Modeling of surface damage by a breakdown event

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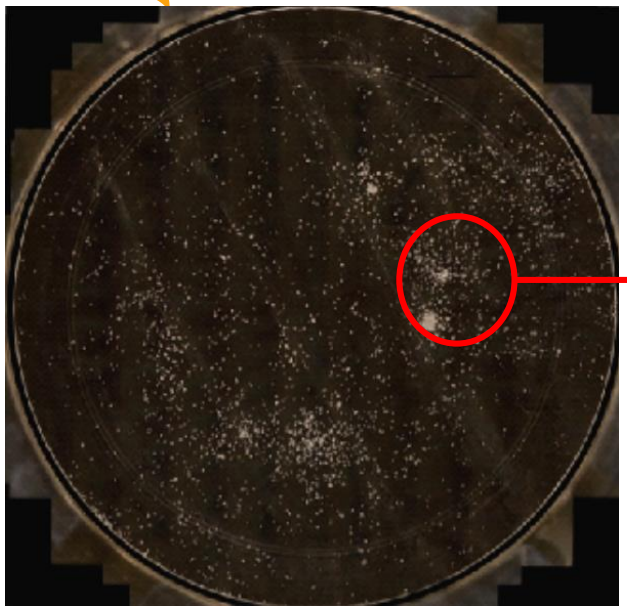
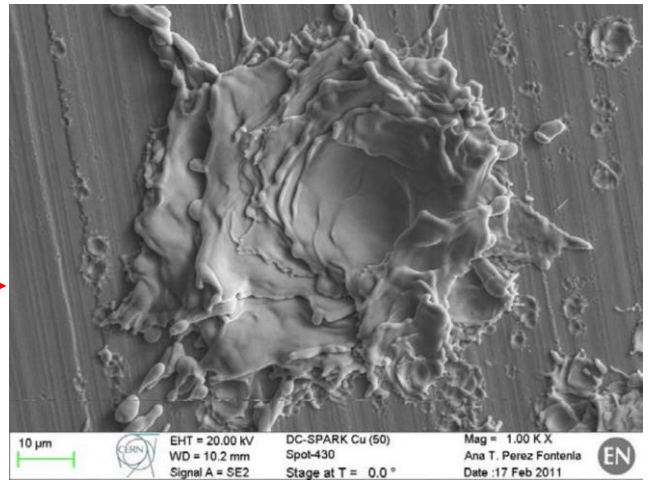
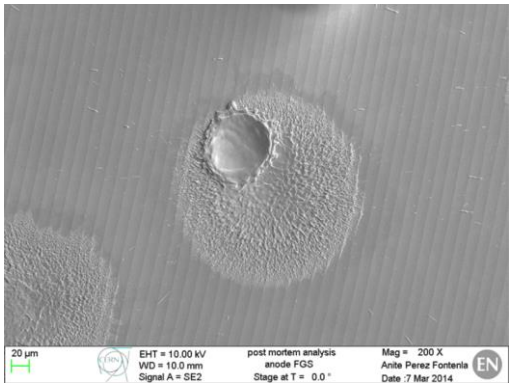
Craters From Experiments

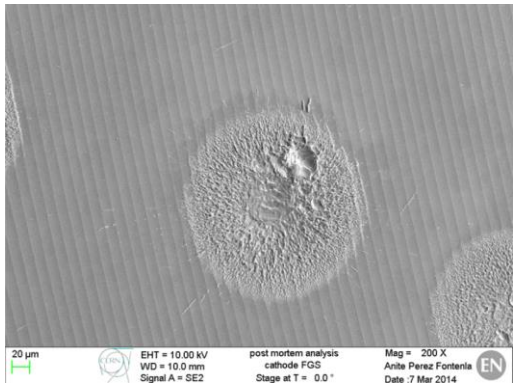
Results from Shipman N C, Thesis, The University of Manchester, 2014







