



Molecular Dynamics Simulations of Ion Irradiation of a Surface under an Electric Field

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Ion irradiation during breakdown

- Breakdown: plasma above surface
- Ions from the plasma are accelerated towards the surface
 - Irradiation
- Plasma sheath, strong electric field
- Irradiation in general is well studied, but what about irradiation under breakdown conditions?
 - Plasma sputtering invented in 1852, but still little data?



What I will tell you

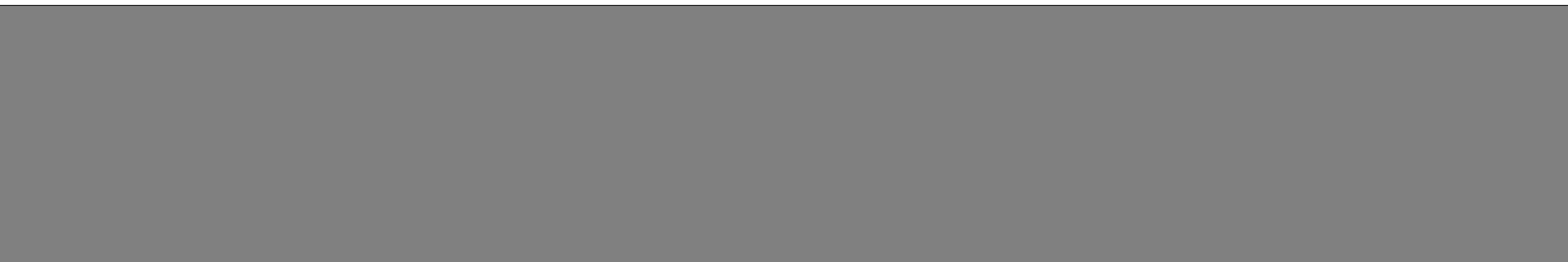
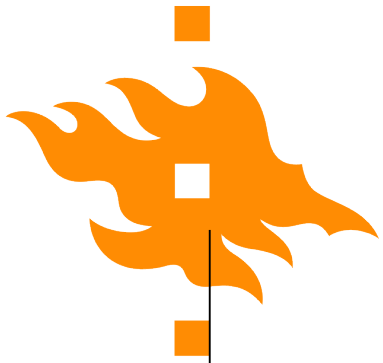
- Sputtering yield (=sputtered atoms/incident ions) is modified by:
 - The presence of an electric field
 - Surface features (e.g. protrusions)
 - Also modifies local flux
- Relevance for breakdown research: plasma is maintained by sputtered atoms
 - Input for plasma simulations
 - So far these have not included the modified yields



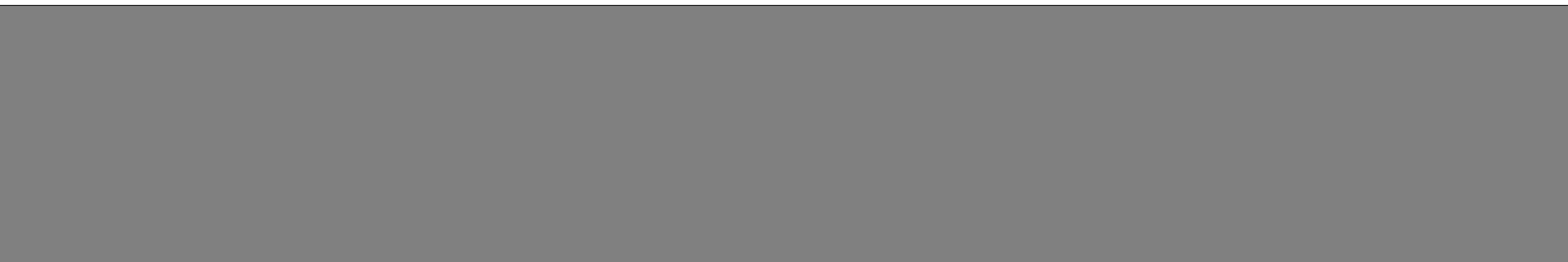
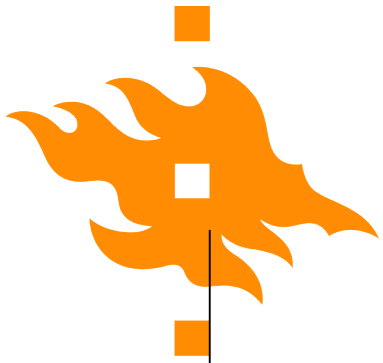
The modeled system

- Flat surface, flat surface w/ protrusion
- Cu^+ ions on Cu surface perpendicular to surface
- DC - constant electric field
- Room temperature
- “Low” flux (No multiple hits in same spot)
- Hybrid Molecular Dynamics - Electrodynamics
 - See Flyura's talk for details

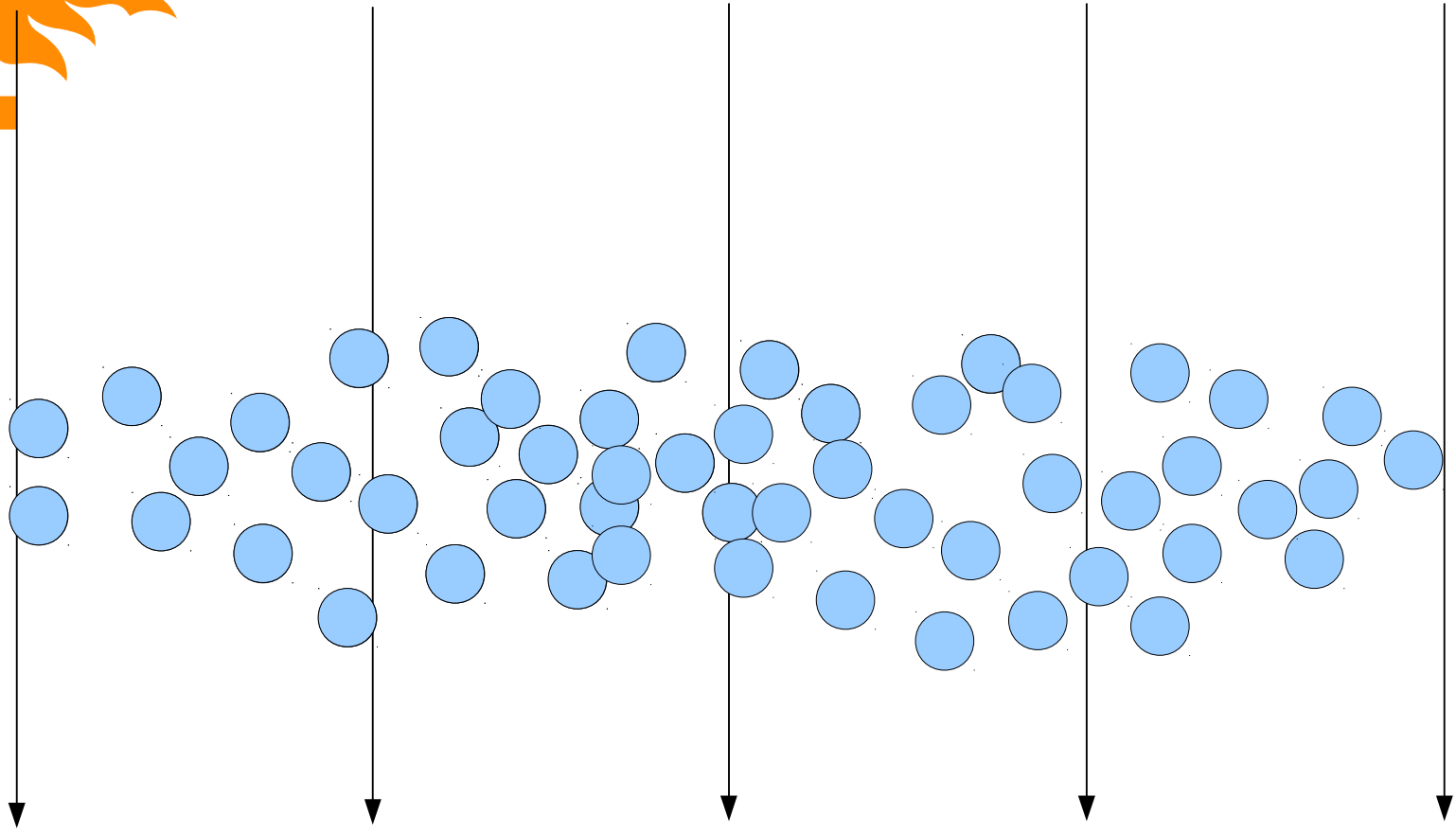
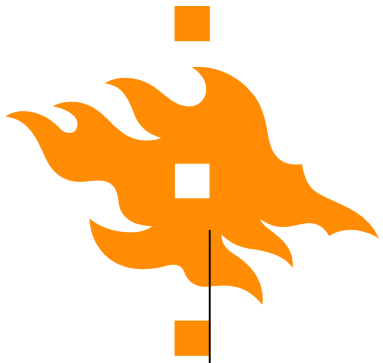
Plasma-surface interaction



