Sputtering in the heat spike and high-temperature regimes

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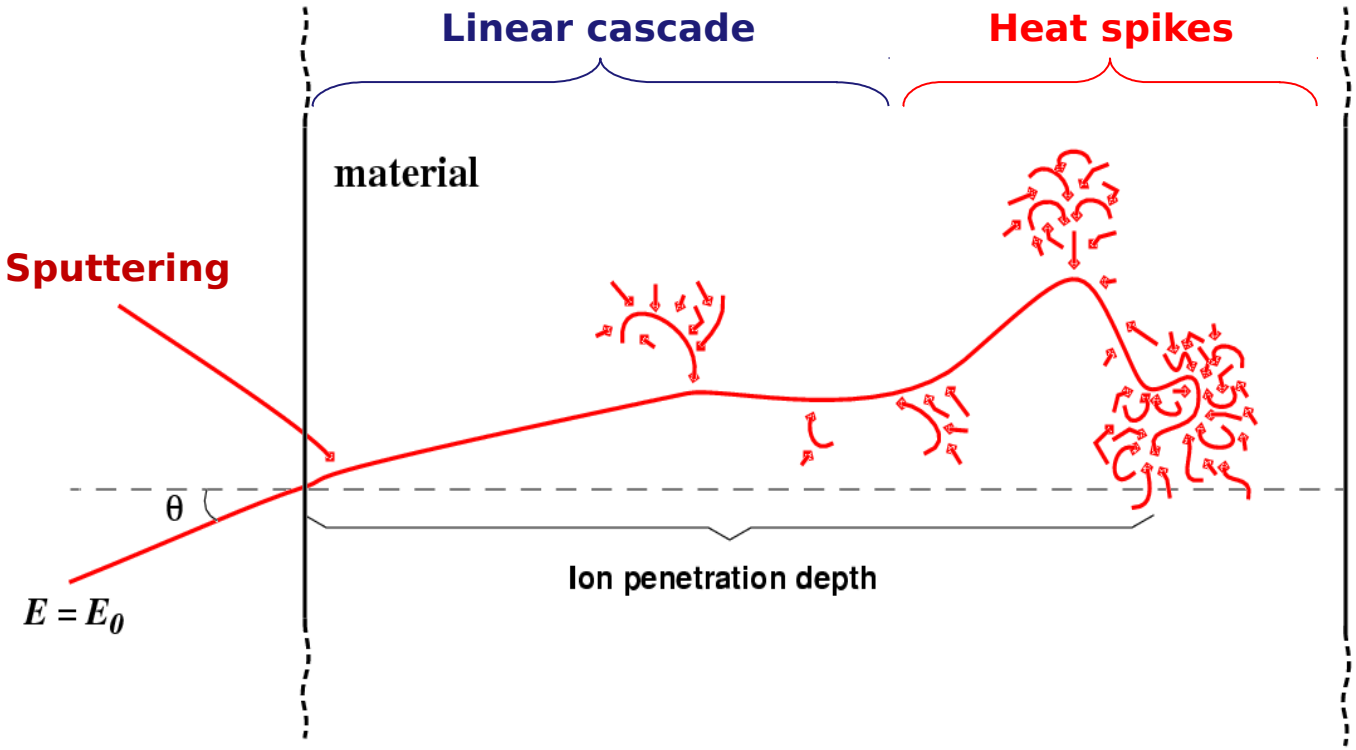
Contents

- Overview of sputtering
  - Linear cascades
  - Heat spikes
  - Sputtering from nanosystems

- Sputtering in the high-temperature regime
  - Experimental observations
  - New work by us