Anode

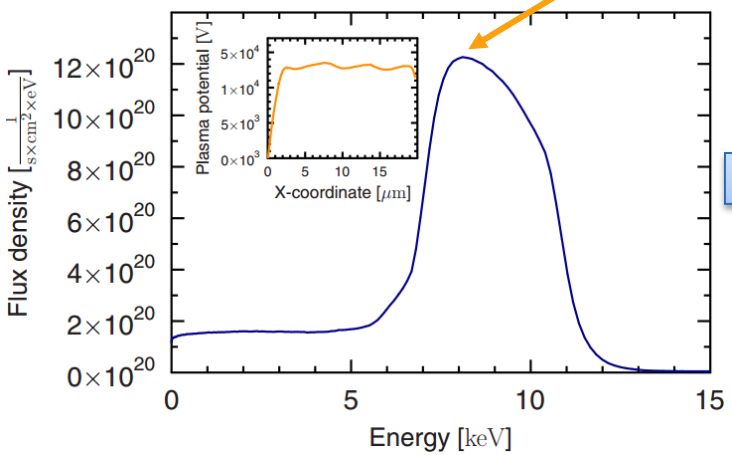


Cathode

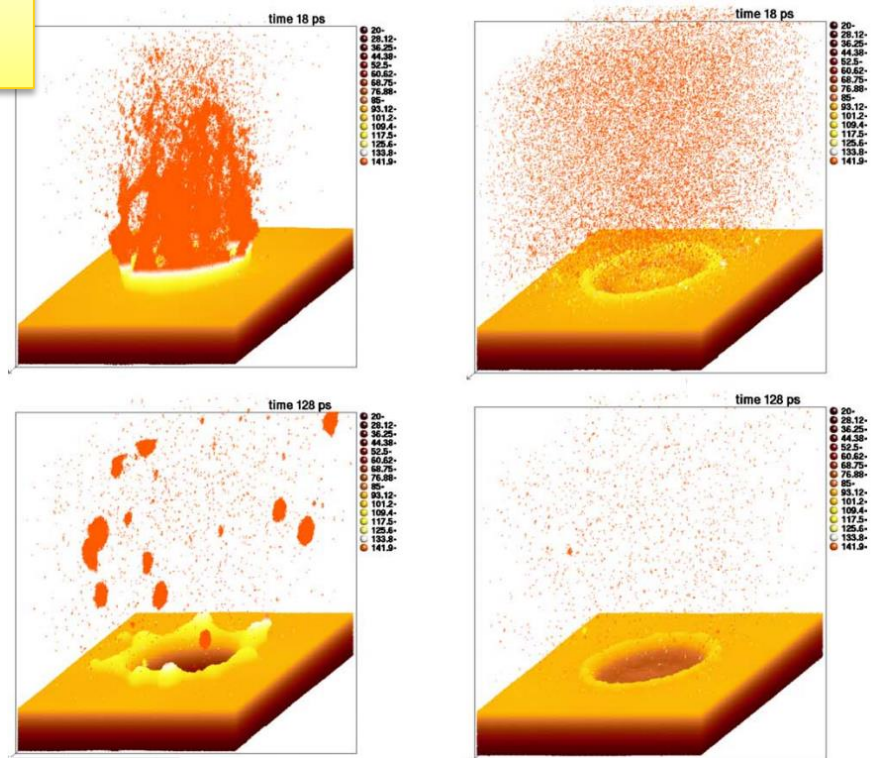
- **Micrometer-sized craters and frozen-in liquid are the final products of BDs on the surface.**
- **A crown-shape crater can be always found when the surface is checked by a SEM after BDs.**
- **The crown-shape craters indicate the metal surface has melted during BDs and the instability of the liquid metal.**
- **Not only the cathode but also the anode is affected by the BDs.**

Previous Modeling

Maximum around the high kinetic energy/atom of 8 keV.