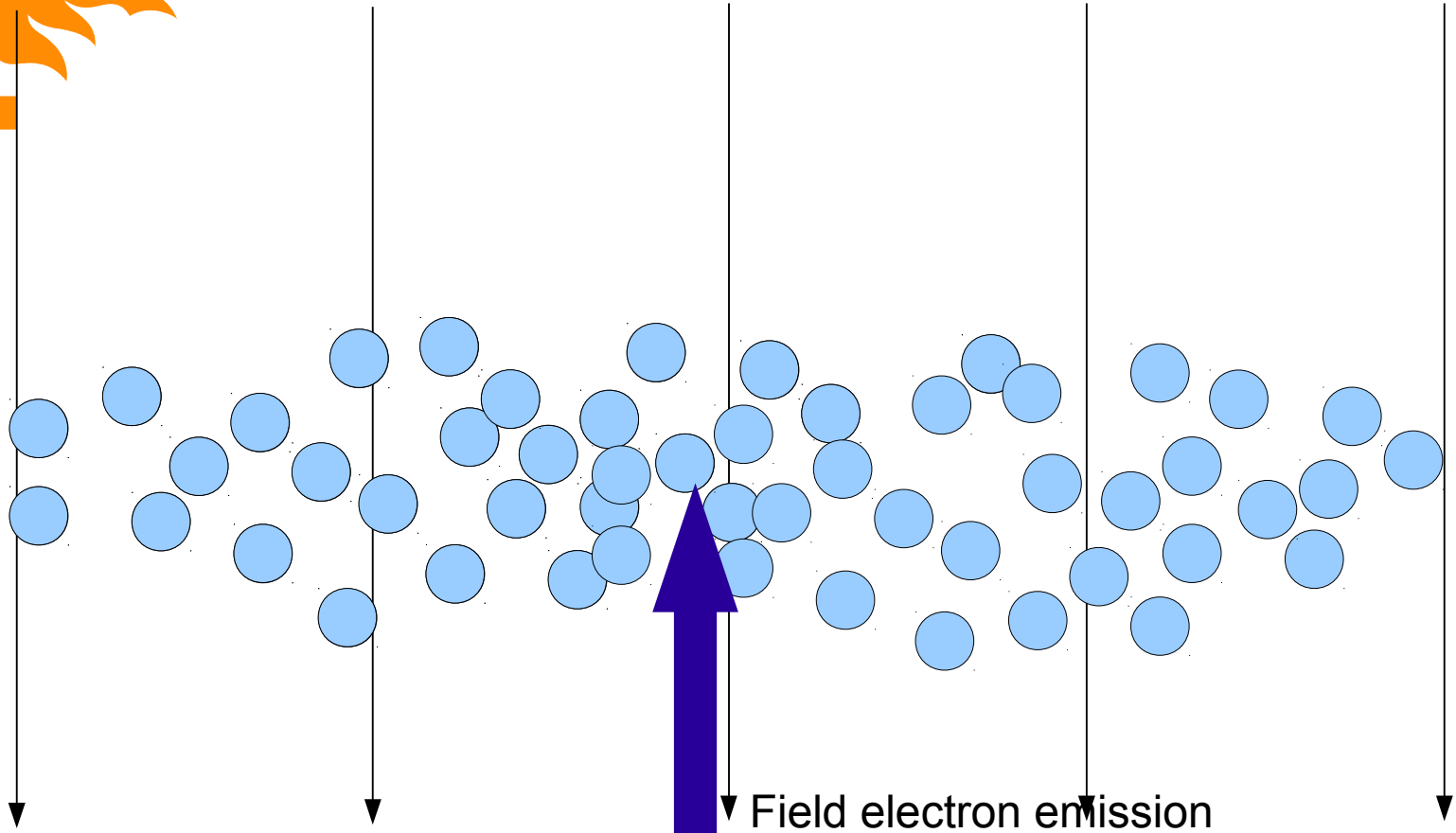
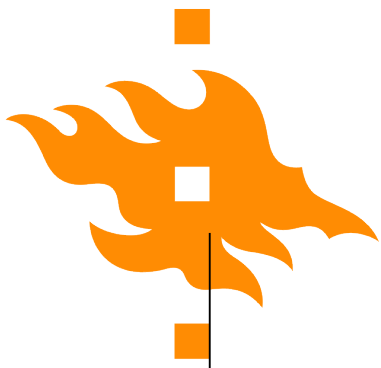
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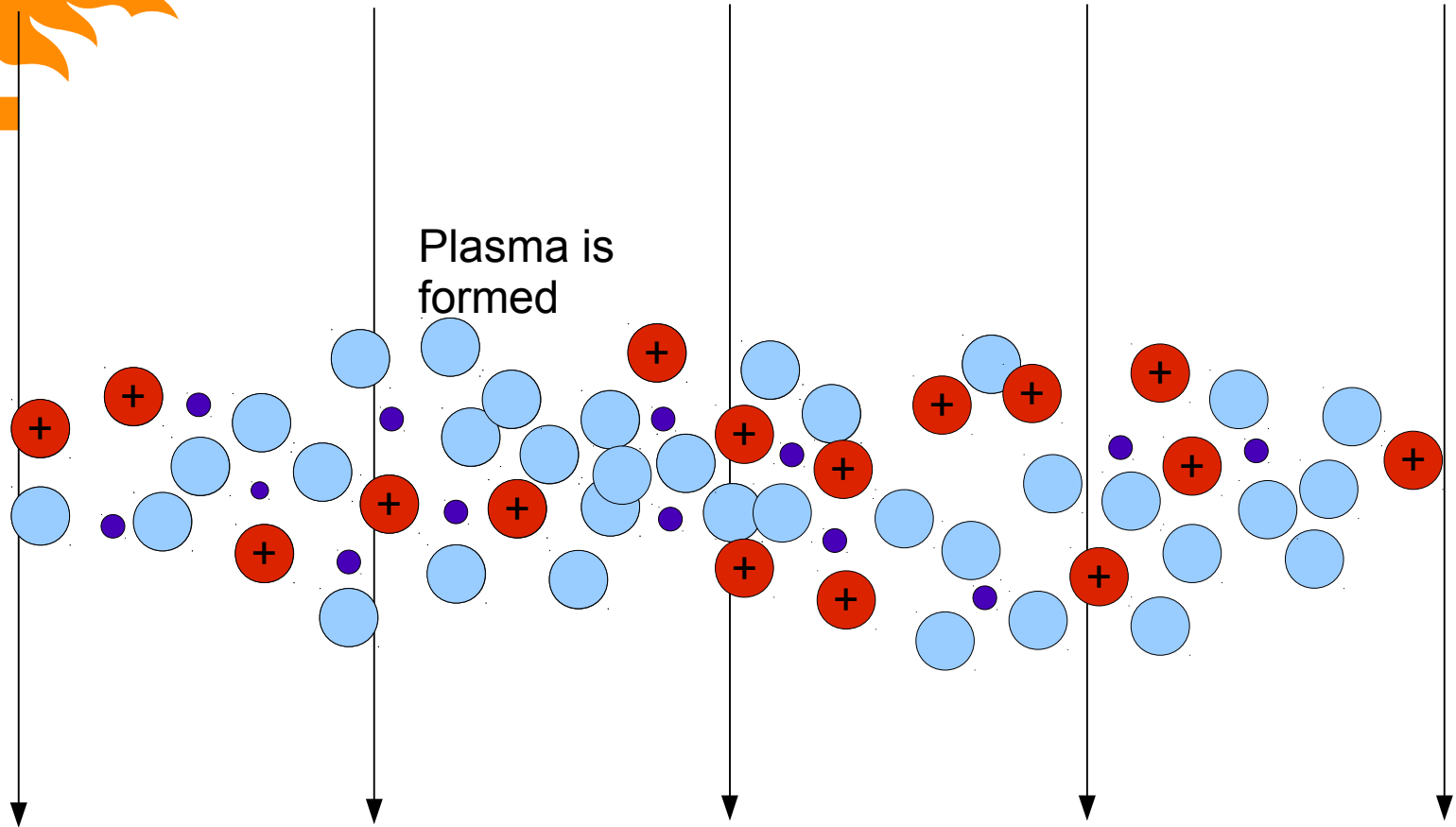
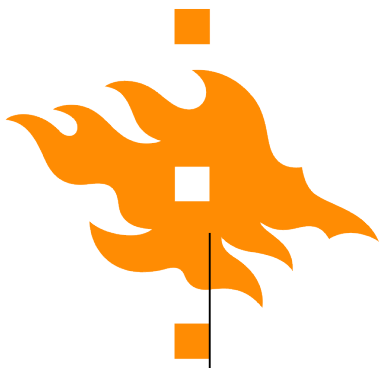


Plasma-surface interaction

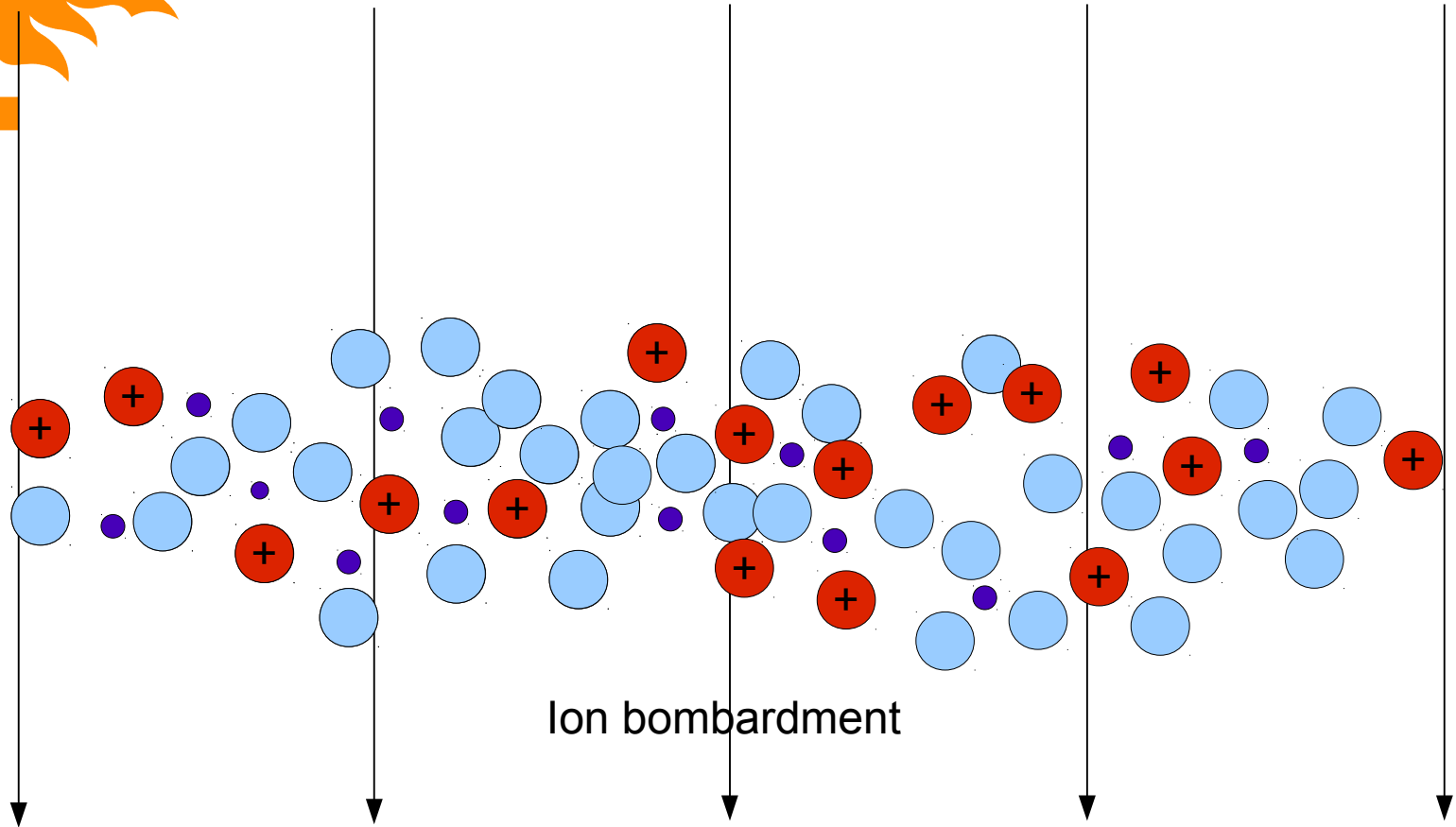
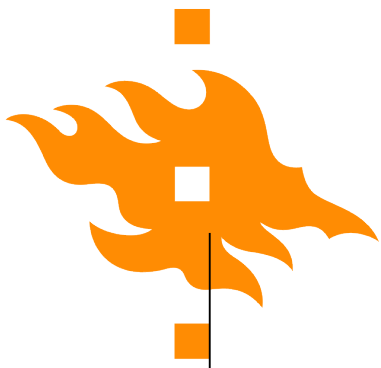


Field electron emission

Plasma-surface interaction

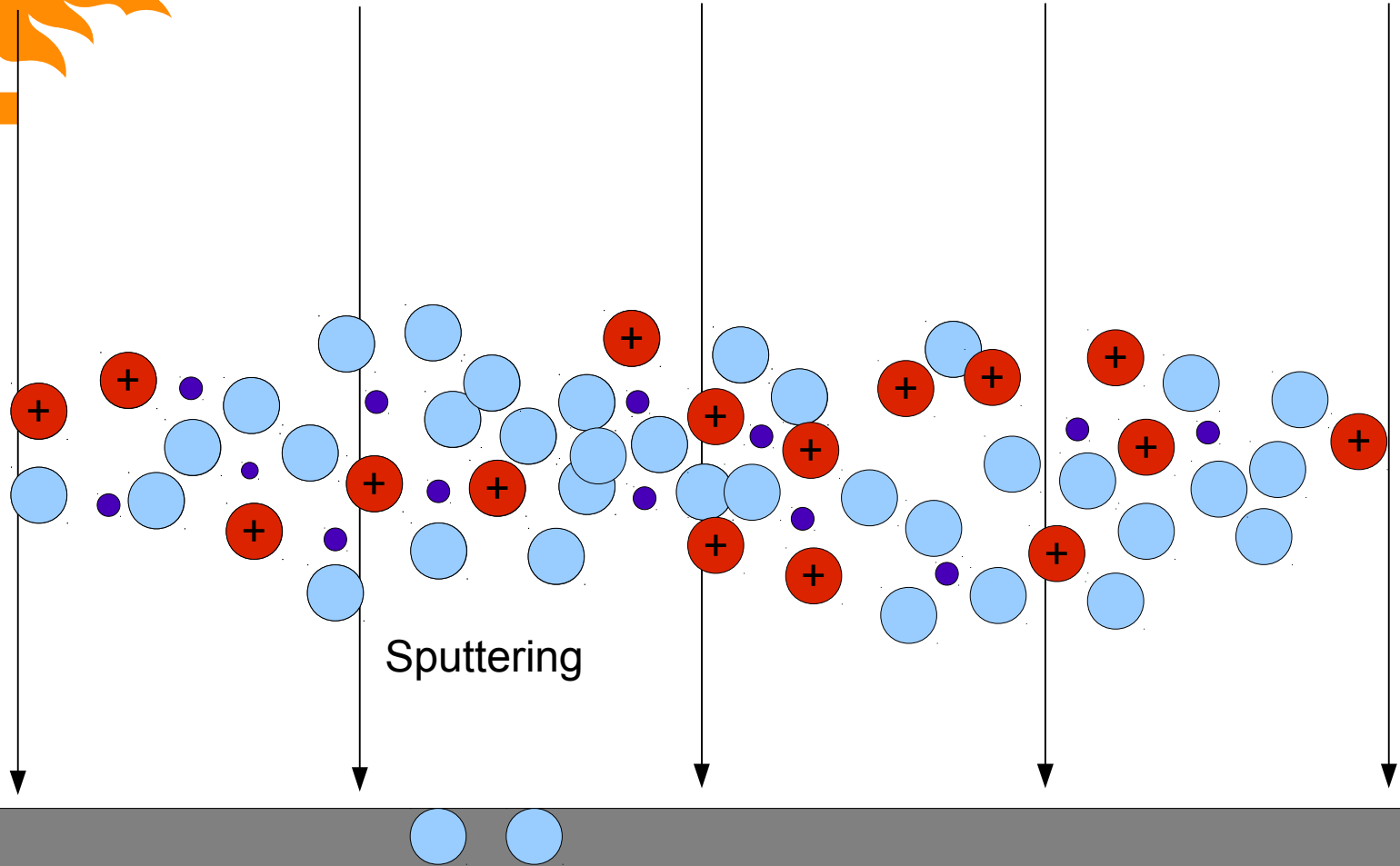
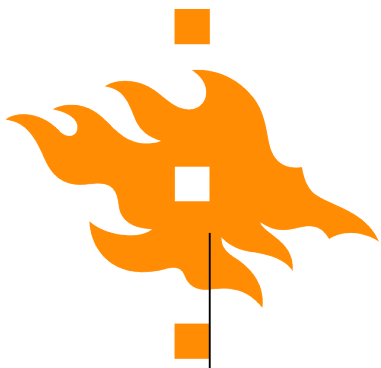


