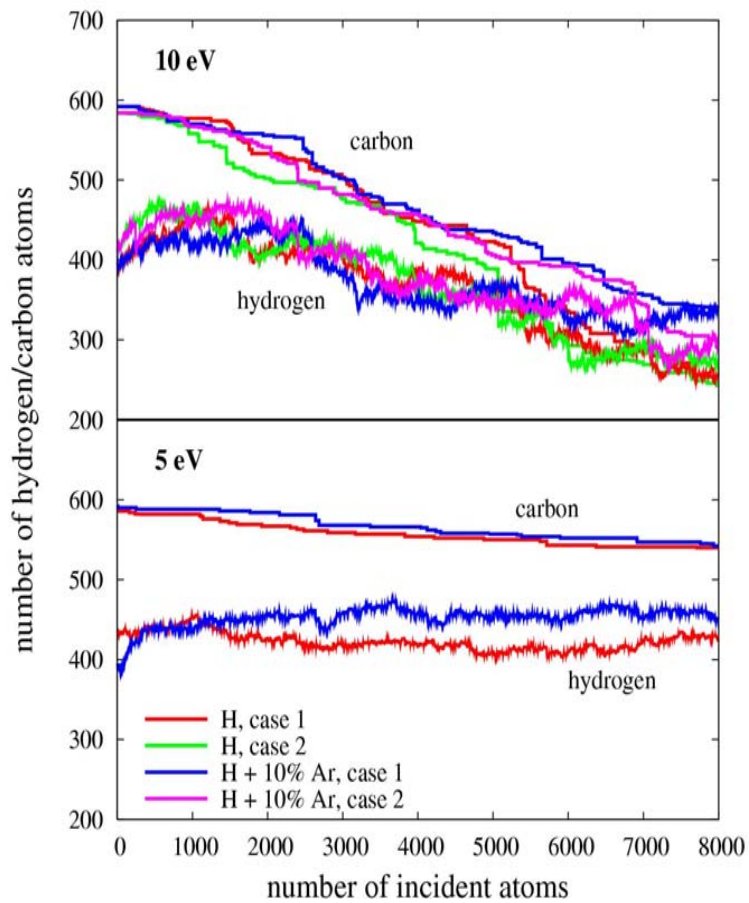
- This mechanism can explain the low-energy erosion of hydrocarbons
- Good agreement with experiments
- We have shown that the mechanism:
  - is not physical sputtering
  - is not model-dependent
  - is not chemical etching



[Salonen et. al, Phys. Rev. B 63 (2001) 195415; Europhys. Lett. 52 (2001) 504; Contrib. Plasma physics 42 (2002) 458]

Noble gas seeding

- What happens if 1-10% He/Ne/Ar is added to the edge plasma?
- We examined this using same energies for H and noble gases
- Result: no effect of up to 10% noble gas
  - Reason: noble gases do not cause much swift chemical sputtering



C:H layer growth

- CH radicals are important growth species in fusion reactors
- Important to how the growth occurs is the sticking probability on dangling bonds
  - But experimental values on this differ a lot
- We have used MD simulations to obtain understanding on the basic sticking mechanism
  - Also try to understand why there is such a large variation in the experiments