Basic irradiation physics

- Sputtering, linear cascades, heat spikes

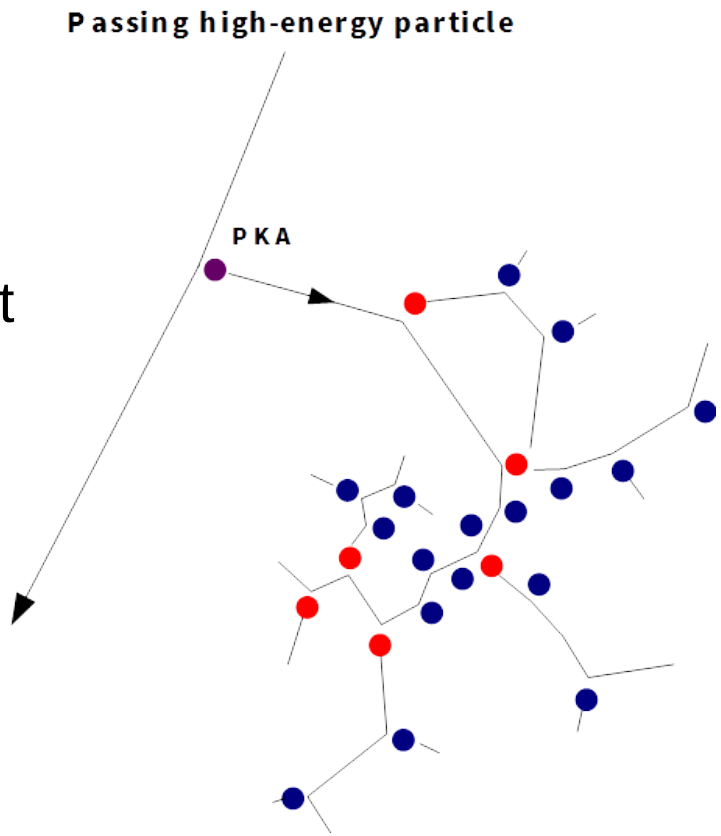


Example: low energy basic sputtering event

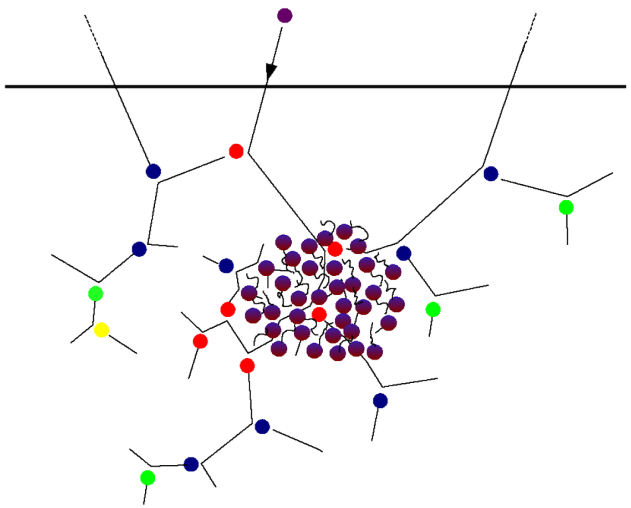
- 500 eV Xe on Au

MD of sputtering: basic motivation

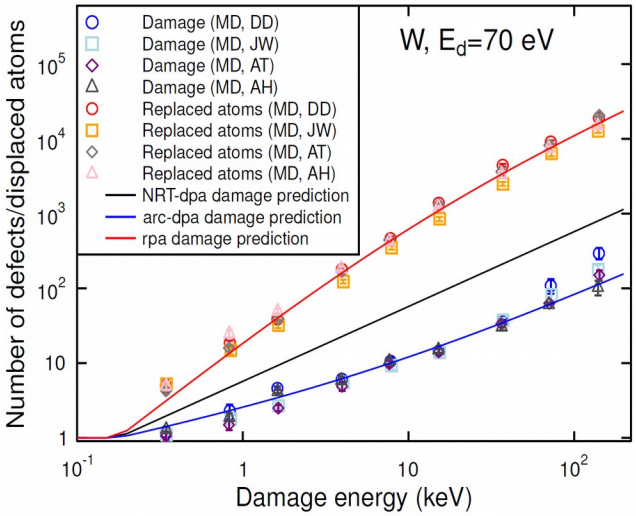
- Molecular dynamics is well suited to study sputtering
  - Regular physical sputtering is an athermal effect (no thermal activation needed)
    so MD time scale limitation
    is not a problem
- Can predict sputtering effects "ab initio", i.e. from models that do not have any empirical inputs from irradiation experiments!
- However, in linear cascade regime, MD is not really needed: all binary collisions