Plasma-surface interaction

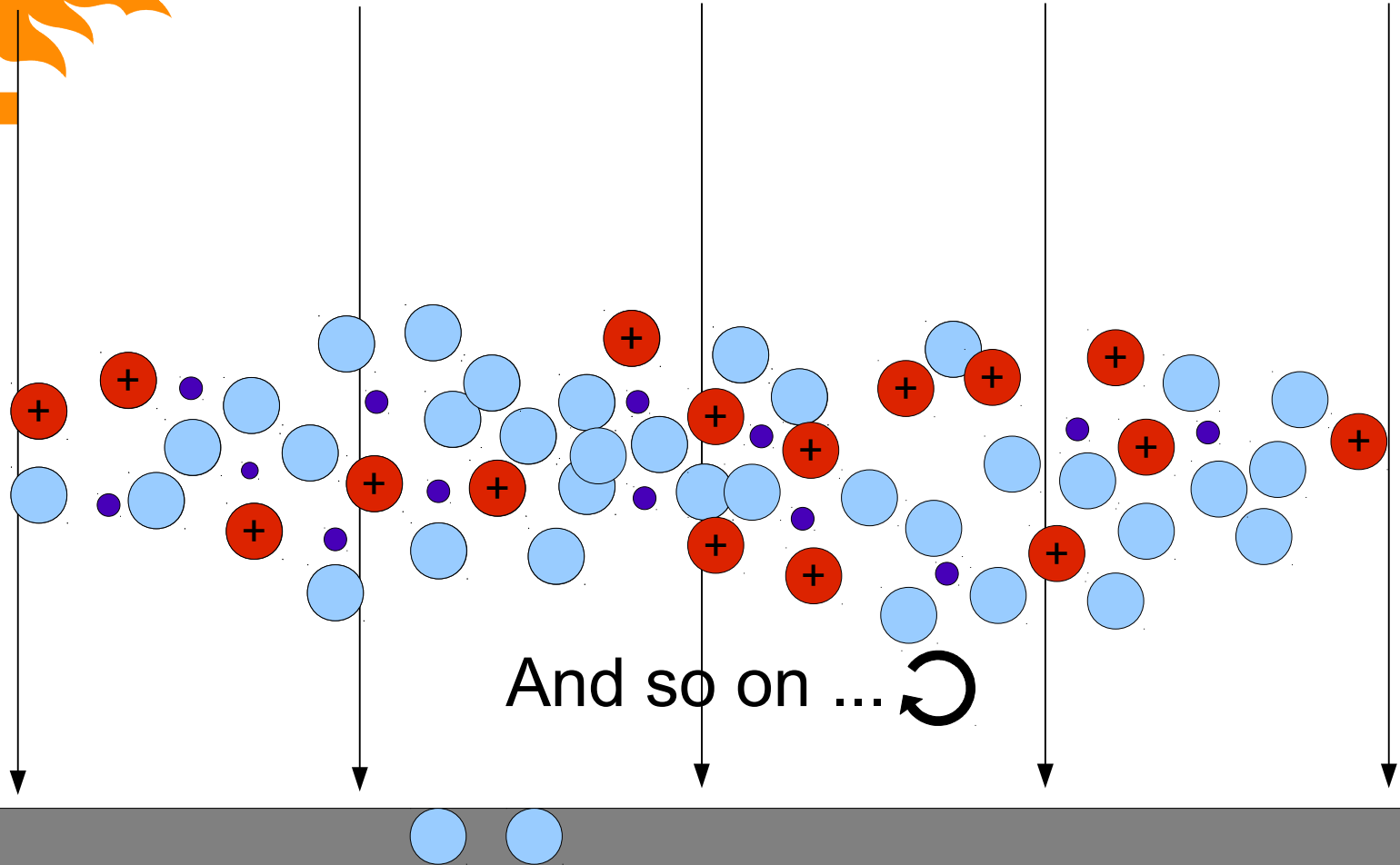
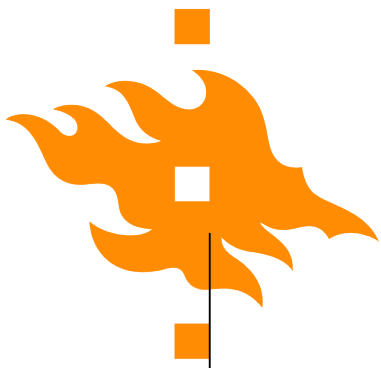