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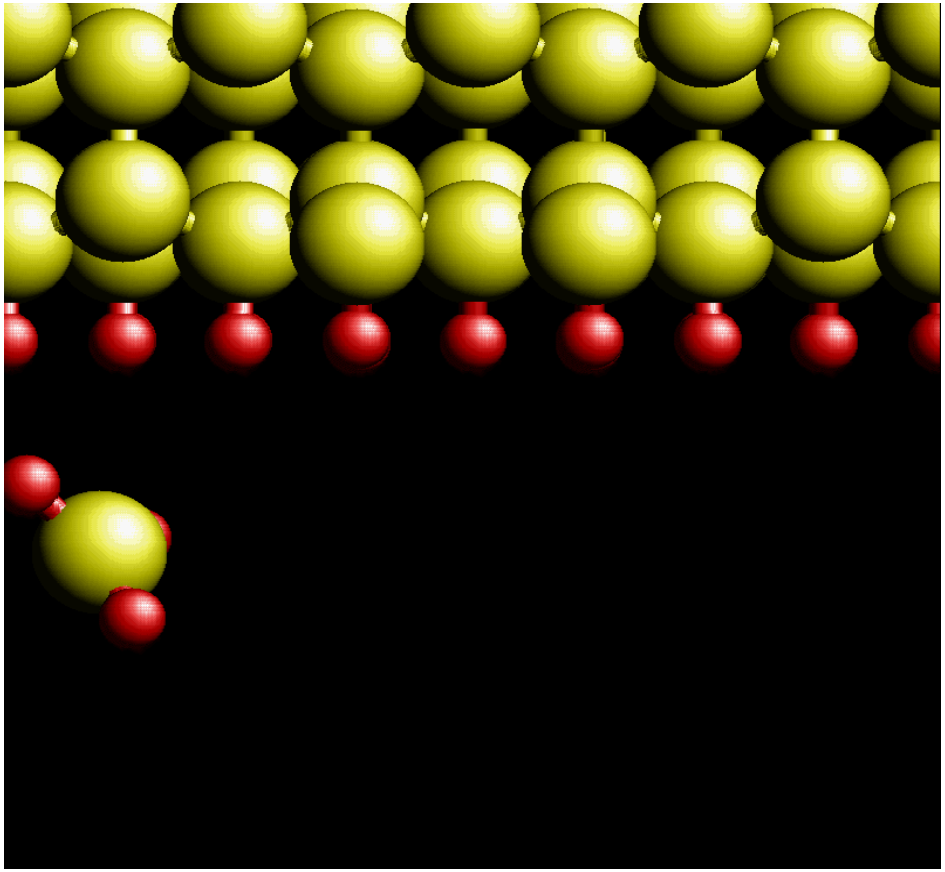
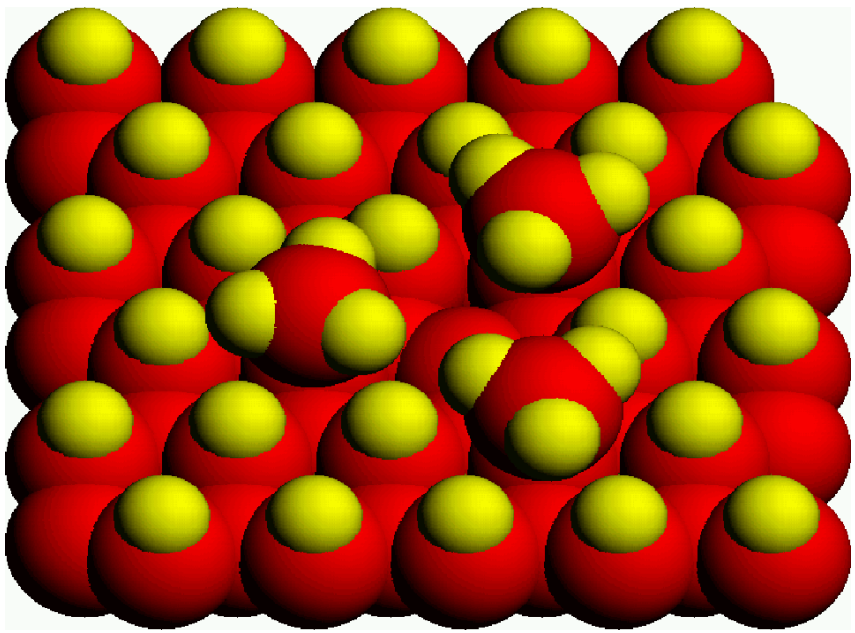
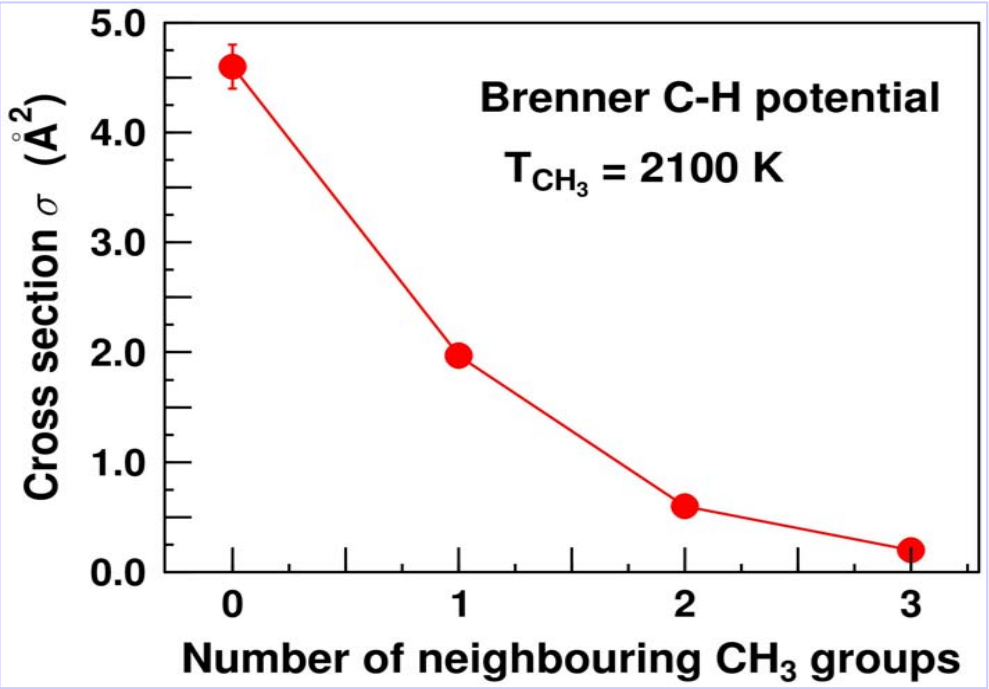
Animation: CH_3 sticking



Effect of dangling bond neighbourhood

- We tested the effect of the dangling bond neighbourhood on the sticking cross section => very strong dependence

