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

Diagram:
- Sputtering
- Linear cascade
- Heat spikes
- Material
- Ion penetration depth
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

Results do depend on interatomic potential, though


[Expt: Szymczak and Wittmaack]
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

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 $Y \sim 1000$
- Simulated $Y = 1000 \pm 200$

Analysis of mechanism

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

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.
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 \{100\} surface irradiated at 300 K and 1200 K with $\theta = 7^\circ$ and $\theta = 20^\circ$ of incident angles.

Fig. 11. Sputtering yield of Cu from the \{110\} face with $\theta = 7^\circ$ 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:

![Graph showing the relationship between target temperature and sputtering yield for different energies.](image-url)
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 Sigmund’s definition of sputtering (cf. first talk this morning).
- But not binary collision!
- We named this mechanism **swift chemical sputtering**

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

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