Ion Energy Distribution Obtained From PIC Simulations

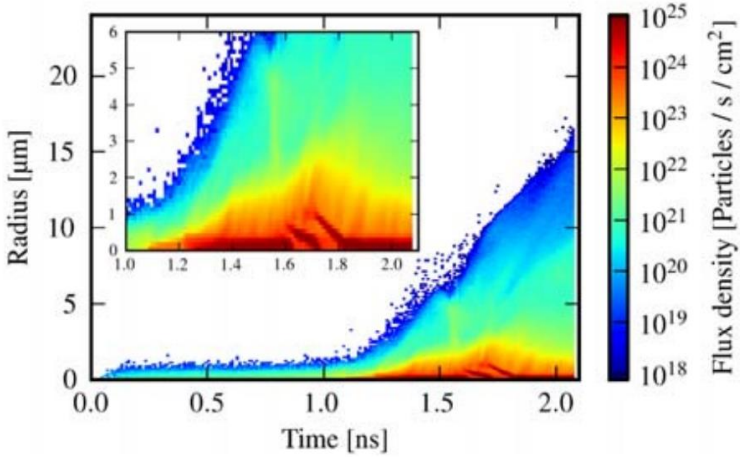


Timko Het al. 2010 Physical Review B 81 184109

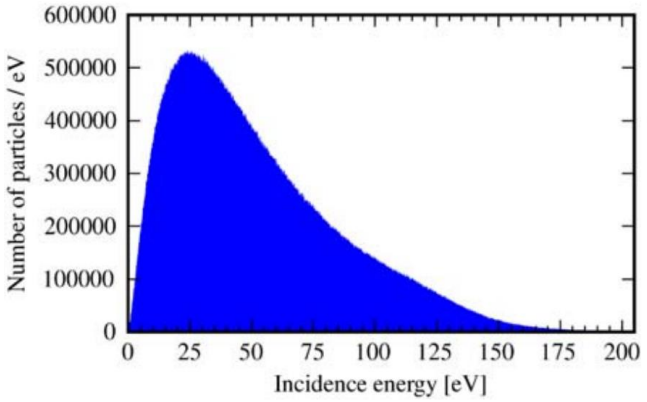
- **The ion energy come from the acceleration of the sheath near the cathode.**
- **The formation of "finger" and break of "finger" were observed in the simulations.**
- **An energetic ion flux leads to a crater and a crown-shape rim on the surface.**

New Question

Timko H, et al. 2015 Contrib. Plasma Phys. 55 299-314



Flux as a function of time and R



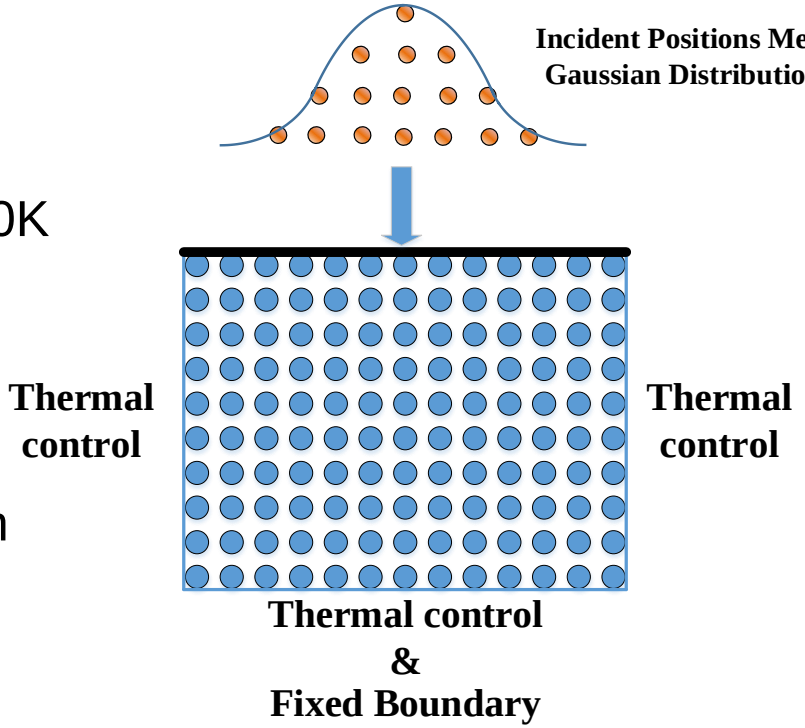
Energy spectrum, integrated over total simulation time

- **However, the 2D PIC simulation shows that the ion energy is no more than 200 eV which is much lower than 8 keV, and the average energy is about 55 eV.**
- **The flux density at 1ns can achieve 10^25 ions/s/cm^2 with a radius of 15 um.**

Is it possible for a crown-shape crater to be produced by an ion shower with such low energy (lower than 200 eV)?