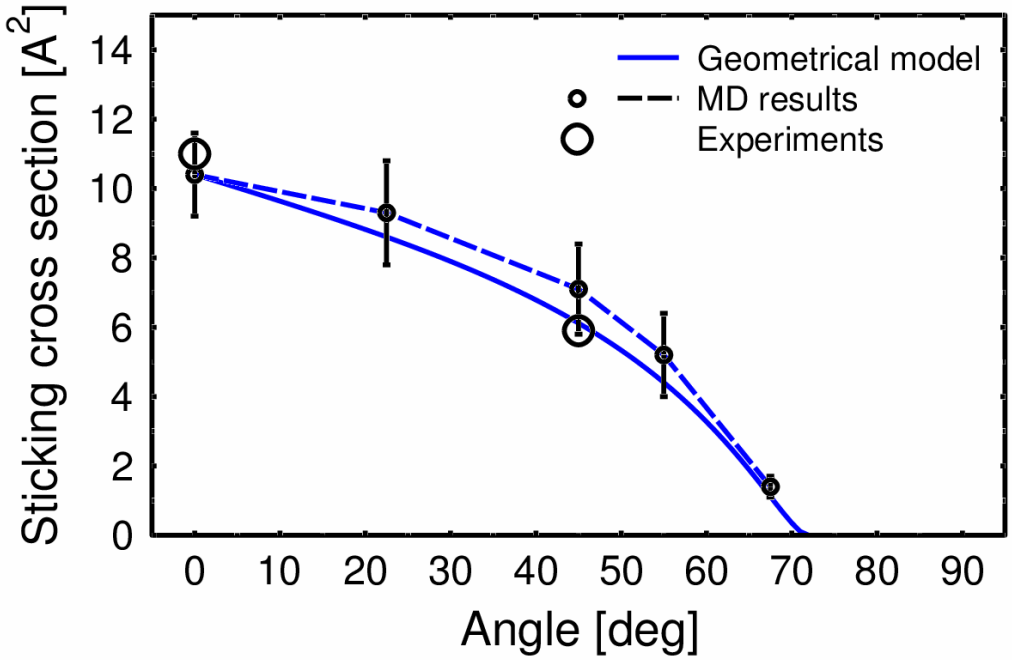




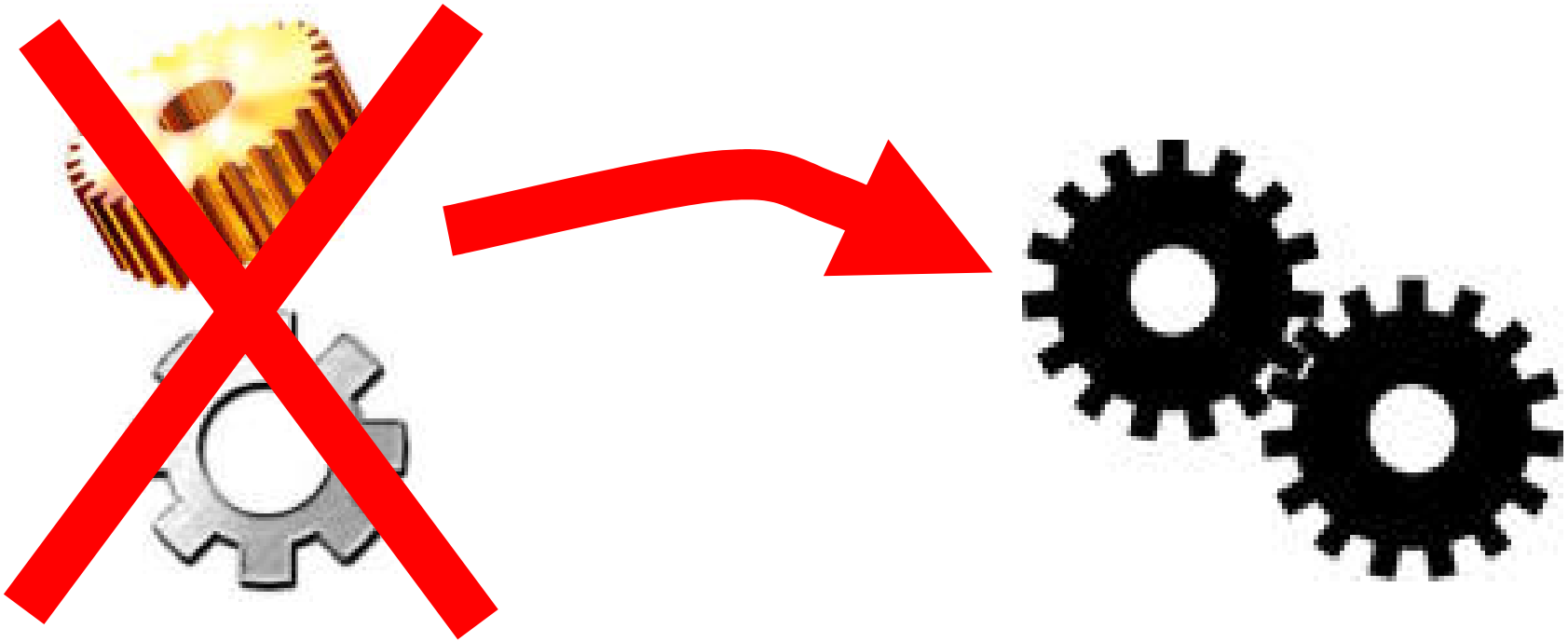
[Träskelin et al, J. Appl. Phys. 93 (2002) 1826]

Angular dependence

- We have also shown that the incoming angle of the CH_3 species has a strong effect on the sticking
- The strong angular and dangling bond neighbourhood dependence are likely explanations of the variation in experimental results (when the dangling bond coverage is the same)



- Let’s change gears…



Bubble formation and blistering in W

- The main divertor material in ITER will be W
- So what about H and He damage in it?
- One of the main advantages of W is that 1-100 eV H and He cause zero damage, very little physical sputtering and no chemical sputtering
- But these ions do produce bubbles and blisters, which eventually rupture and might cause erosion

Difference of H and He bubble formation

- Depth of blisters vastly different.
  - H: at micrometer depths
  - He: close to Rp (<100 Å)
- Why is this?
- We considered many possibilities:
  - Damage different: no, since also non-damaging irr. produces bubbles!!
  - Difference in diffusivity: no, about the same
  - Thermal gradients: no
  - Different kinds of W samples in experiments: no
- But how about differences in trapping behaviour?

H vs. He self-trapping

- The simplest possible trap is the self-trap: two mobile atoms A and A clustering with each other
  - Becomes immobile, acts as seed for further bubble growth
- To examine this, we used classical MD simulations and quantum-mechanical DFT calculations to examine the energy of two H or He atoms at different distances

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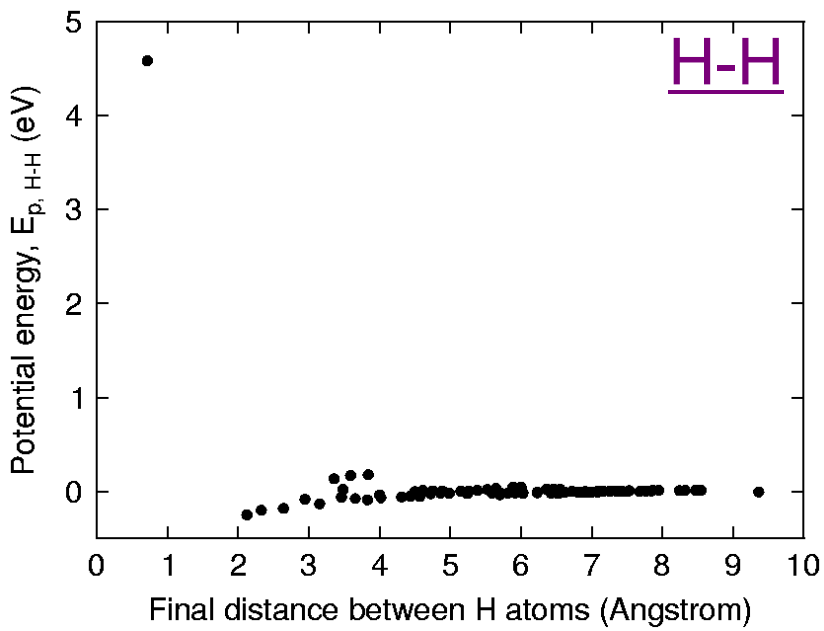
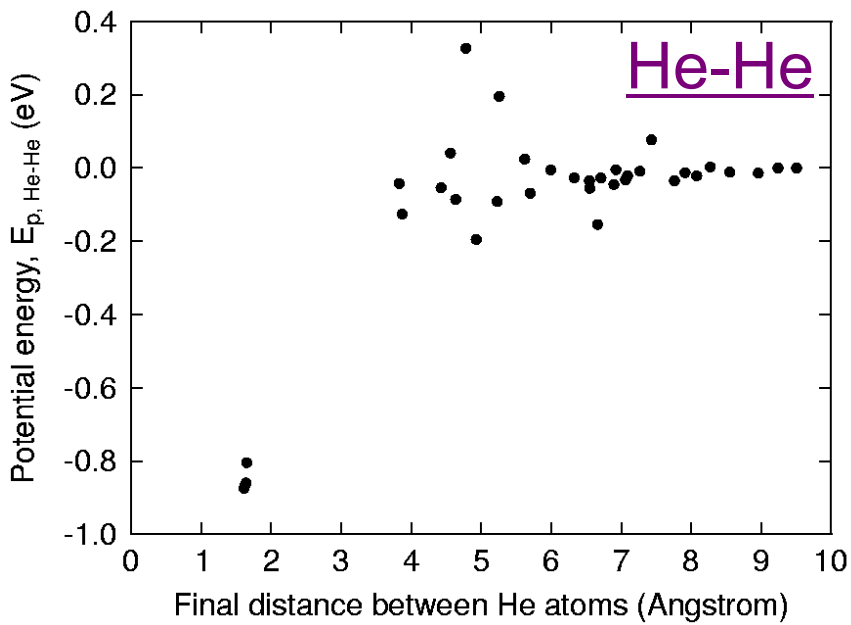
H vs. He self-trapping: energetics results