Ion bombardment

Plasma-surface interaction



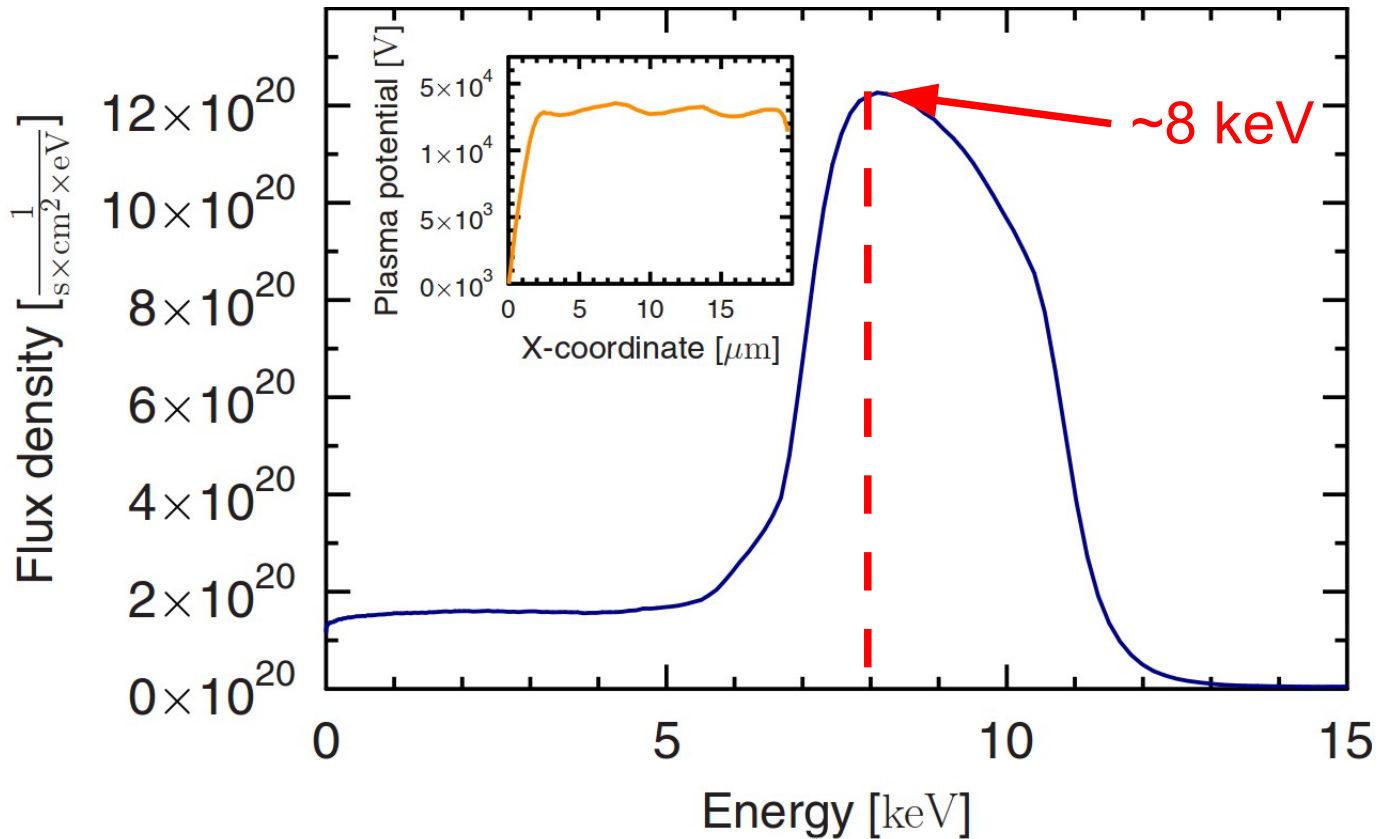
Plasma-surface interaction



And so on ... ↻



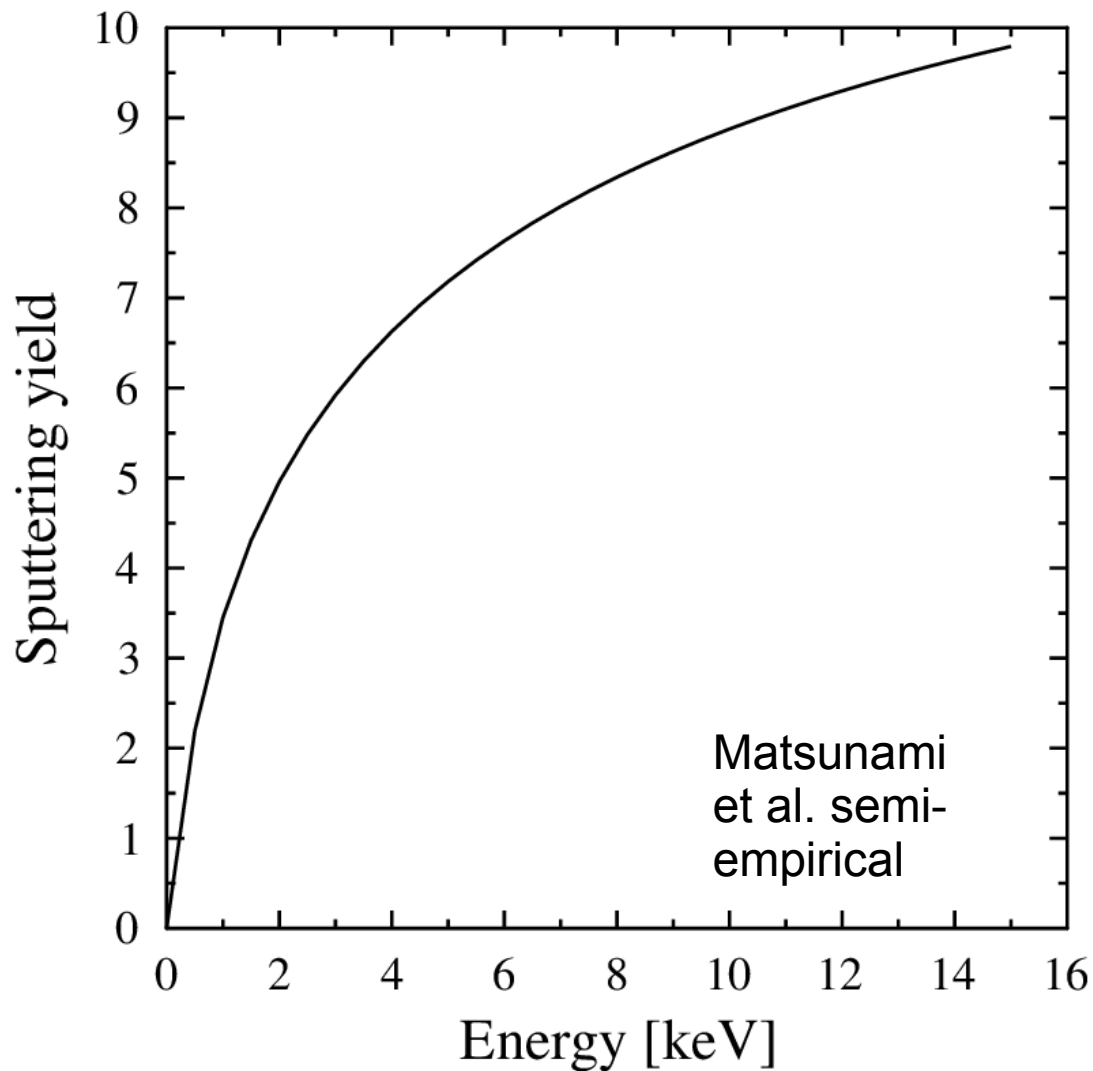
Energy of incident ions

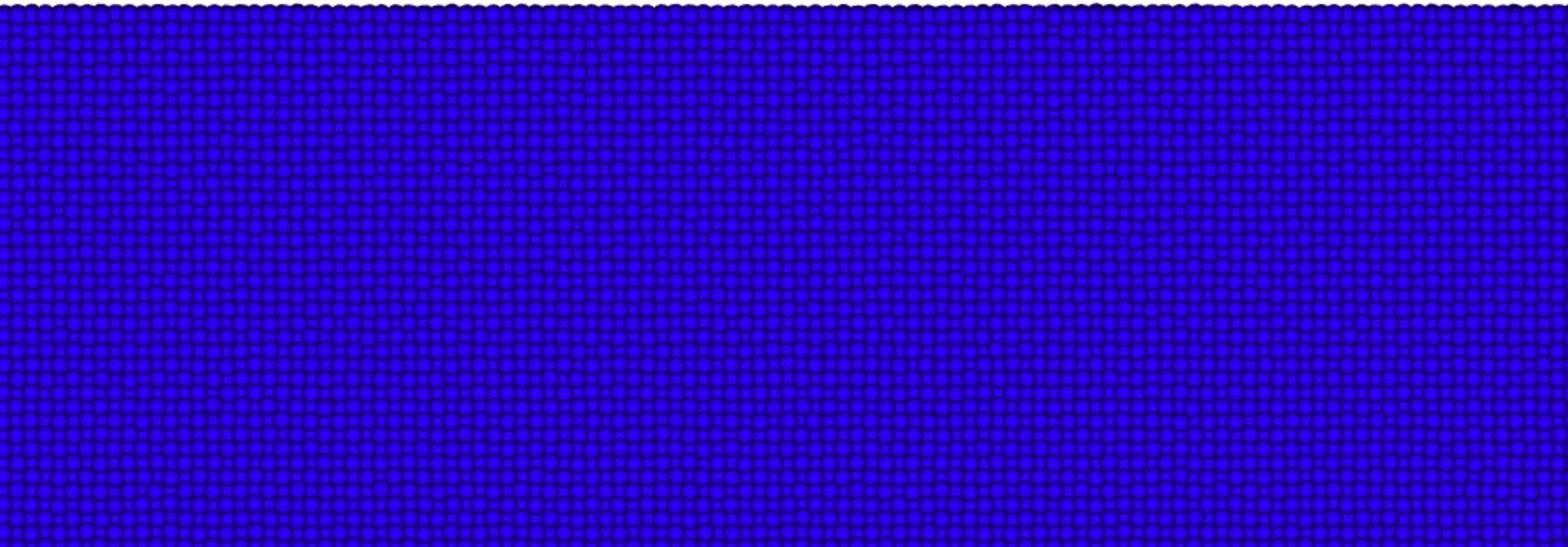


(H. Timkó)

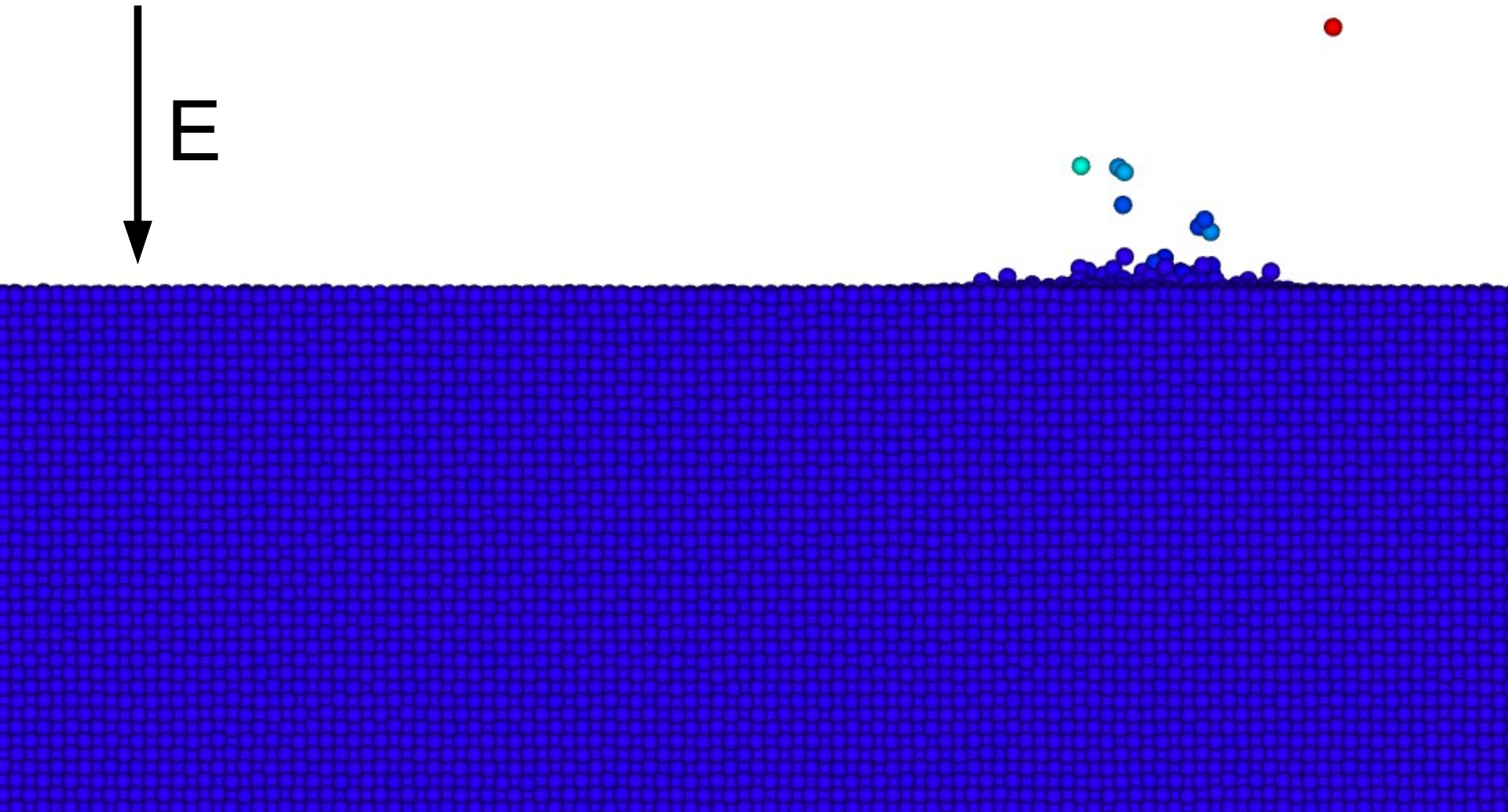


Sputtering yield (Cu on Cu)