Heat spikes

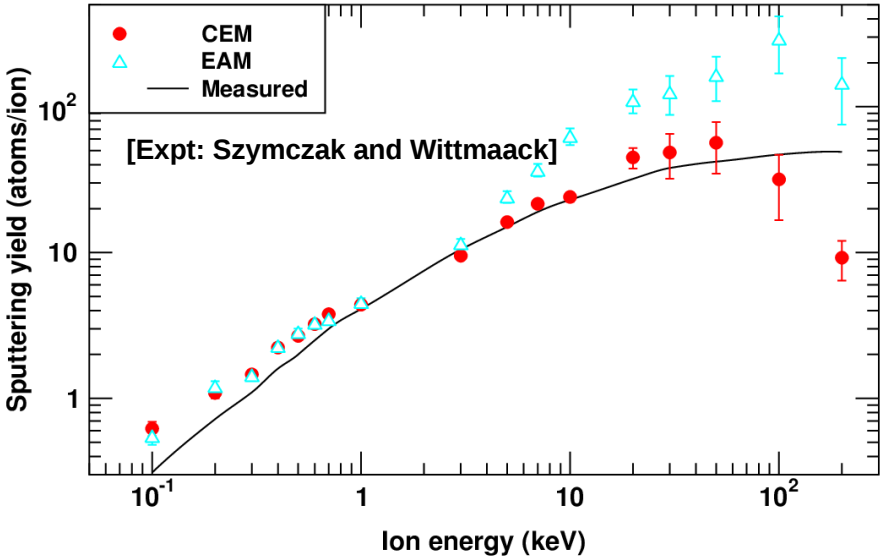


- If the collisions occurs very close to each other, one gets a single zone of many-body collisions = “heat spike” or “thermal spike”
  - Temperature about 10000 K
- Radiation damage gives a good view of when heat spikes become important: there is major damage recombination in them
- In a recent other work, we analyzed this systematically in several metals [Nordlund et al, Nature Comm. **9**, 1084 (2018)]
- Result: heat spikes important already at ~ 1 keV!



Heat spike sputtering effects

- The heat spikes can cause a major enhancement of sputtering

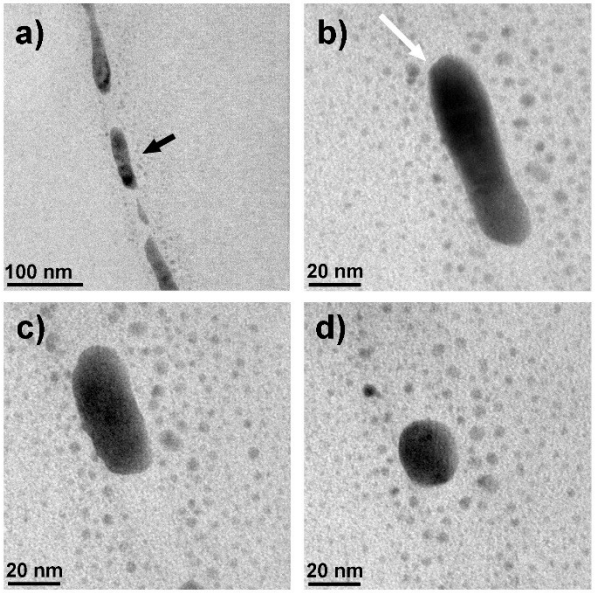


[Samela et al, Nucl. Instr. Meth. Phys. Res. B (2005

- Results do depend on interatomic potential, though

Extreme case of heat spike sputtering: 80 keV Xe on Au nanowires

- Recent experiments by Donnelly *et al* show that the sputtering yield of Au nanowires is dramatically enhanced compared to the bulk!
  - 80 keV Xe ion
  - Single nanowire observed in TEM in situ
- Experiments give for some cases Y = 1000 to 2000 !
- Bulk experimental yield Y = 50
- Factor of 20 enhancement - why??
- Enhancement by inclined angle
  - Was considered by us, does enhance yield, but not enough



[G. Greaves et al, Phys. Rev. Lett. 111 (2013) 065504]

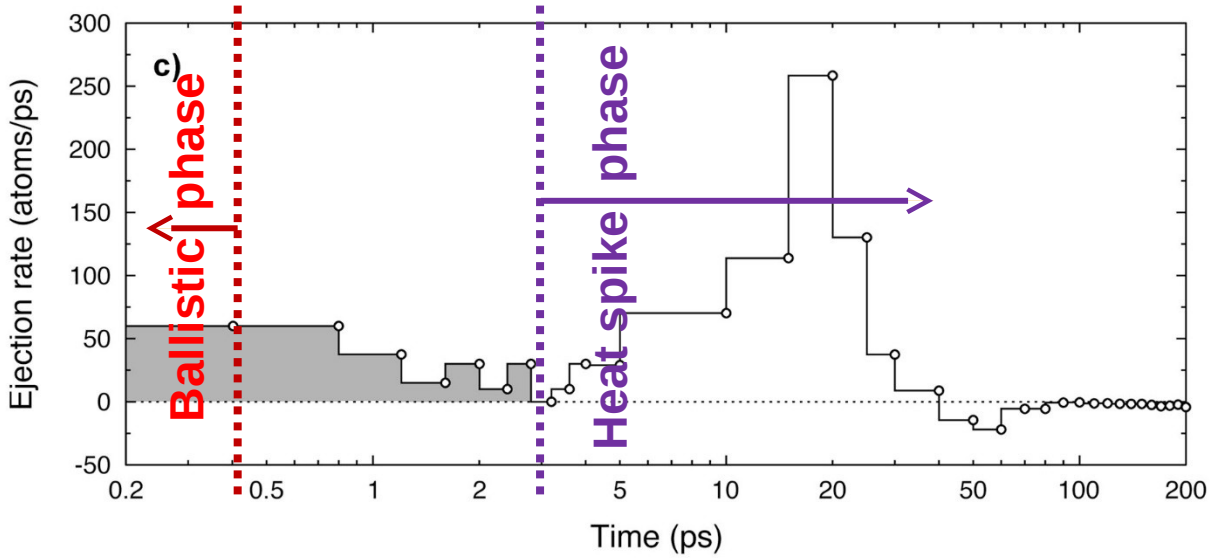
Explanation: Heat spike sputtering enhanced at surfaces