- MD energetics of H-H or He-He pair:
  - Most important features confirmed by DFT





- Almost no binding for H-H, but strong (1 eV) binding for He-He!

Kinetic Monte Carlo

- Kinetic Monte Carlo (KMC) is the ideal tool to simulate processes which occur at a certain rate
  - Typically migration
- In Object KMC only the mobile objects are simulated
- For each mobile object the migration activation energy and prefactor need to be known:

$$r_i = w_0 e^{-E_A / k_B T}$$

- Once all r_i are known, processes are selected proportional to their rate, and the atoms allowed to jump
- There is no approximation involved if the r_i are correct!

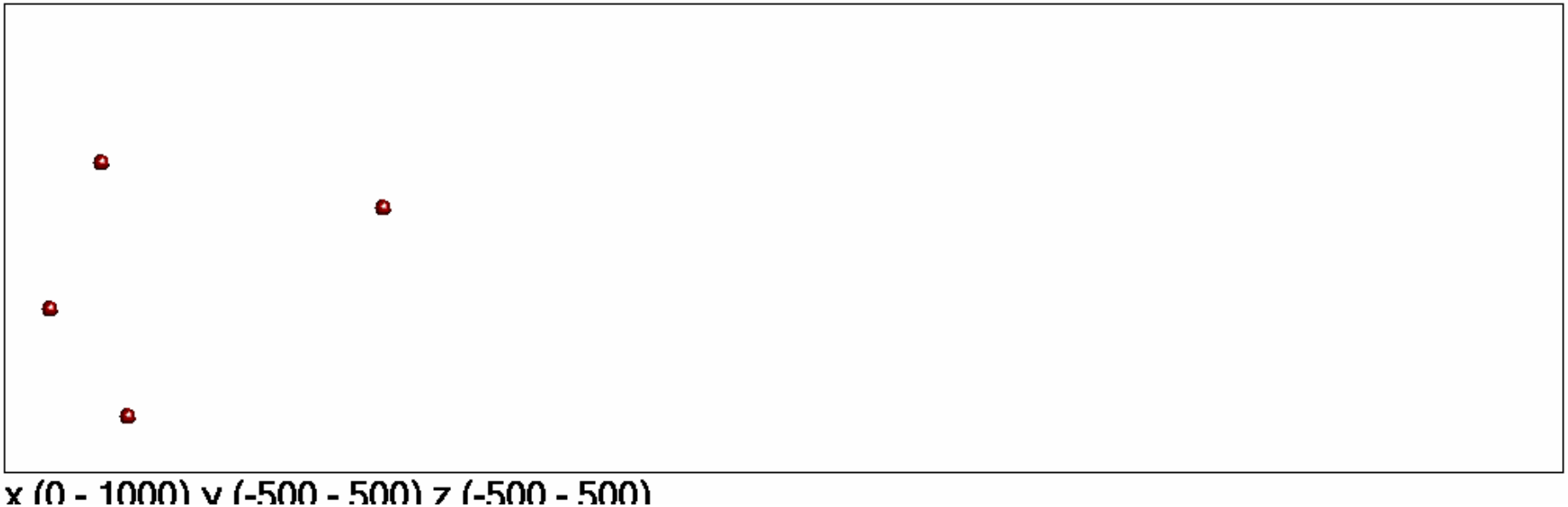
He bubble depths

- This shows that He can self-trap, while H can not
- Enough to explain qualitatively He-H difference
- But to be on the safe side we also used Kinetic Monte Carlo (KMC) simulations of He migration in W to check whether He bubble depths obtained with self-trapping are the same as in experiments
- Results:

T(K)	Our KMC	Expt.	Reference
300	100 Å	62 Å	Nicholson and Walls 1978
2370	2200 Å	0 – 5000 Å	Chernikov and Zakharov 1989

Animation of KMC bubble formation

- He bubble formation: mobile atoms red, immobile He in clusters orange, large clusters green or blue