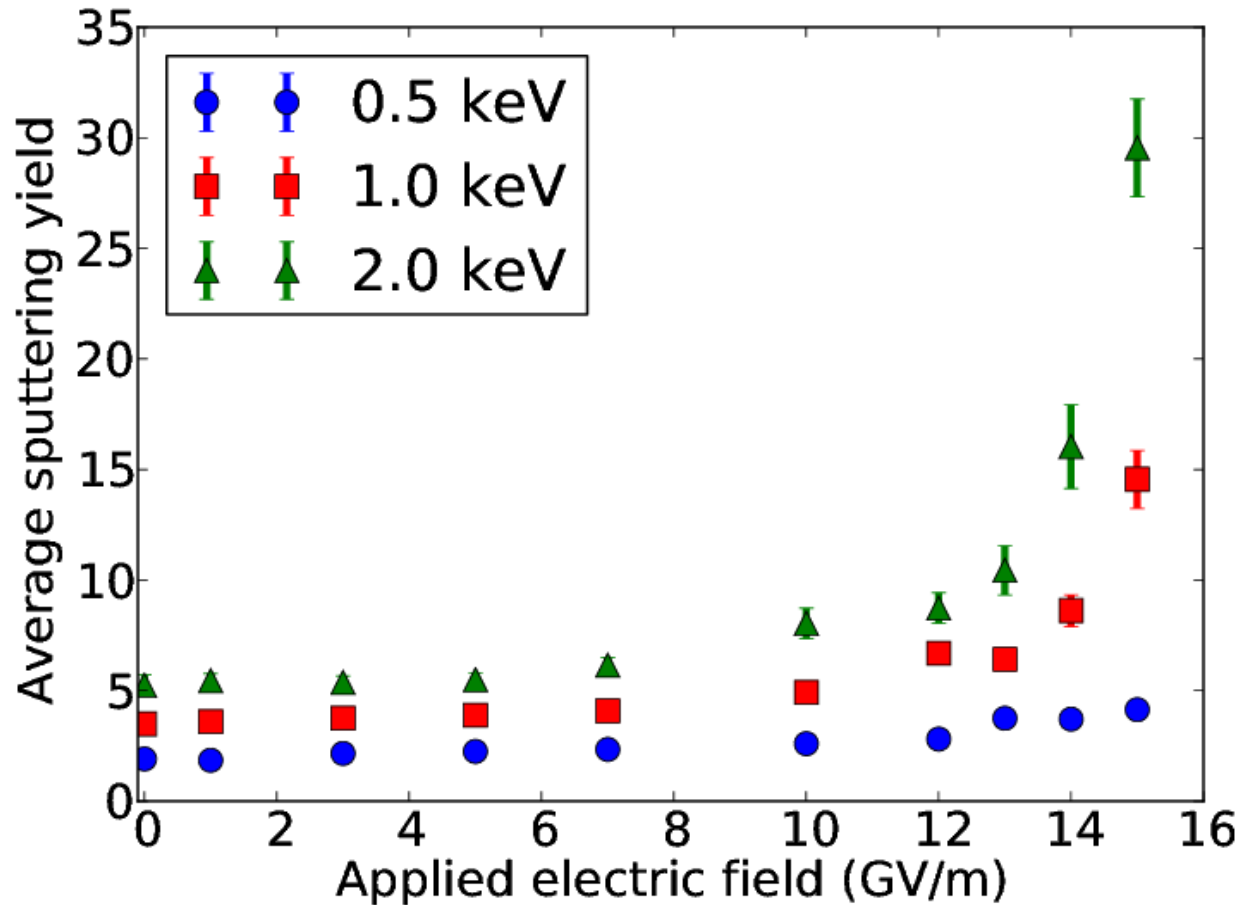
Color indicates kinetic energy

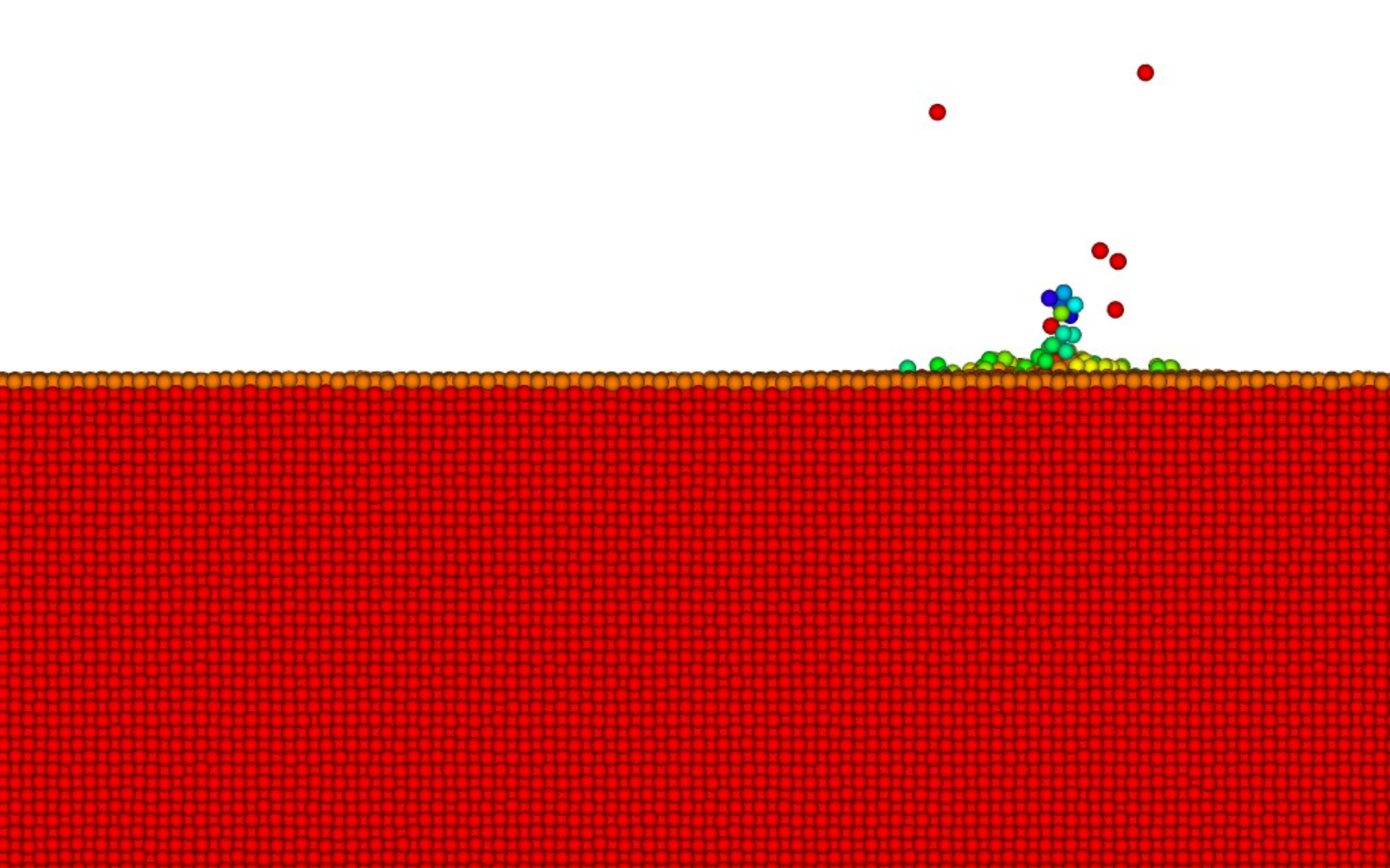


Color indicates kinetic energy

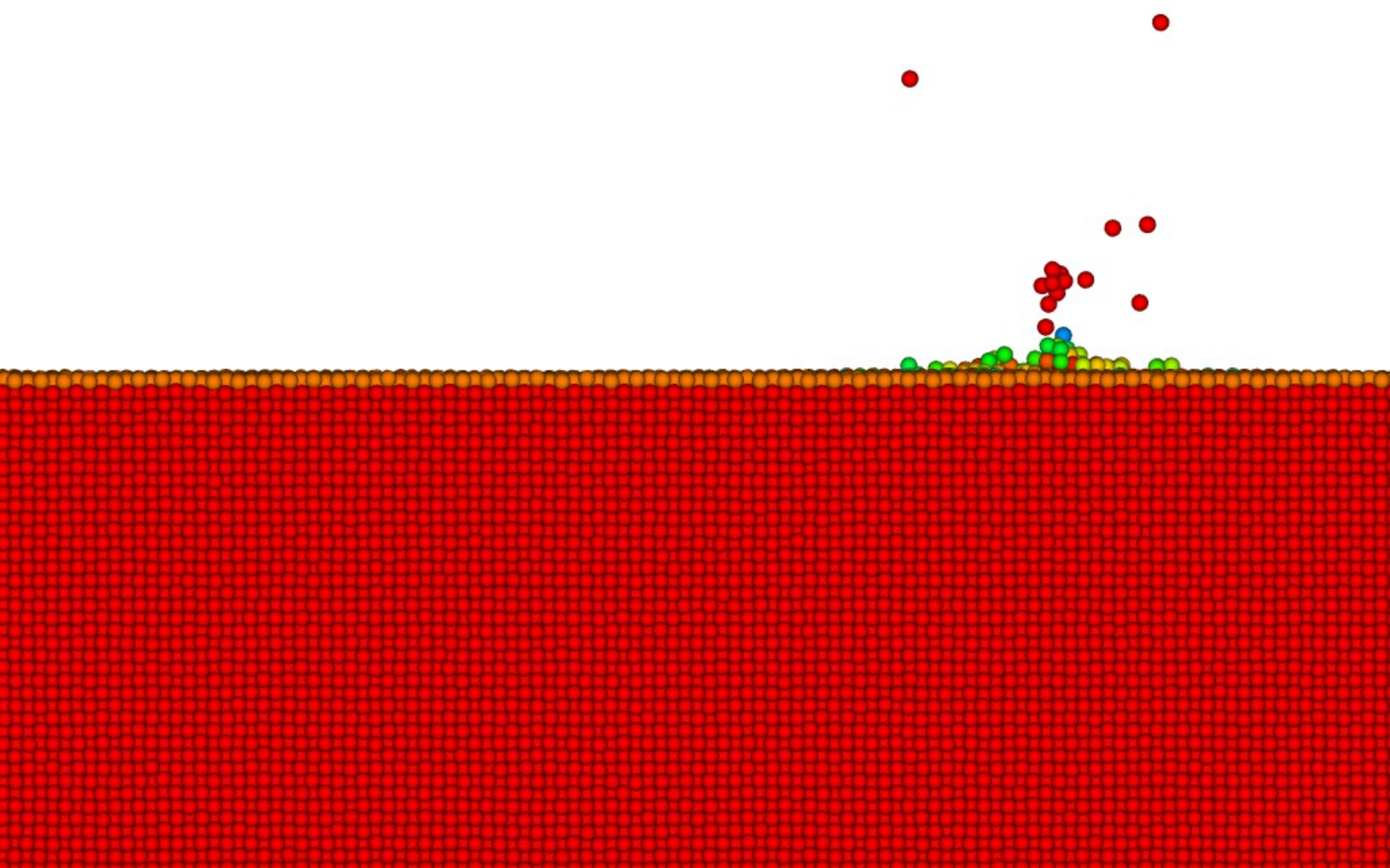


Sputtering yield vs. field





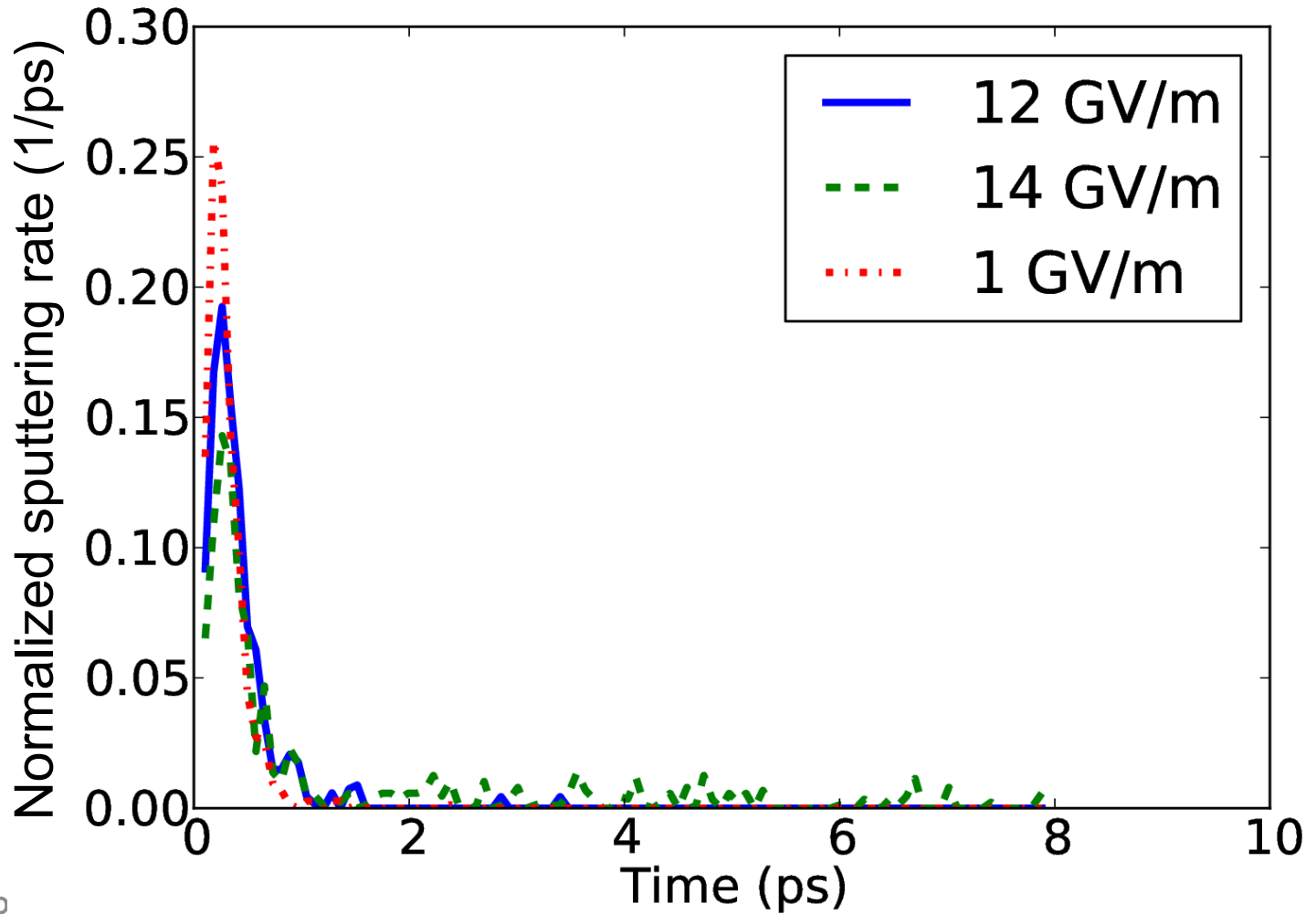
Color indicates charge



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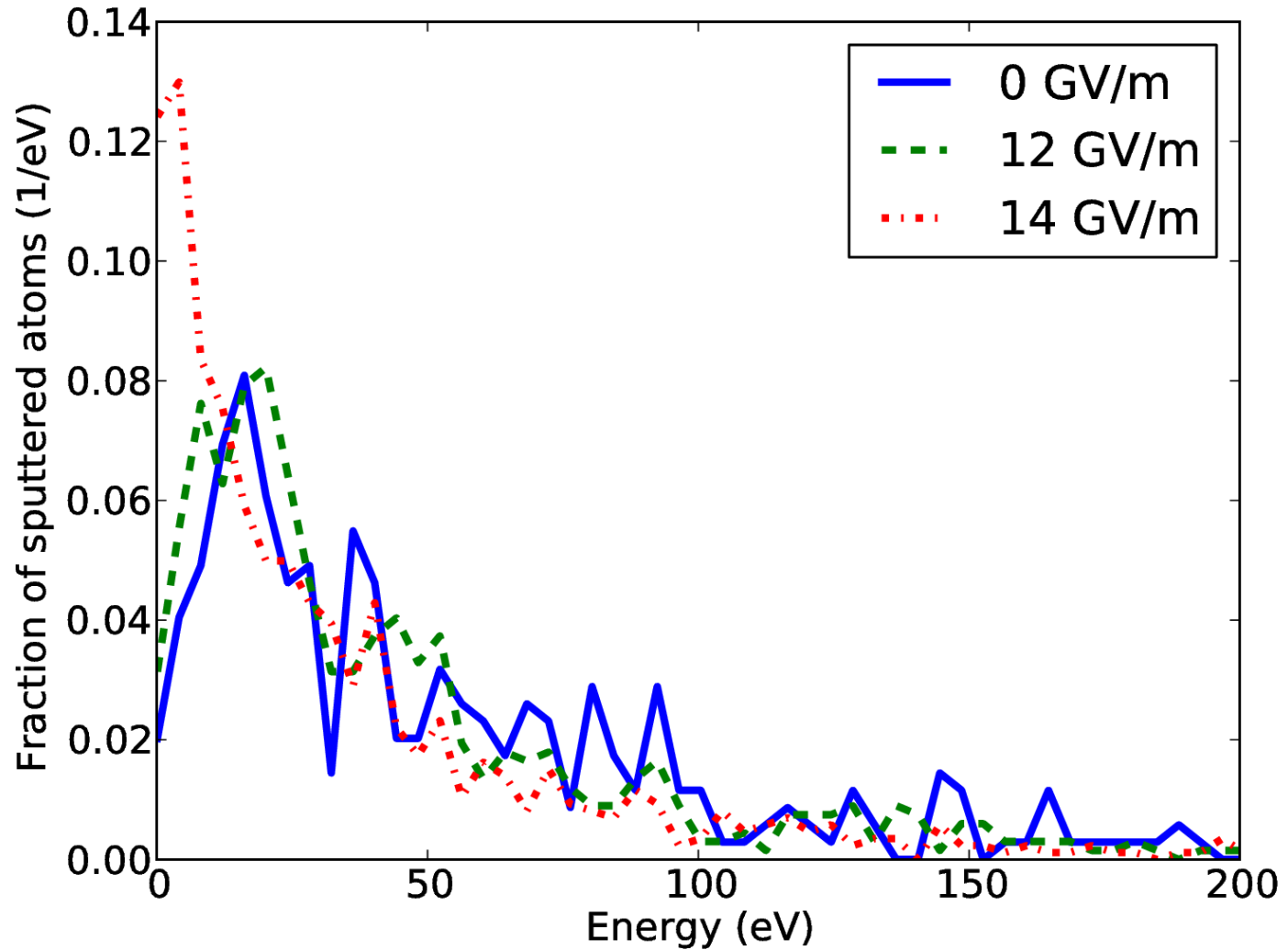


Sputtering or evaporation?