- We simulated ***exactly*** the experimental condition with MD
- We found major explosive emission of atoms due to heat spike sputtering
- Experimental Y ~ **1000**
- Simulated Y = **1000 ± 200**

[G. Greaves et al, Phys. Rev. Lett. 111 (2013) 065504]

Analysis of mechanism

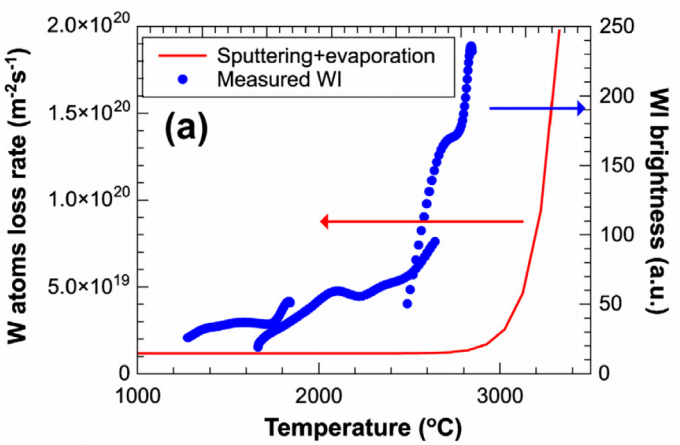
- Analysis of the time dependence shows the major sputtering is clearly a heat spike effect
  - Majority of sputtering late in cascade

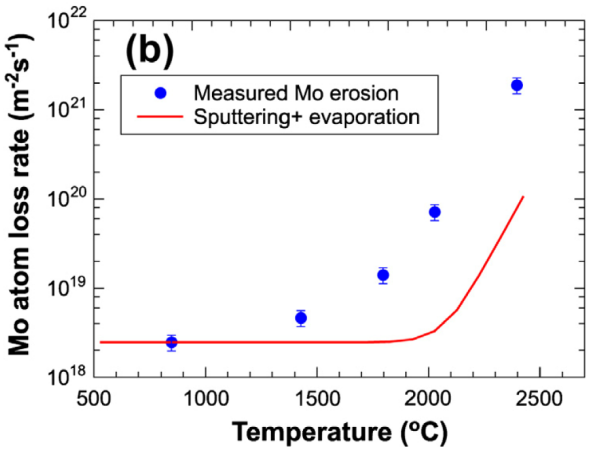


[G. Greaves et al, Phys. Rev. Lett. 111 (2013) 065504]

Enhanced sputtering at equilibrium high T

- In fusion reactors the inner surface materials are often quite hot, and hence knowing the sputtering yield from elevated temperatures is of interest.
- Results on 2 wall materials
  - Reasons not fully understood: simple equilibrium evaporation model not enough to explain result
  - Possible explanation: formation of loose adatoms that evaporate easier



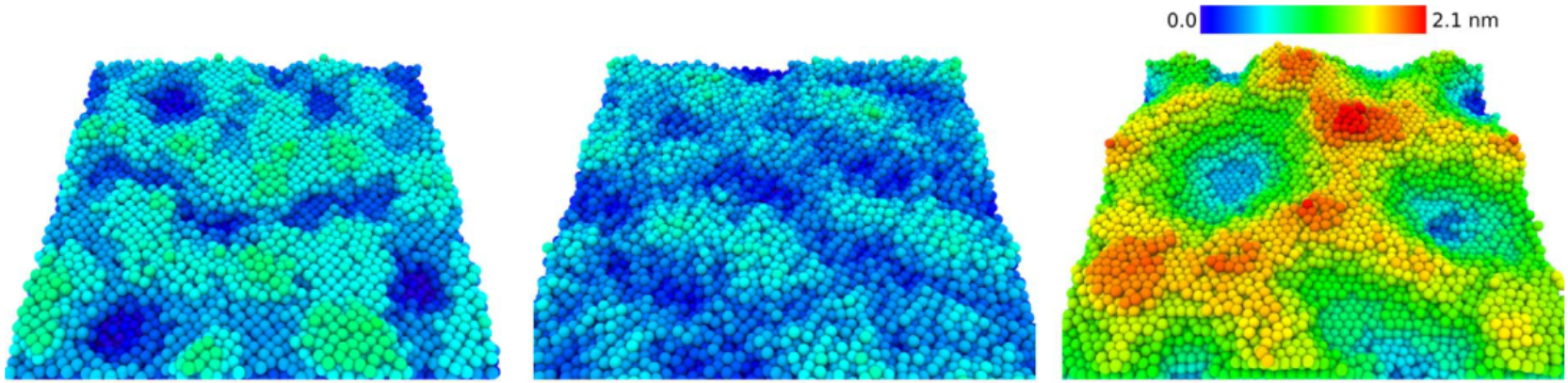


[Temmermann *et al*, JNM 438 (2013) 578]