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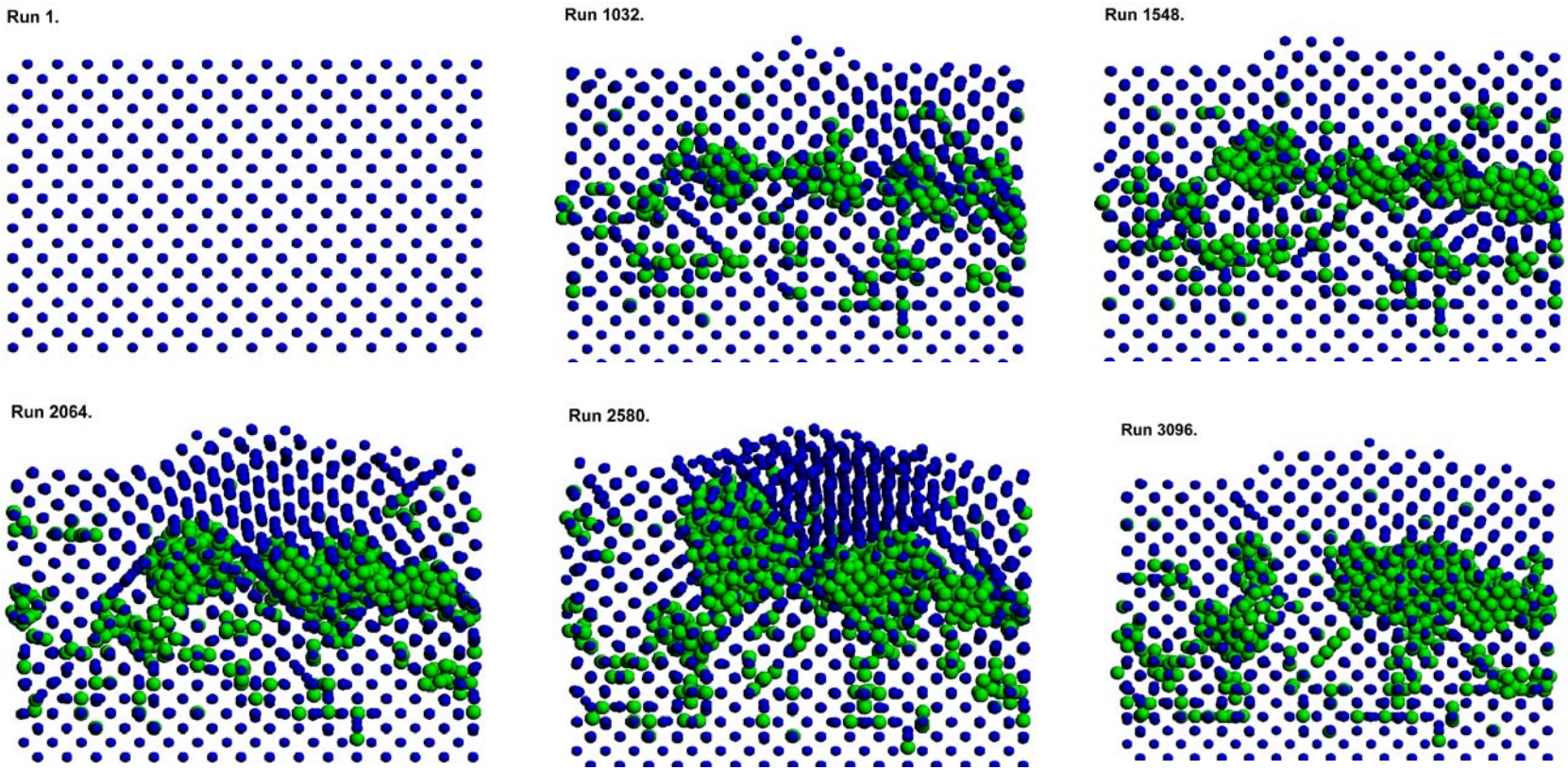
Near-surface blistering of W by He

- MD simulation of 100 eV He -> W:



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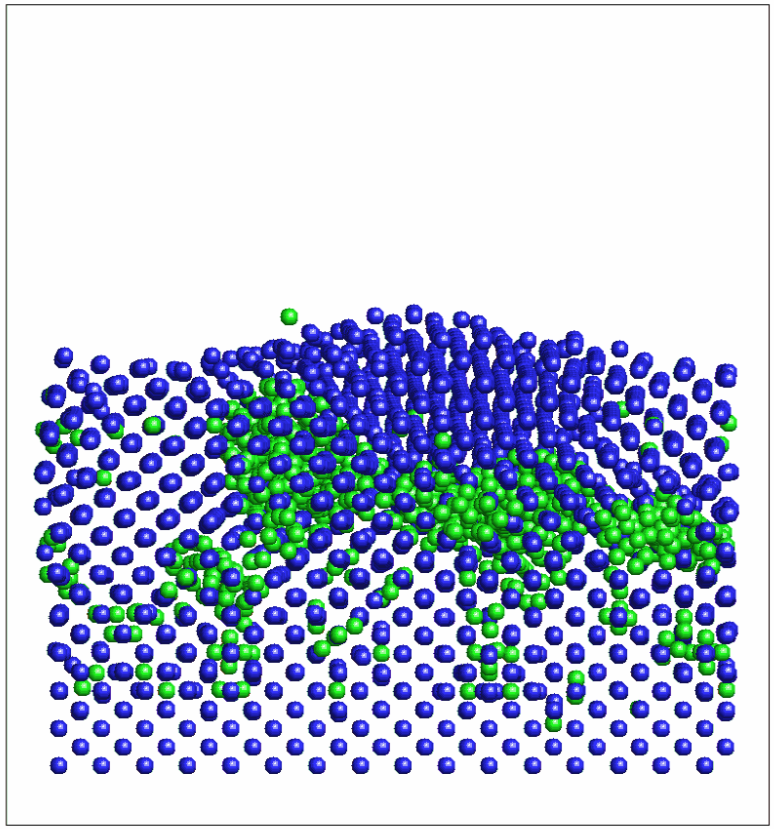
What happened after run 2580?



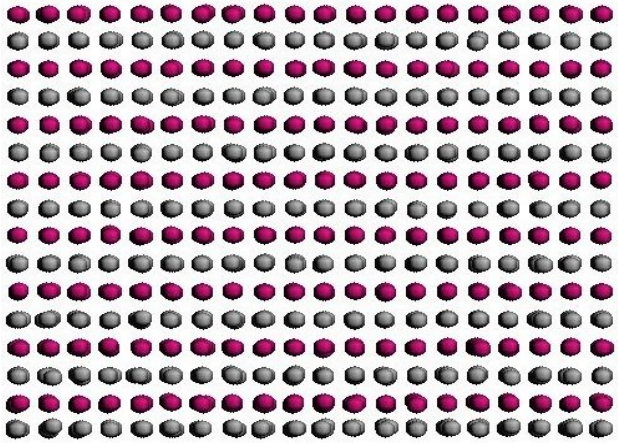
Blistering results

- In the He-induced blistering events observed so far, no W erosion associated with the bubble rupture has occurred
  - Sounds encouraging: low-E bombardment bubble rupture may not cause much erosion