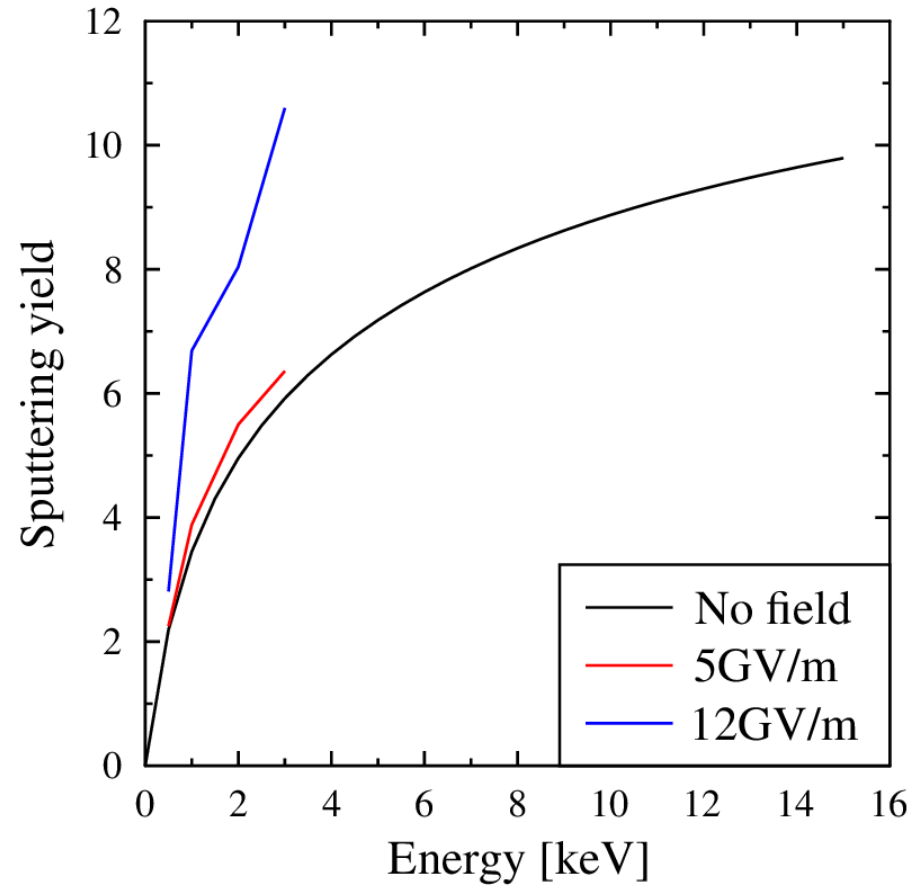


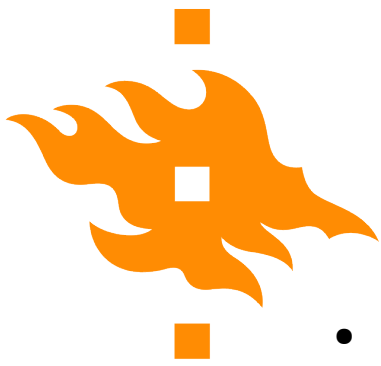
Sputtering or evaporation?





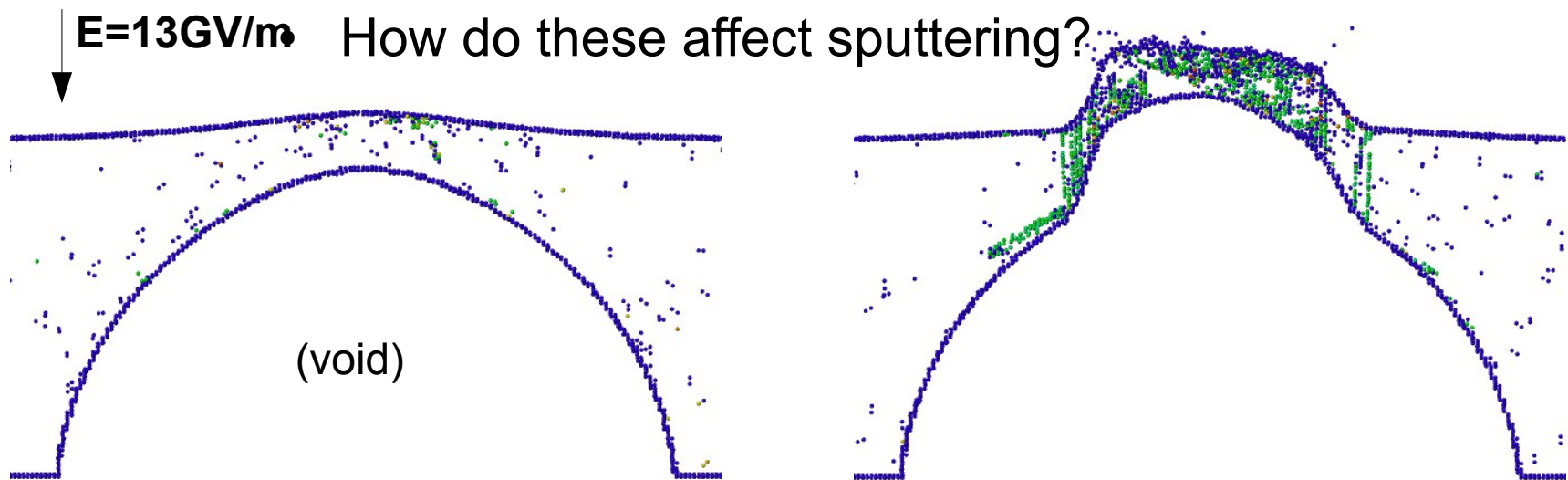
Modified sputtering yield



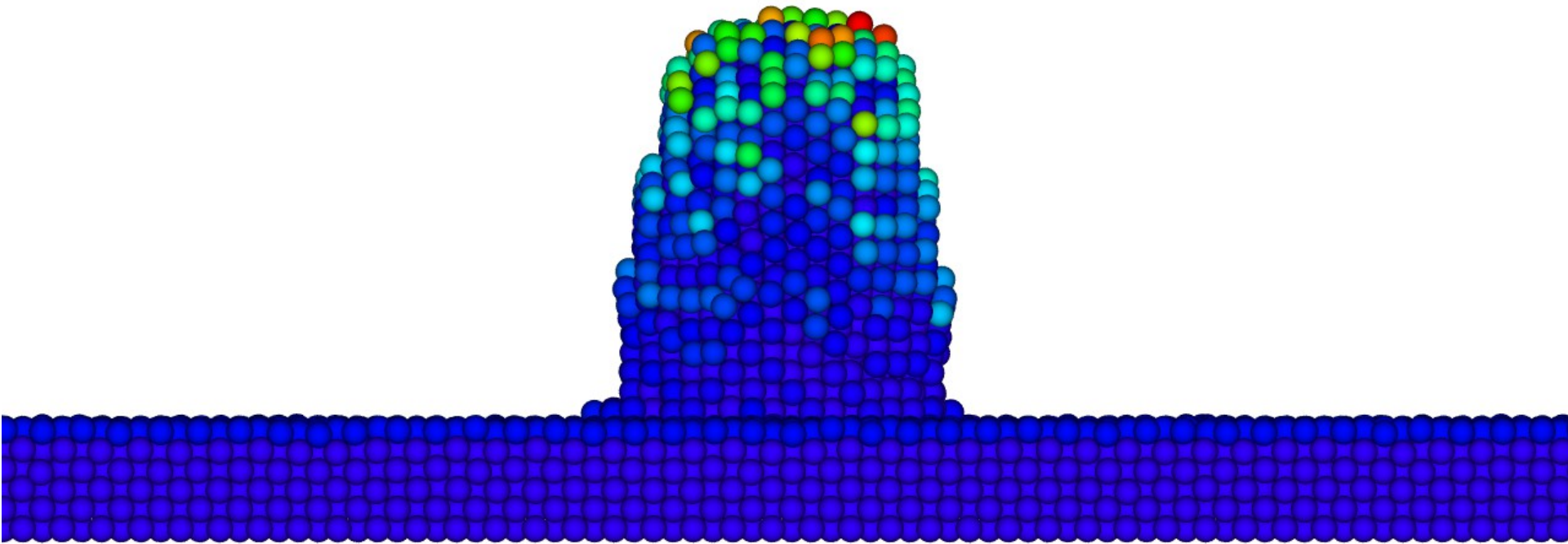


Surface features

- Field emitters are present on surface
- e.g. Protrusions may appear on an initially flat surface in the presence of a strong electric field