Systematic studies of T effects on sputtering in Cu

- We examined systematically the self-sputtering of Cu at high temperatures (1200K), at different surface orientations, and for rough surfaces for CLIC conditions

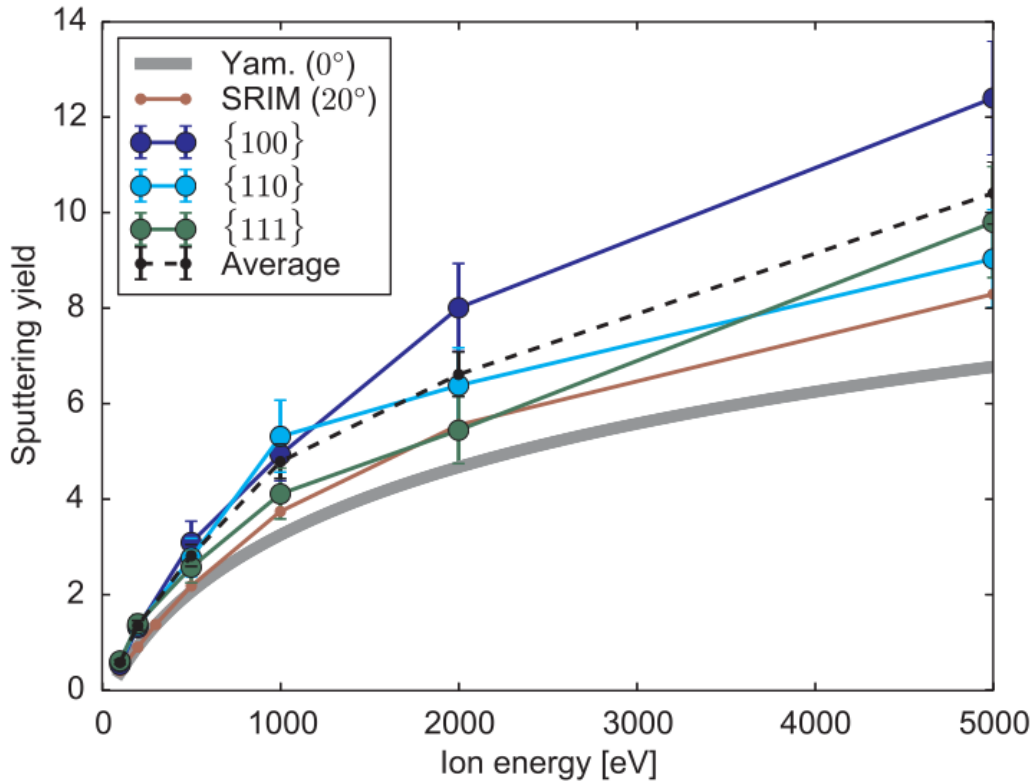
100 110 111



(a) (b) (c)

Results: surface orientation, 300 K

- The results depend on surface orientation, but not too strongly



Results on temperature dependence

- There is some enhancement of the sputtering with temperature – but the effect is weak and comparable to surface orientation effects

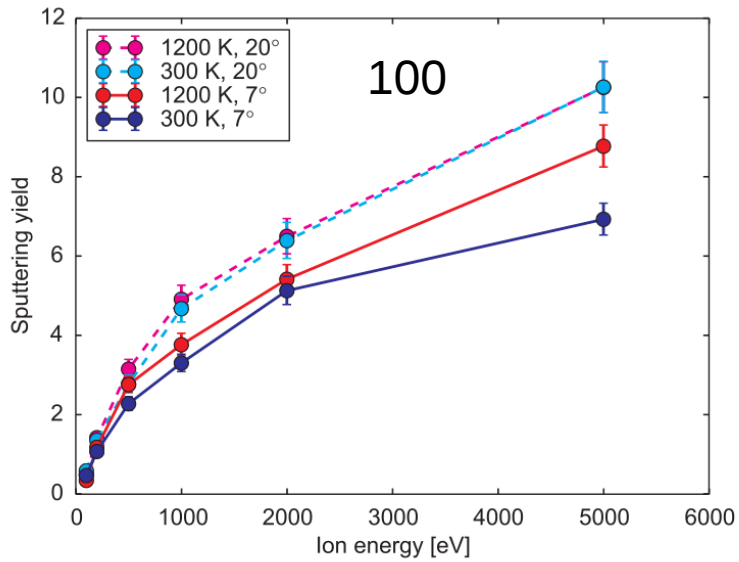


Fig. 10. Sputtering yield of Cu from the {1 0 0} surface irradiated at 300 K and 1200 K with $\theta = 7°$ and $\theta = 20°$ of incident angles.