WC

- Since the ITER divertor contains both W and C, WC may form either at the C-W-interface or due to C drifting in the reactor forming WC thin films
- So how about erosion of WC?
  - Does it behave more like a metal (no chemical sputtering) or carbon with loose hydrocarbon formation and swift chemical sputtering?
- To model this we have developed parameters for W-W, W-C and W-H
  - Effort needed about 2 person-years of work
- For C-C, H-H and C-H we use the well tested parameters by Brenner

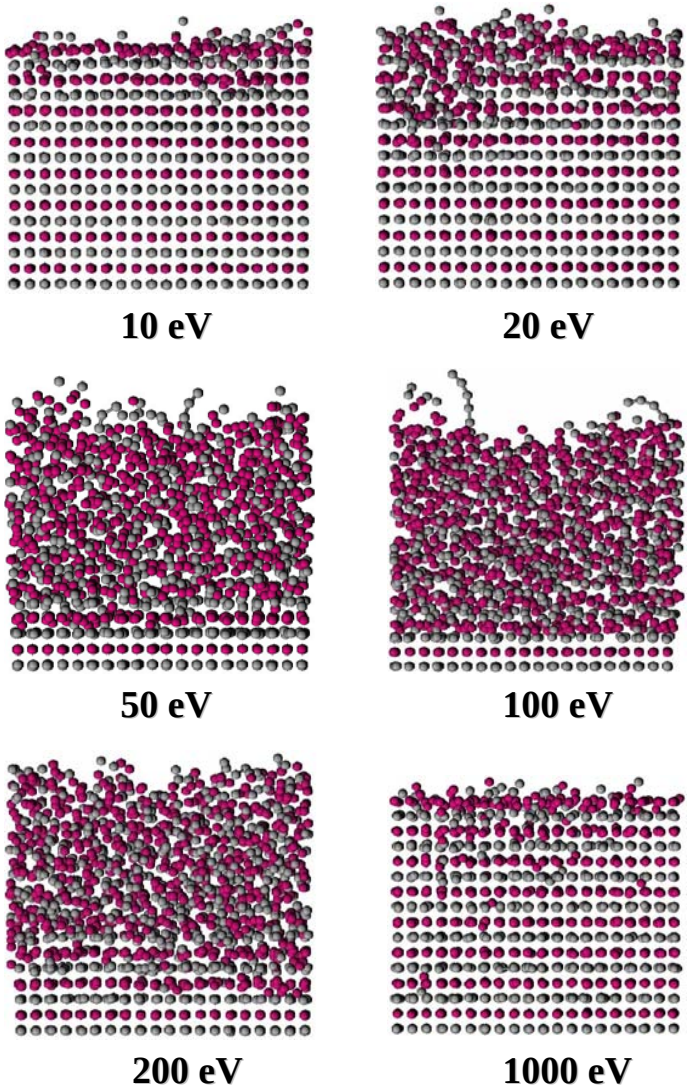
Simulation cells



- Simulation box:
  - 1600 (W) or 1920 (WC) atoms
  - Periodic boundaries in two directions
  - Open surface
  - In tungsten carbide both tungsten and carbon as the outermost layer: WC and CW
- In the *non-cumulative simulations* we bombard a clean surface for every new simulation run
- In the *cumulative simulations* we use the surface from a previous run, simulating a surface being bombarded several times

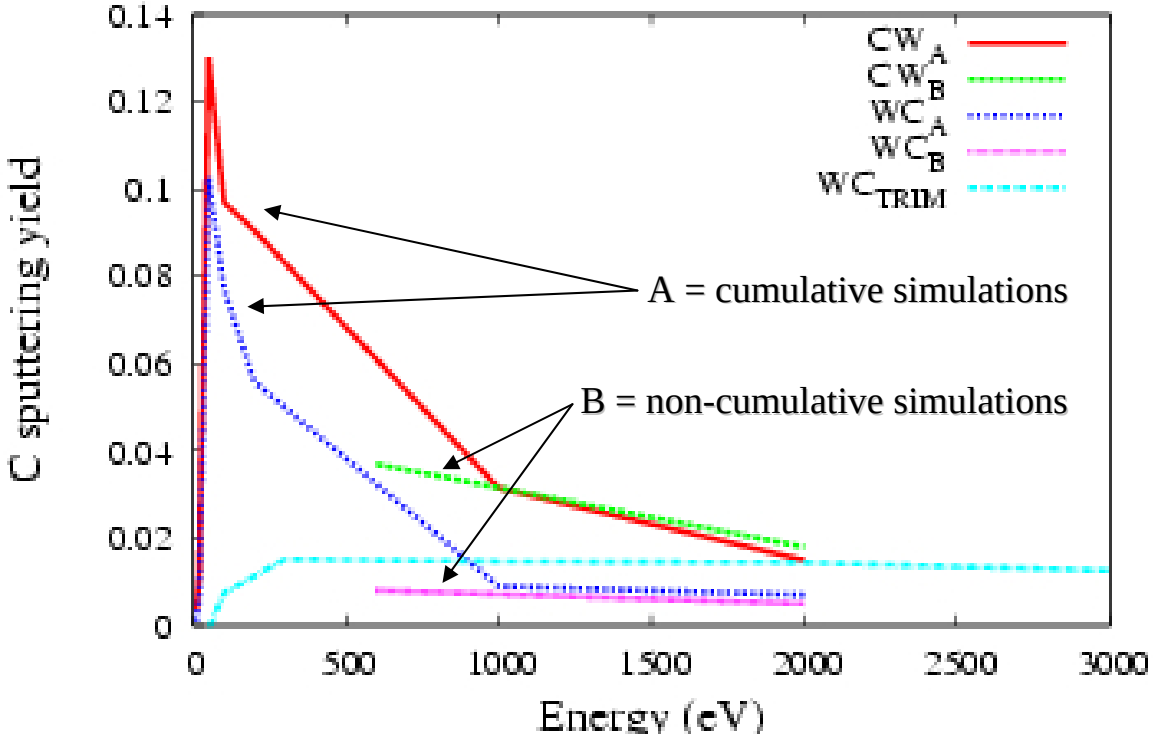
Results for WC

- Snapshots after 1000 impact events for different energy D
- Sample amorphizes!
- Loose hydrocarbon chains form on surface!