MD Simulation Condition(1)

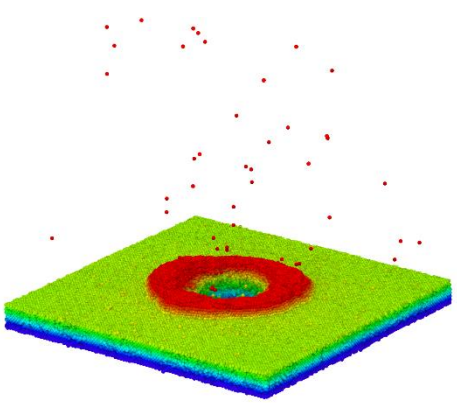
- Atom Structure: (1 0 0)
- Potential: Sabochick-Lam
- Sample Temperature: 300K, 1300K,1350K
- Ion Shower:
  - ✓ Radius:10nm
  - ✓ Ion Energy: 200 eV
  - ✓ Ion positions are generated by Gaussian distribution
  - ✓ Flux: 1e25 ions/cm^2/s



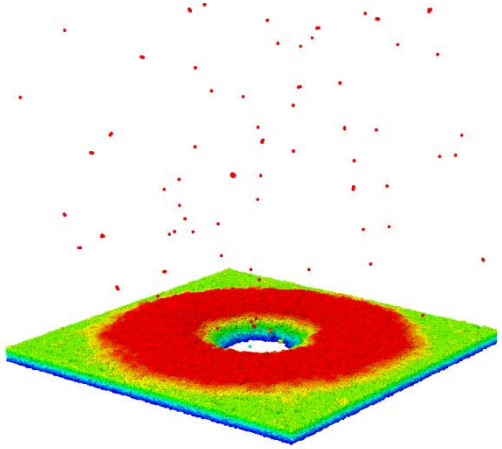
Temperature(K)	Number of Atoms	Size(nm)	Lattice Constant (A)
300	1.6m	32.6*32.6*18.1	3.63564
1300	3.4m	44.6*44.6*22.3	3.72478
1350	6.2m	52.2*52.2*29.8	3.7303