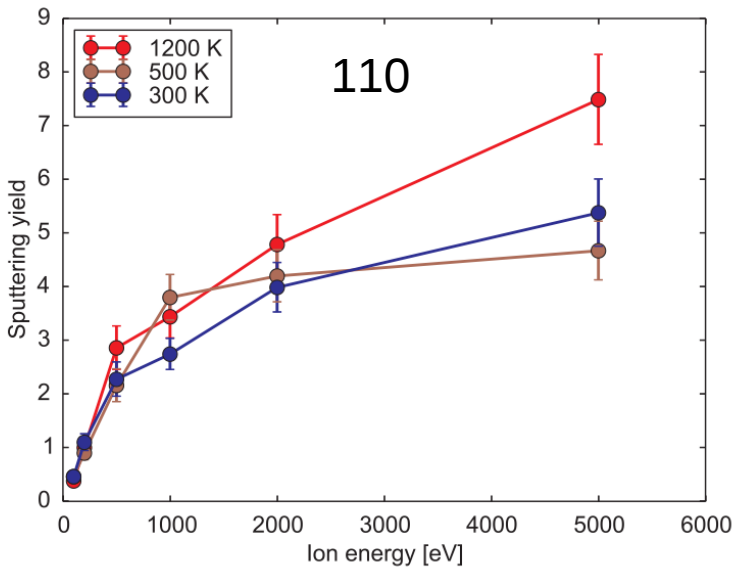
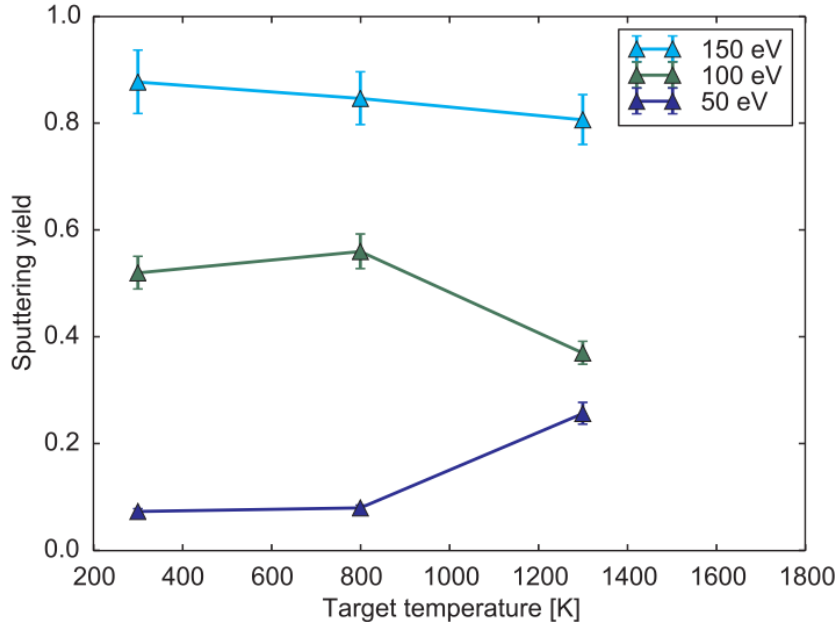


Fig. 11. Sputtering yield of Cu from the {1 1 0} face with $\theta = 7°$ at different temperatures.

Results on T dependence at low energies

- In a typical arc, the sheath potential is believed to be around ~100 eV
- At these energies, the T effect is weak and can go in both directions:



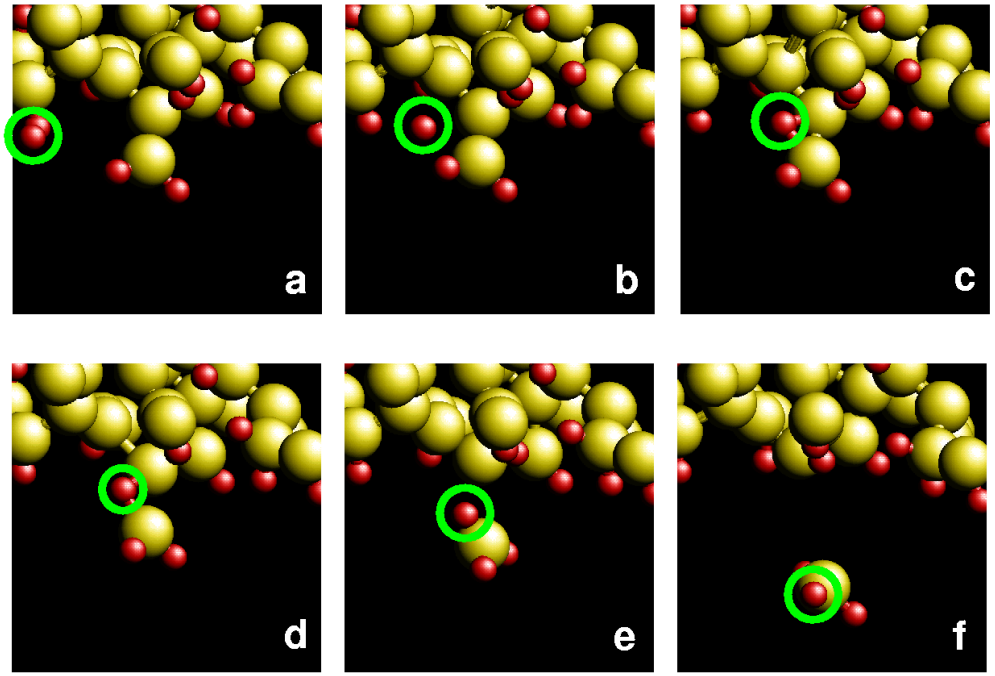
Conclusions

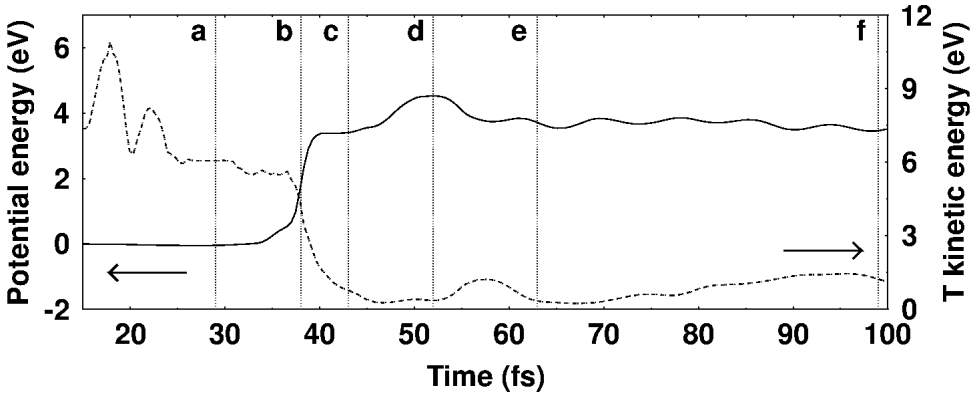
- Heat spike effects can strongly enhance sputtering yields
- Also enhanced evaporation of adatoms can enhance ’sputtering’
- The current work shows the prompt sputtering by single ion impacts on an equilibrated surface; the T effects are weak, however
- Hence the enhanced sputtering needed to feed an arc plasma are likely due to either overlapping cascades [Timko, PRB 2009] or enhanced evaporation due to high T
  - Or a combination of both

Backup slides

Chemical effects: swift chemical sputtering of carbon

- In 1999-2000 we found that if an H ion hits the middle of a C-C bond, it raises the energy enough to break the chemical bond
- Process is energetically unfavorable (endothermal) – barrier too high for thermal evaporation.
- Fulfills Peter Sigmunds definition of sputtering (cf. first talk this morning)
- But not binary collision!
- We named this mechanism ***swift chemical sputtering***