Erosion yields

- Because of the formation of the loosely bound carbon chains, swift chemical sputtering can occur!
  - Large sputtering yields at low energies
- For pristine samples (non-cumulative runs) no such effect



Erosion yields

- No major difference between WC and CW: amorphization removes initial difference
- But practically no W erosion despite chemical sputtering

  => VERY GOOD!

W

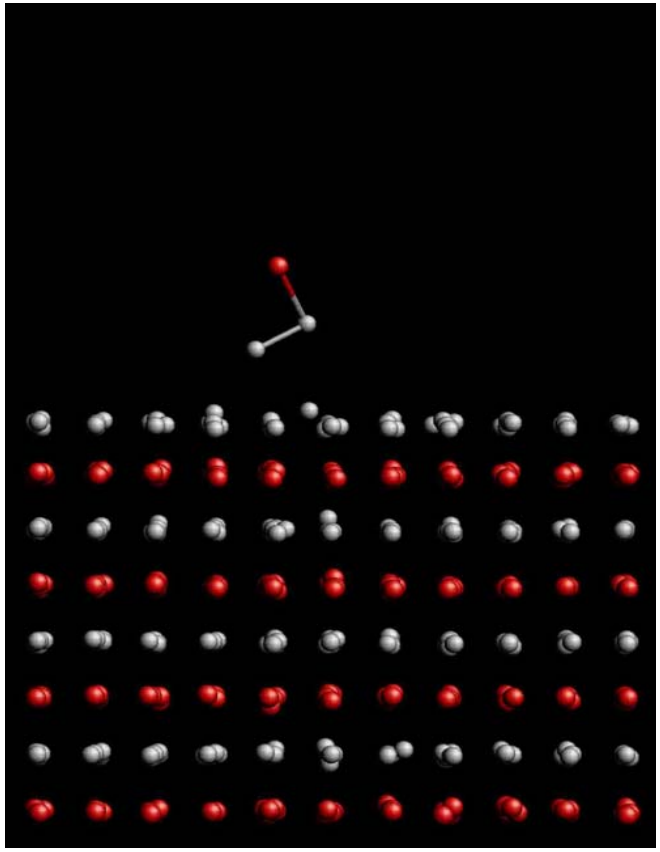
Energy	Y(W)	Reflected D
600 eV	0.0006	0.09
2k eV	-	0.016

WC

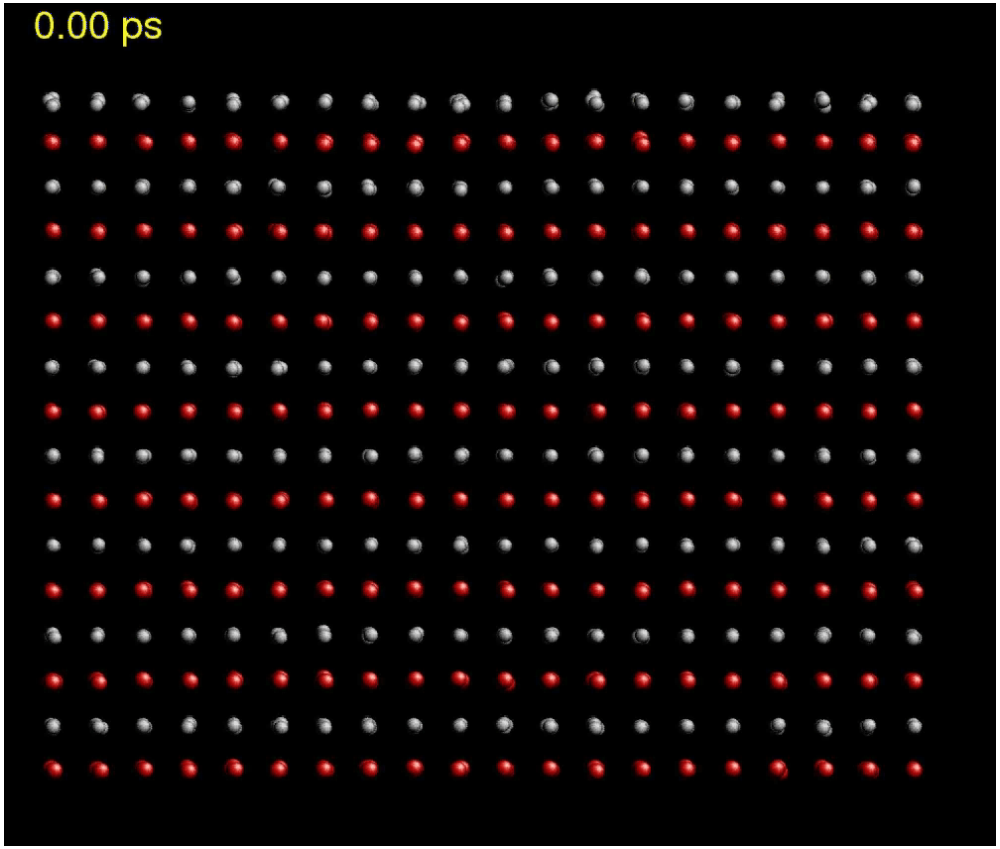
CW

Energy	Y(W)	Y(C)	Reflected D
600 eV	-	0.008	0.044
2 keV	-	0.005	0.015
600 eV	-	0.037	0.054
2 keV	-	0.018	0.012

Animation of WC erosion



0.37 ps



Conclusion

- Molecular dynamics simulations can be used to model:
  - metallic fusion reactor first wall materials
  - C-based fusion reactor first wall materials
  - Their mixtures

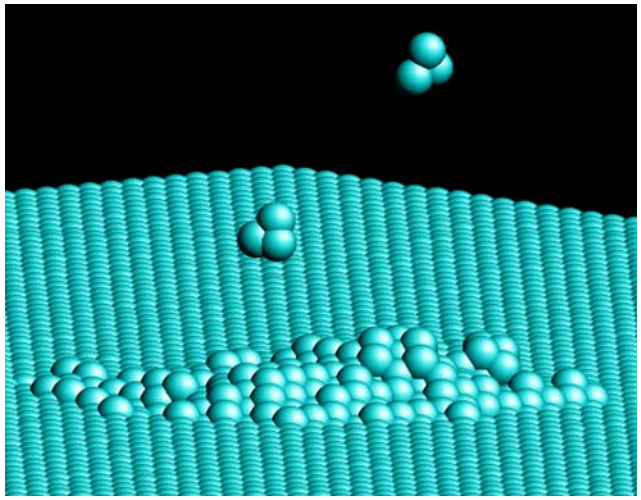
  and
  - sputtering
  - sticking/growth
  - blistering

  in all of these classes of materials

The END

Cluster sputtering in W?