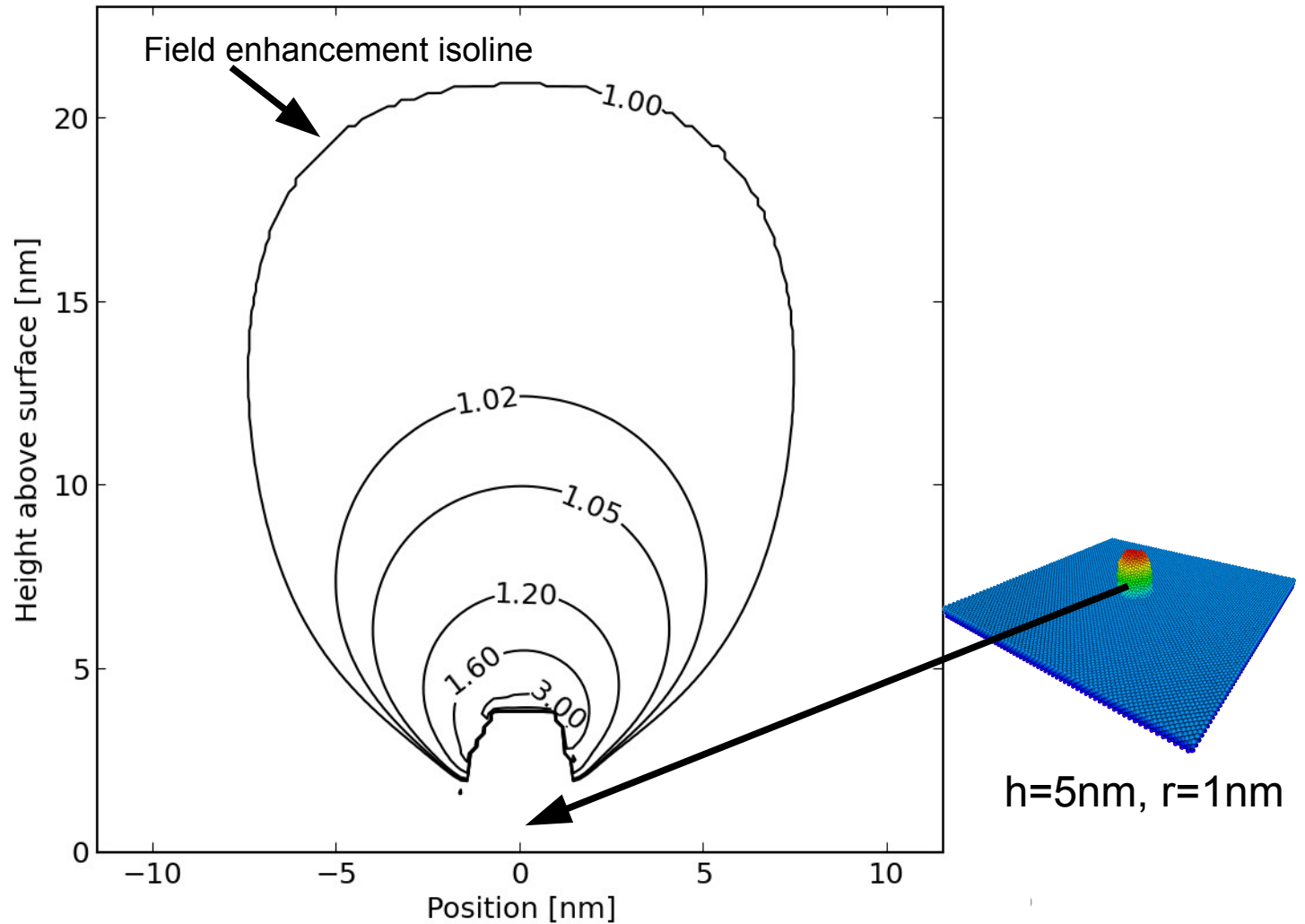


A. Pohjonen et al., J. Appl. Phys. 114, 033519 (2013)



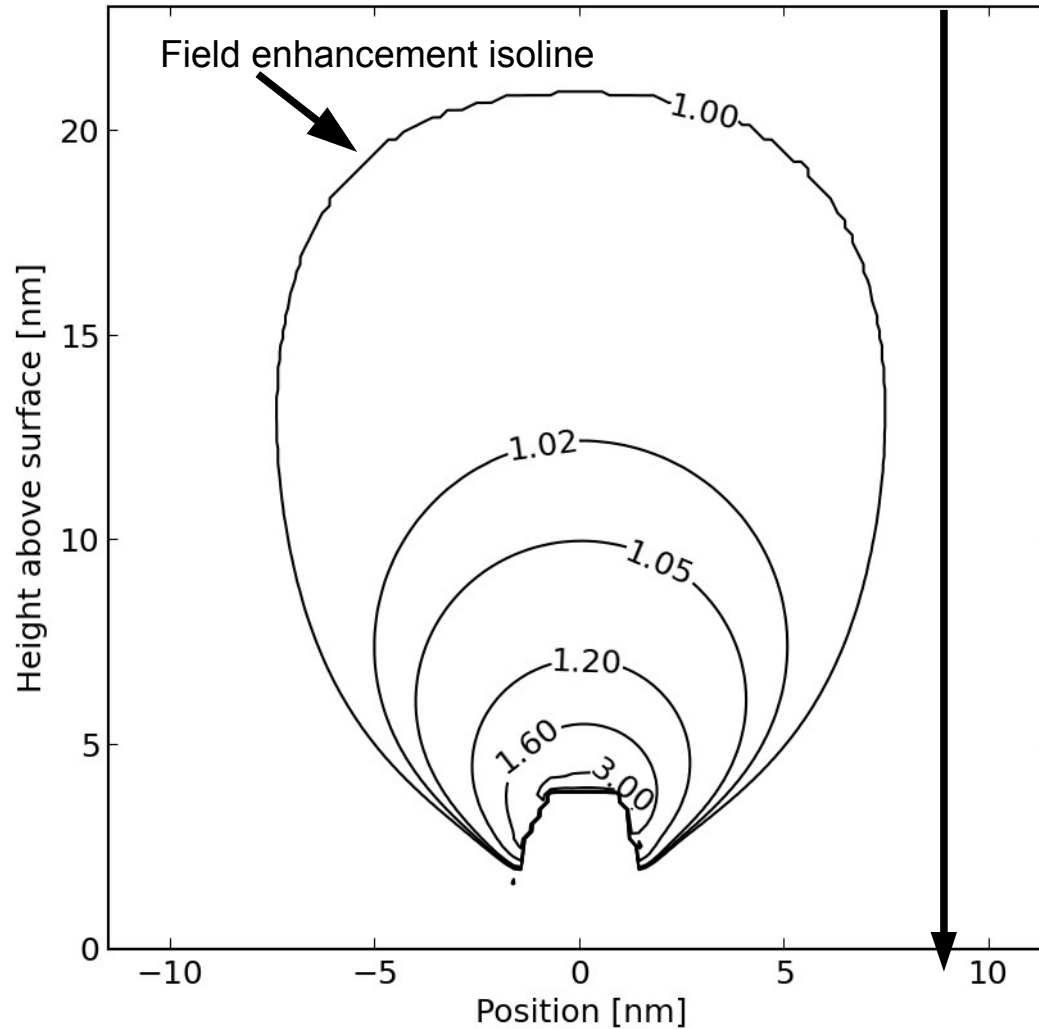


Surface features





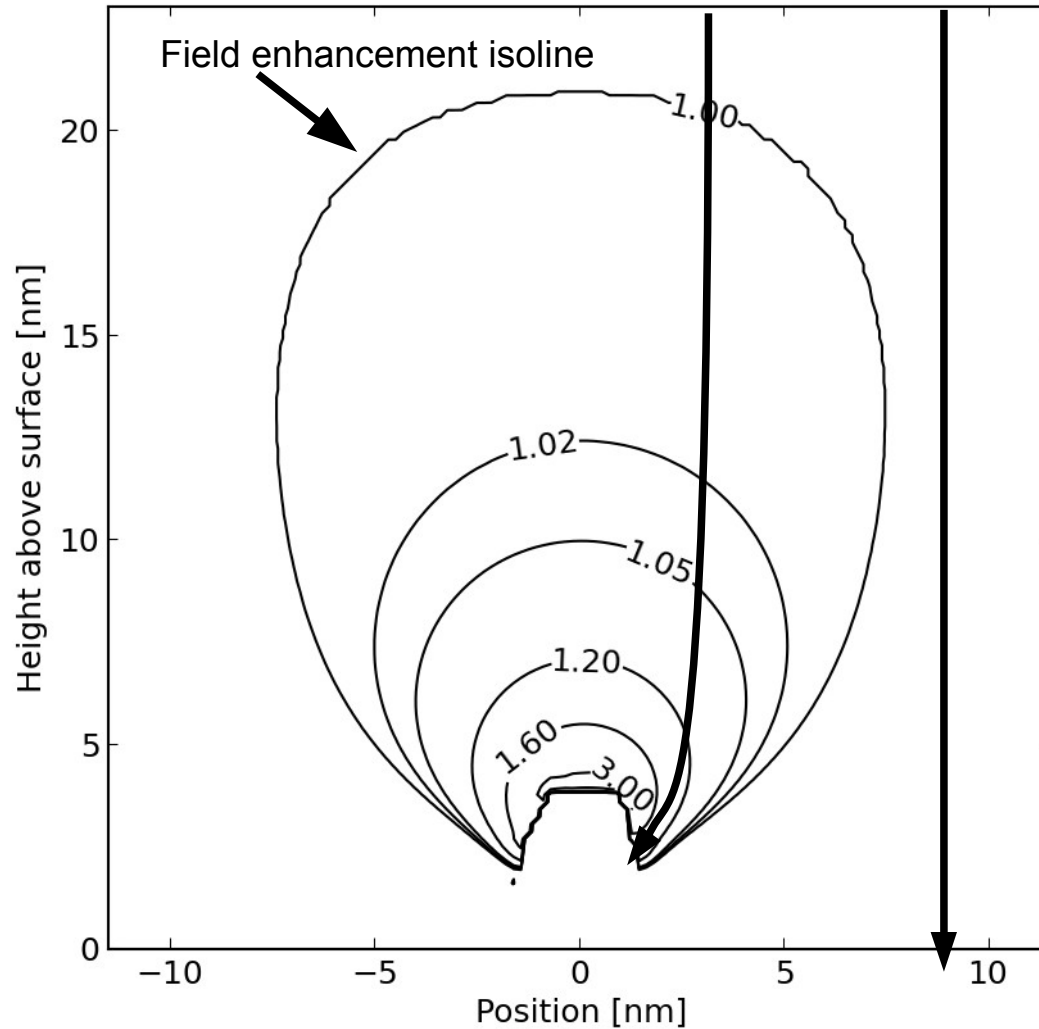
Surface features



$h=5\text{nm}$, $r=1\text{nm}$



Surface features

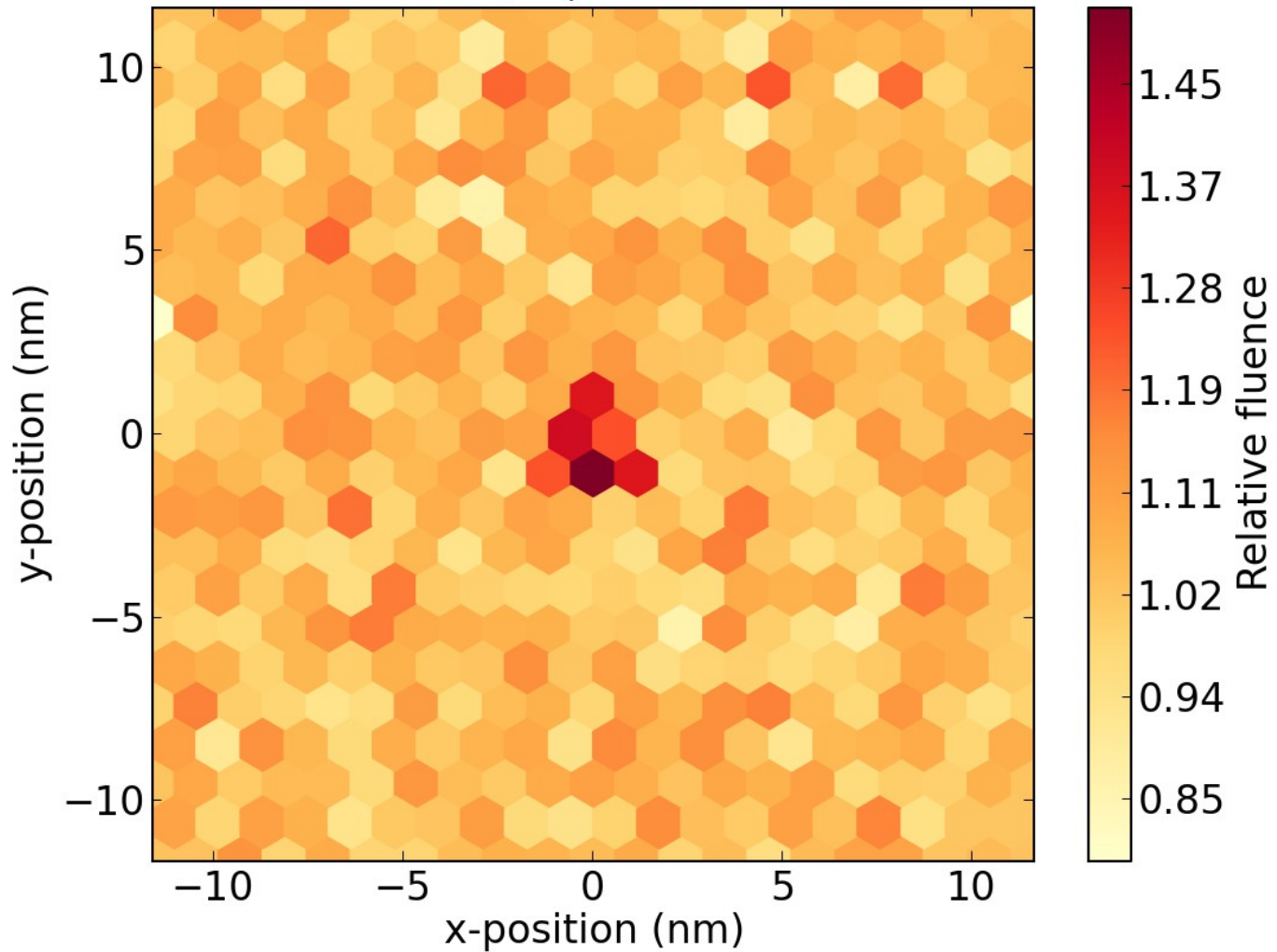


$h=5\text{nm}$, $r=1\text{nm}$



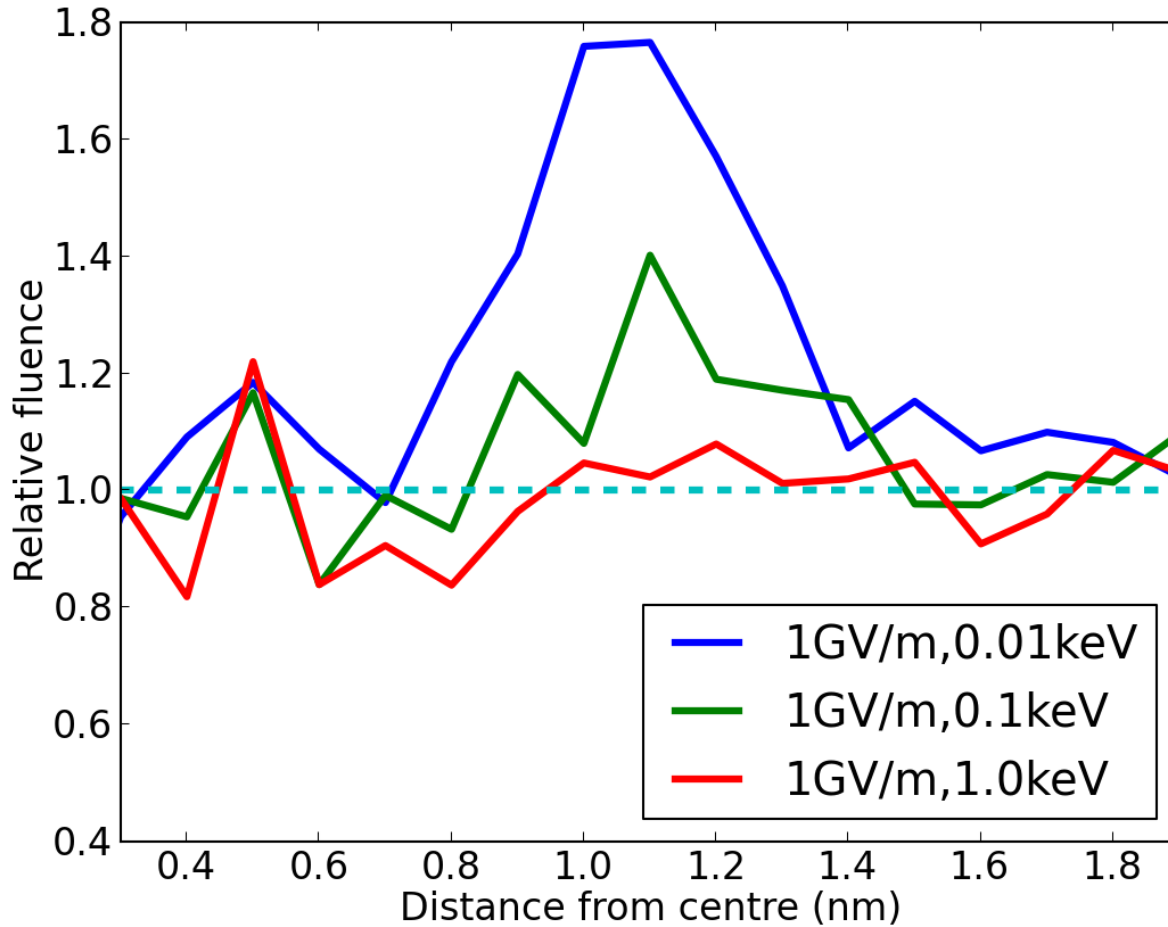
Local fluence

1GV/m, 0.01keV



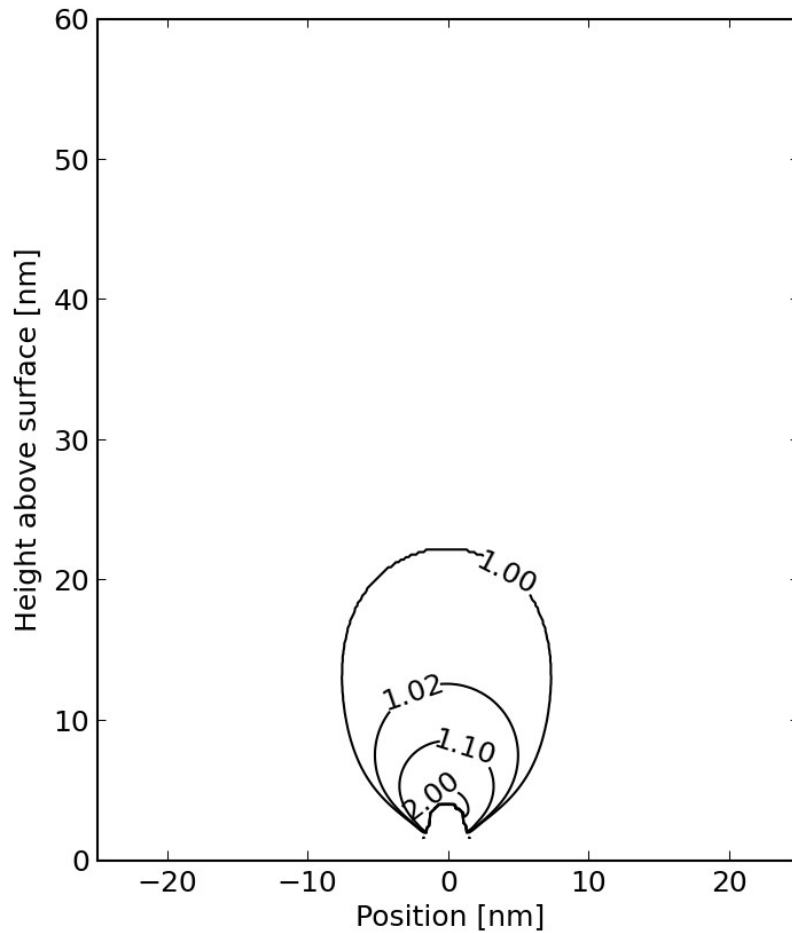


Local fluence

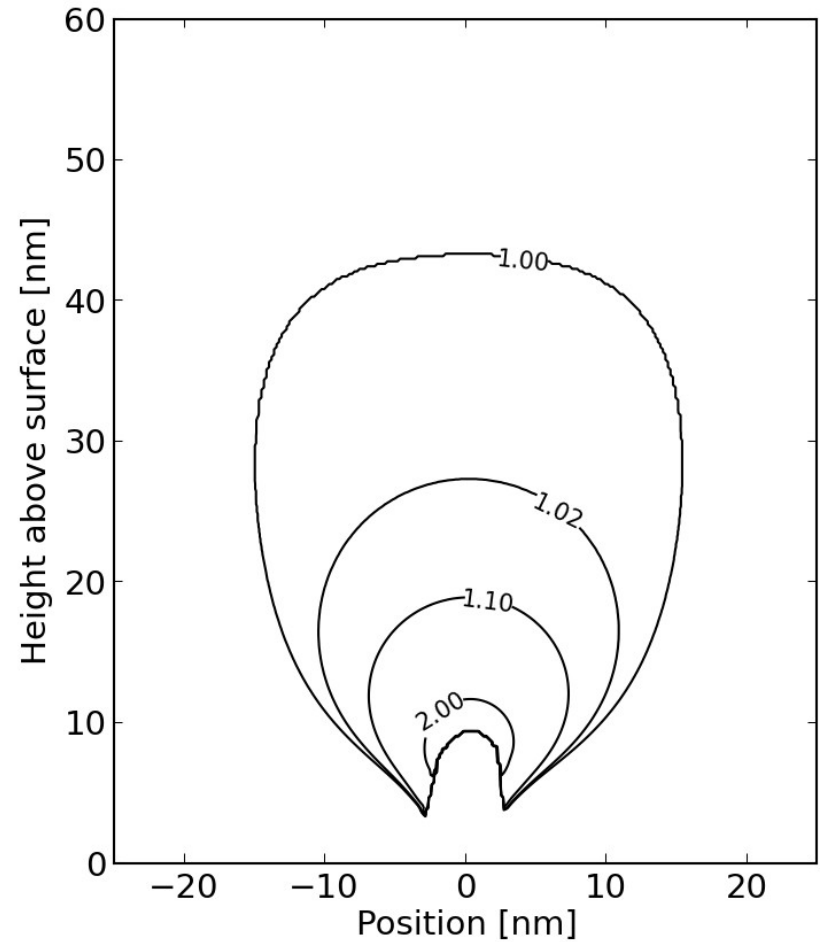




Effect of tip size



$r=1\text{nm}$, $h=5\text{nm}$



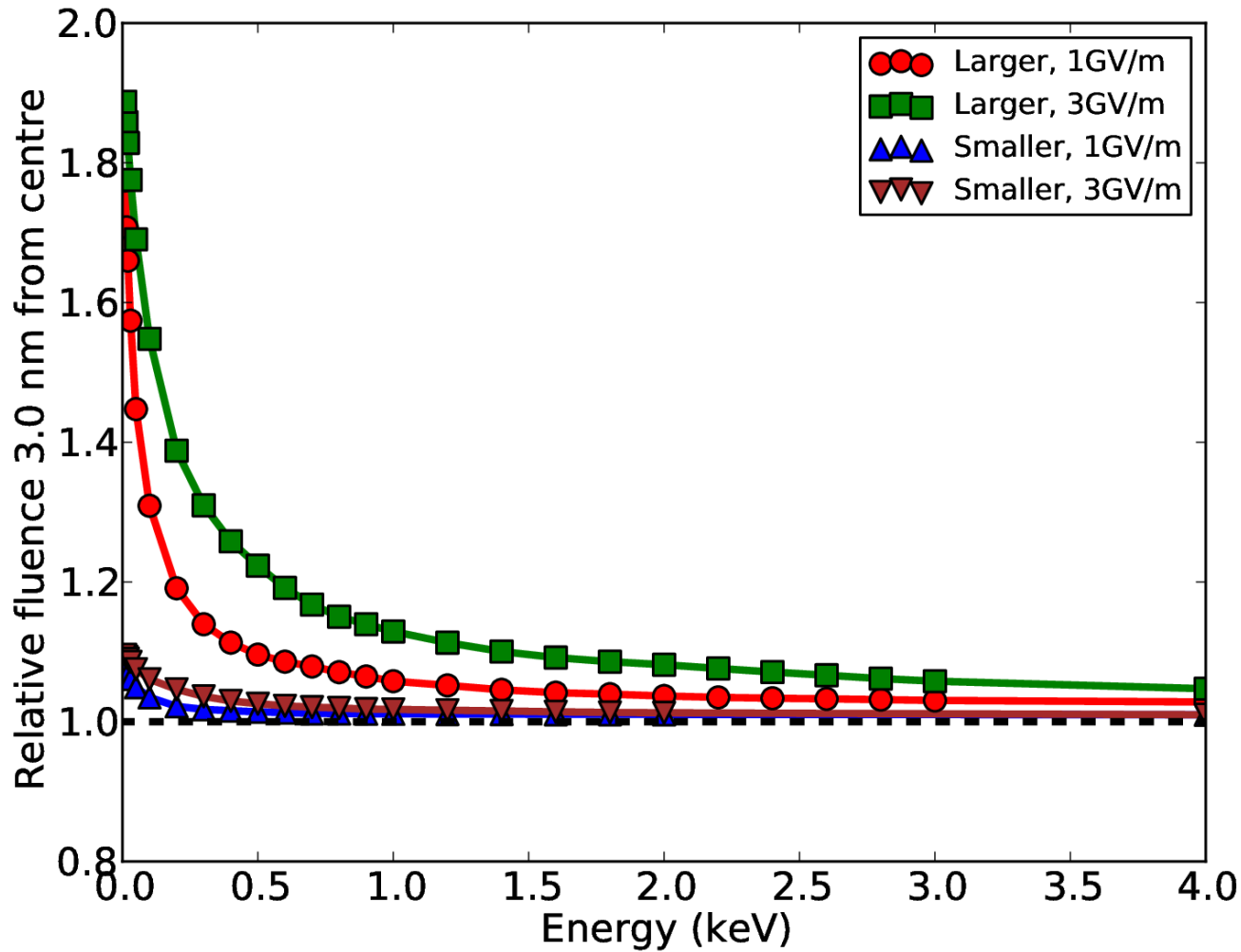
$r=2\text{nm}$, $h=10\text{nm}$



Effect of tip size

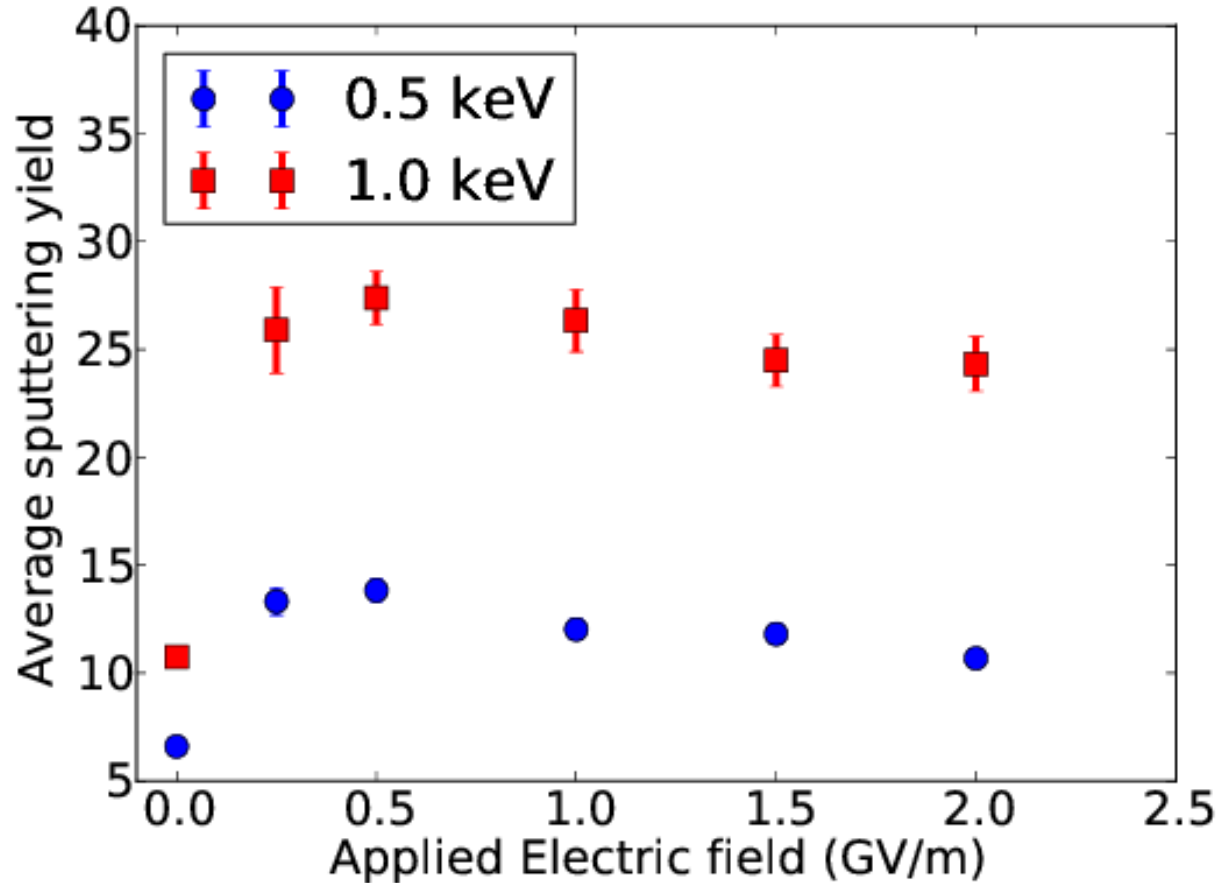
- Stronger electric field can grab faster ions

Larger: $h=10\text{nm}$, $d=4\text{nm}$
Smaller: $h=5\text{nm}$, $d=2\text{nm}$





Sputtering yield on protrusion





For the future

- Energy of incident ions much lower than thought
 - See Kyrre's talk tomorrow
 - ~10-100eV
 - New simulations in this range
 - First results by tomorrow?
- Study other geometries



Conclusions

- Sputtering yield is enhanced significantly when an electric field is applied
 - Increase several hundred percent at high fields
 - This should be considered in e.g. plasma calculations
 - “Sputtering” yield a bit misleading: actually from field evaporation
- Sputtering yield is much higher from protrusions than flat surface
- The local flux is also increased locally around protrusions
 - i.e. probability of hitting a protrusion (if they exist) is increased