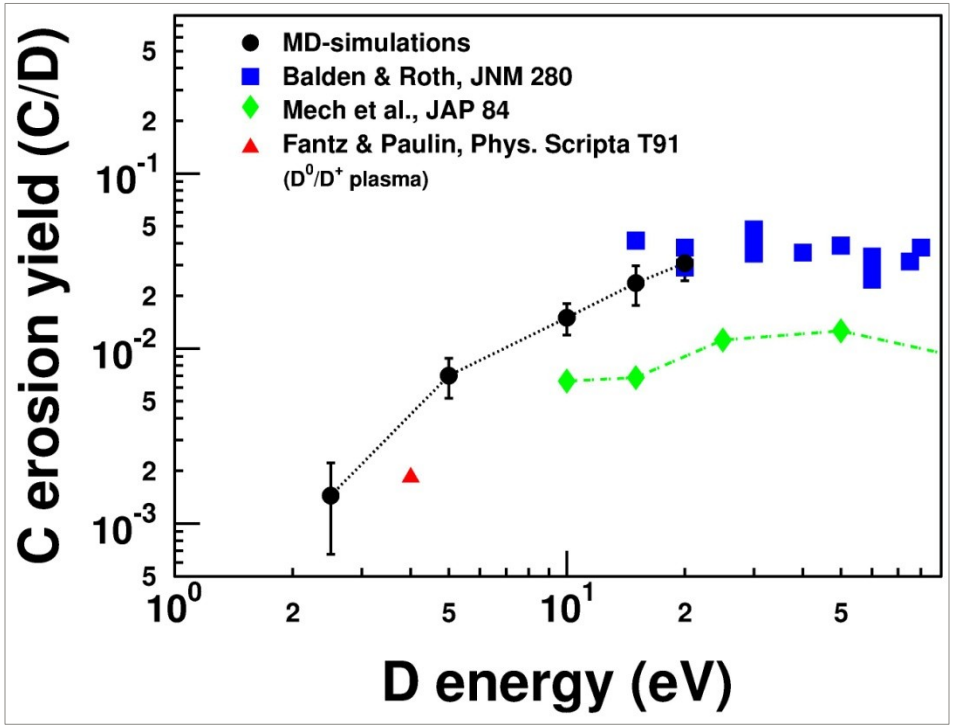




[Salonen et al, Europhys. Lett. 52 (2000) 504; Phys. Rev. B 63 (2001) 195415; A. Krasheninnikov et al, Comput. Mater. Sci. 25 (2004) 427]

Swift chemical sputtering of carbon

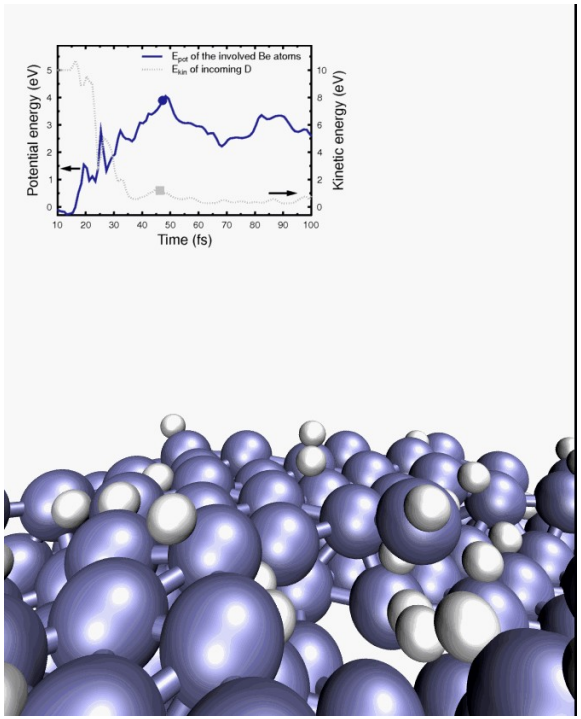
- The sputtering we observed is in decent agreement with experiments!
  - Even better agreement demonstrated later by P. Krstic [ORNL]
- At higher E and T also other mechanisms certainly are active

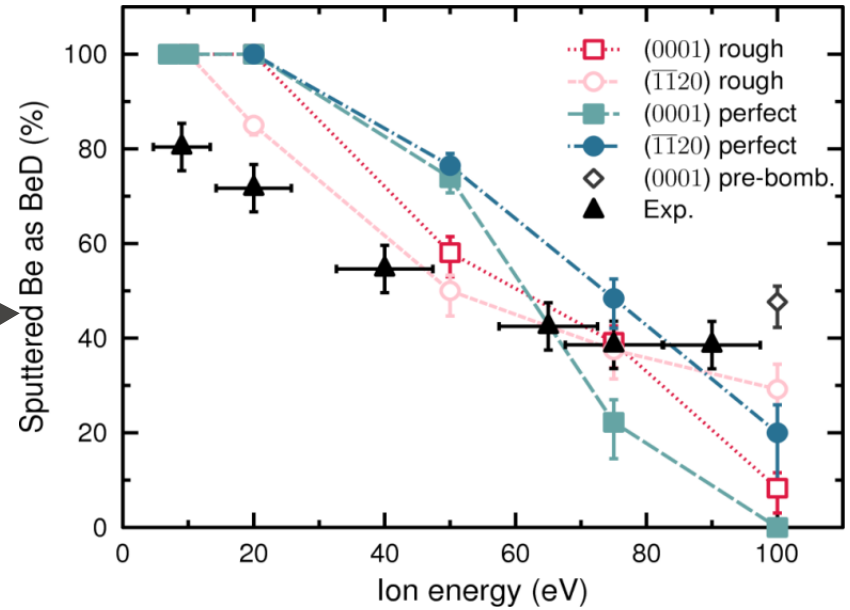


[Salonen, Physica Scripta T111 (2004) 133; Krasheninnikov et al, Comput. Mater. Sci. 25 (2004) 427; Nordlund et al, Pure and Appl. Chem. 78 (2005) 1203]

Swift chemical sputtering of metals

- **Using classical molecular dynamics and experiments, we showed in 2009-2011 that also pure metals can sputter chemically**
  - 10 – 100 eV D on Be





[Björkas et al, New J. Phys. 11, 123017 (2009); Nordlund et al, NIM B 269, 1257 (2011)]