- Recent experiments by Andersen have shown that heat spikes can lead to dramatic enhancement of sputtering yields during cluster bomdardment in dense FCC metals
- We studied whether this would true in W
  - If it were, that would have to be accounted for in the modeling of W sputtering in reactors



[J. Nucl. Mater. 15 (2003) 5845]

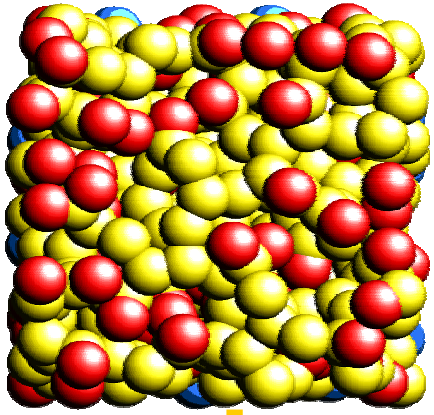
- Our result:
  - Yes, cluster sputtering enhancements can occur in W
  - But if the incoming W energies are < 2 keV the numbers are not self-sustaining => should be no problem in reactors

High-dose H bombardment

- What happens after prolonged H bombardment?

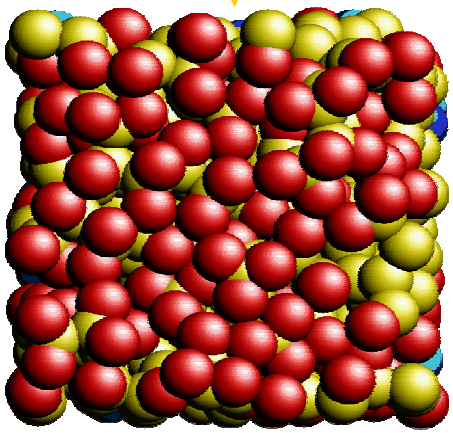
Erosion yield:

0.01



Erosion yield:

0.001 !



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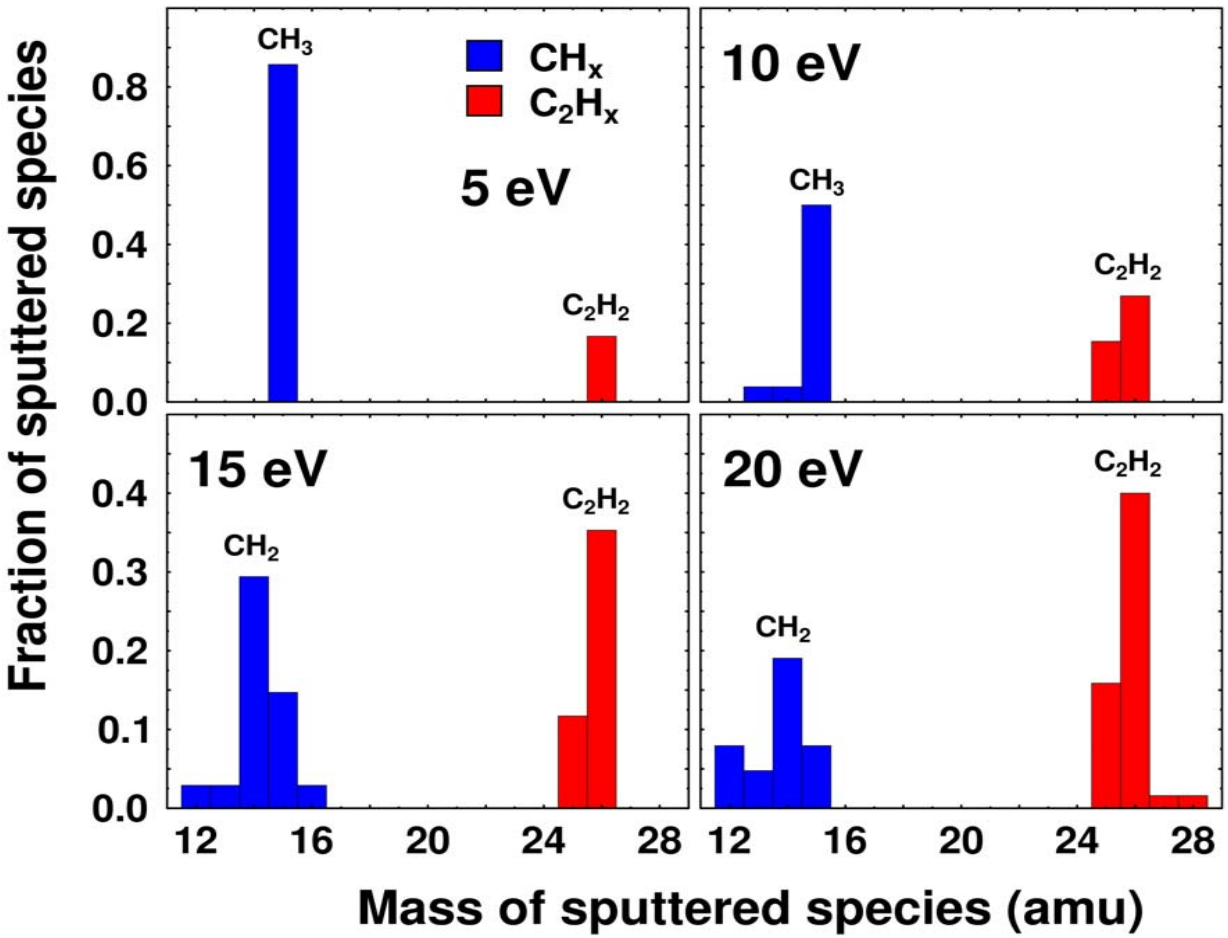
What comes out?