MD Results(1)-Crater

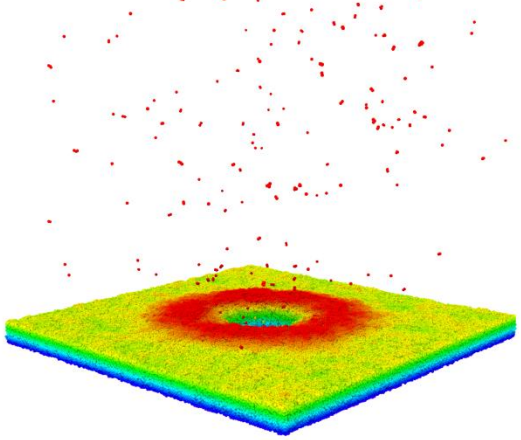
300K

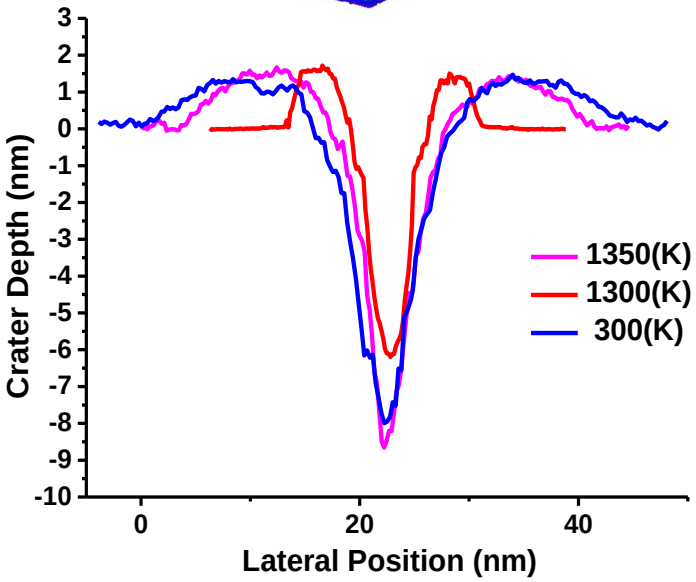


1300K



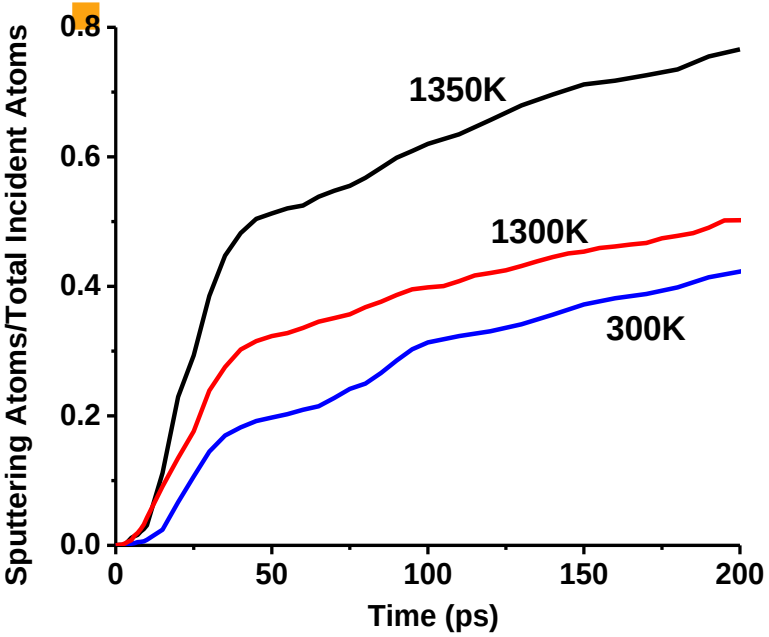
1350K



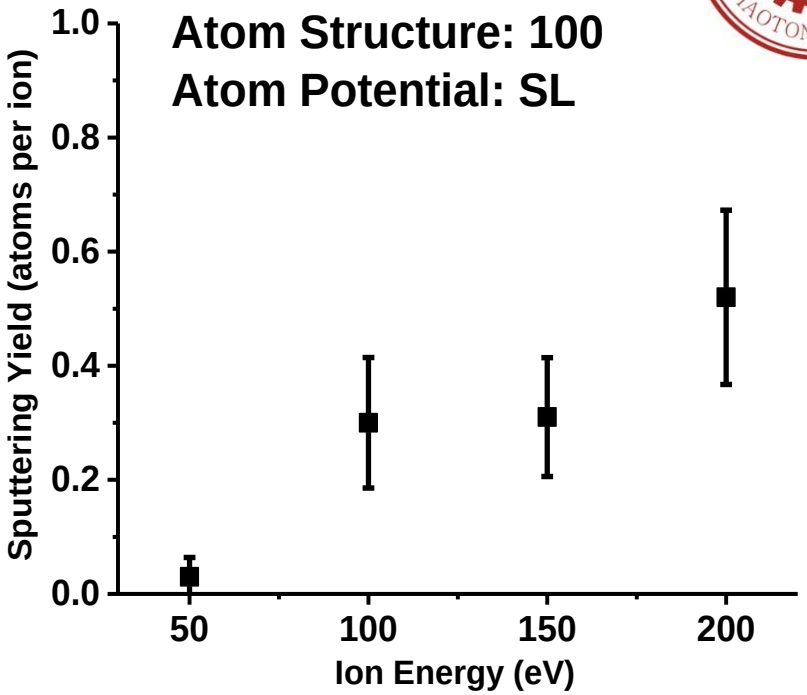


- A small crater is formed on the surface regardless of the sample temperatures.
- Higher temperature may lead to a bigger crater, but the differences are not obvious.
- There is a smooth and stable rim formed on the surface without any fingers or instability.

MD Results(1)-Sputtering Yield



Ion shower results



Compared with previous results:
single ion with different energy

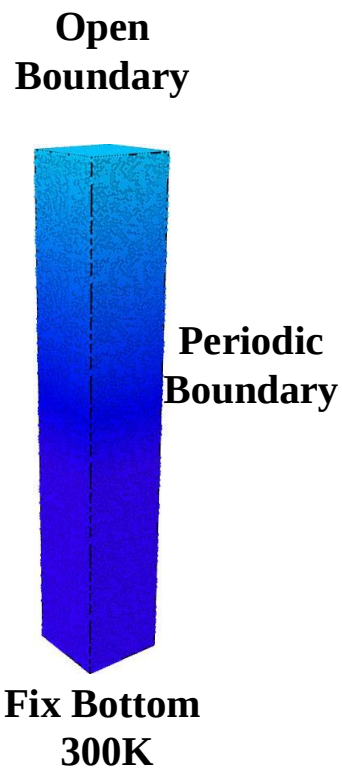
- **There is no intensive sputtering yield even compared with a single ion bombardment.**
- **The sputtering yield is lower than 1 which is below the level to sustain a plasma.**
- **Sputtering yield increases with temperature, but the effect of temperature is limited.**

MD Simulation Condition(2)

The thermal control over the boundary may cool down the sample unrealistically.

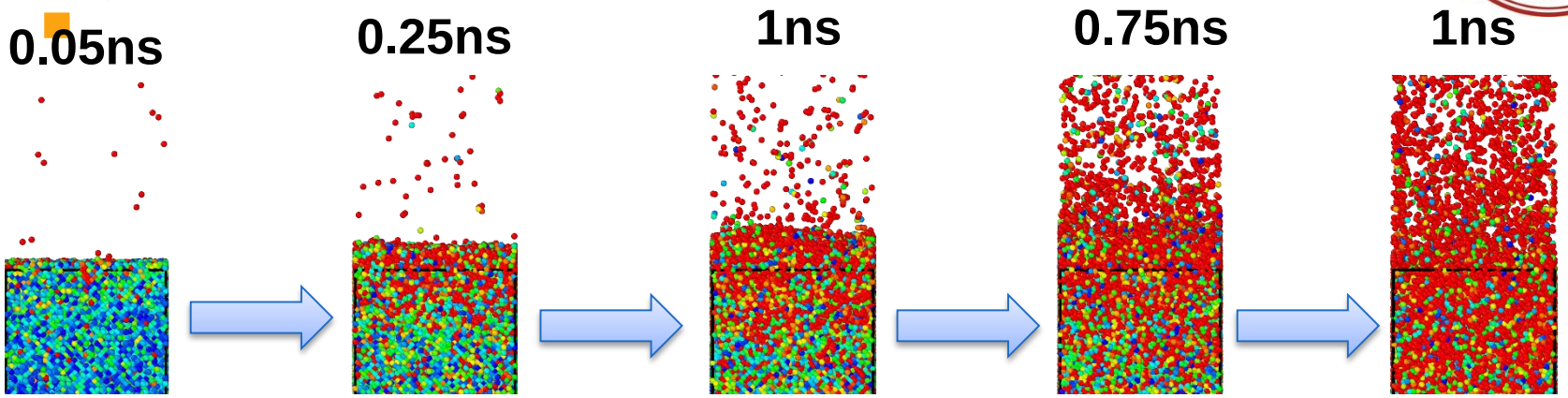
- **Atom Structure: (1 0 0)**
- **Potential: CEM**
- **Sample Size:10nm*10nm*60nm**
- **Fixing the temperature to 300 K at the bottom**
- **Only applying periodic boundary condition upon the X, Y direction**
- **Opening the upper surface in Z direction**

- **Ion Shower:**
- ✓ **Ion Energy: 55 eV**
- ✓ **Ion shower bombards the whole surface uniformly.**
- ✓ **Flux: 1e24-6e24 ions/cm^2/s**

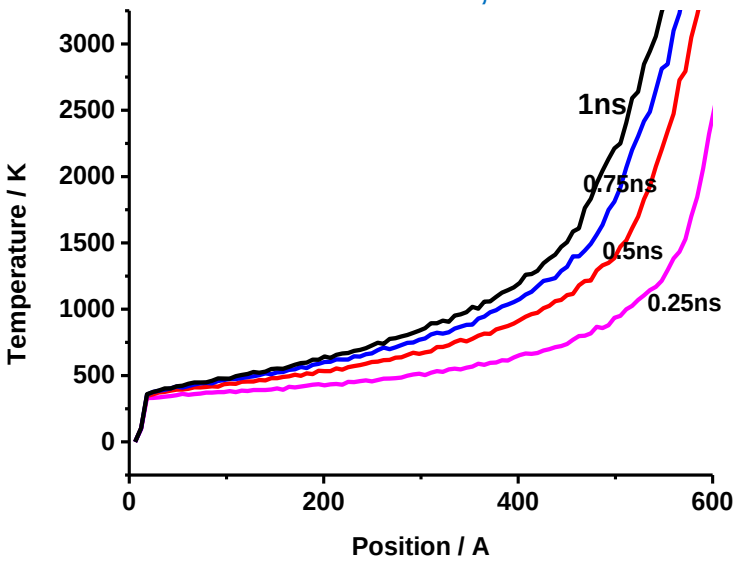


Picking up only one small slice of sample from a relative infinite surface.

MD Results(2)-Temperature



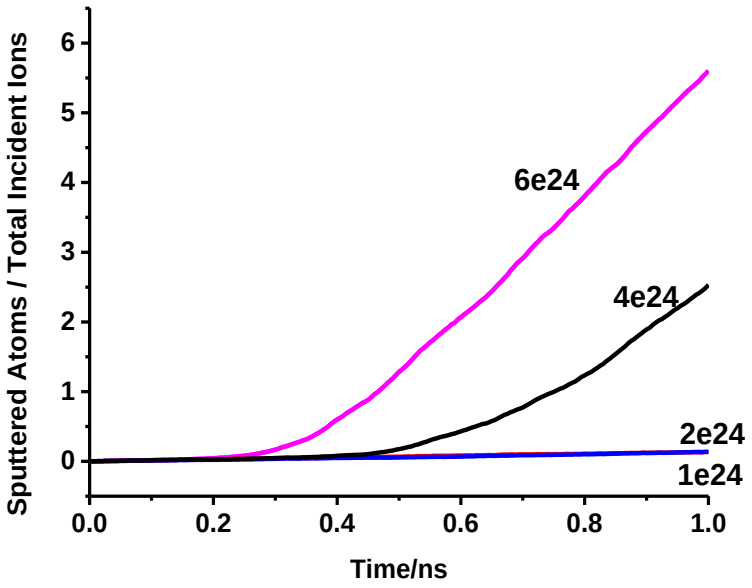
6e24 ions/cm^2/s, 55 eV



Temperature Distribution

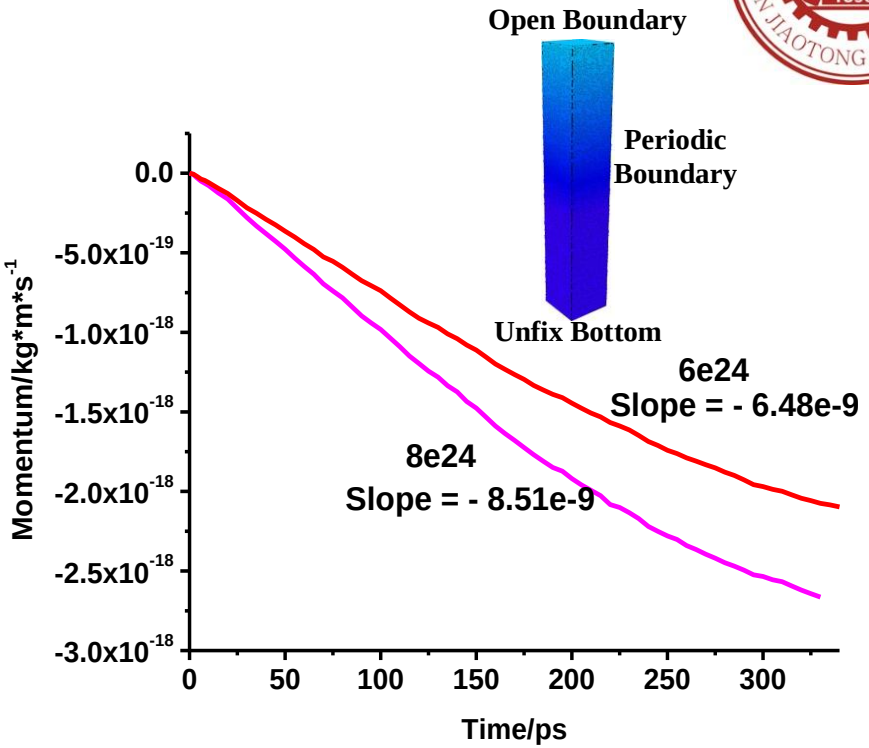
- More and more energy coming from the ion shower is deposited on the surface.
- The surface begins to melt after 0.25ns.
- The surface temperature can even achieve the boiling point.
- Intensive evaporation is observed.
- Time scale and bombarding area of ion shower may be the critical factors to obtain a crater under a condition of low ion energy.

MD Results(2)-Sputtering Yield and Pressure



Sputtering Yield

- **Sputtering yield increase with time and temperature, and can achieve above 1 for the flux density of 4e24 ions/cm^2/s.**
- **The ion shower flux densities have significant impact on the sputtering yields.**



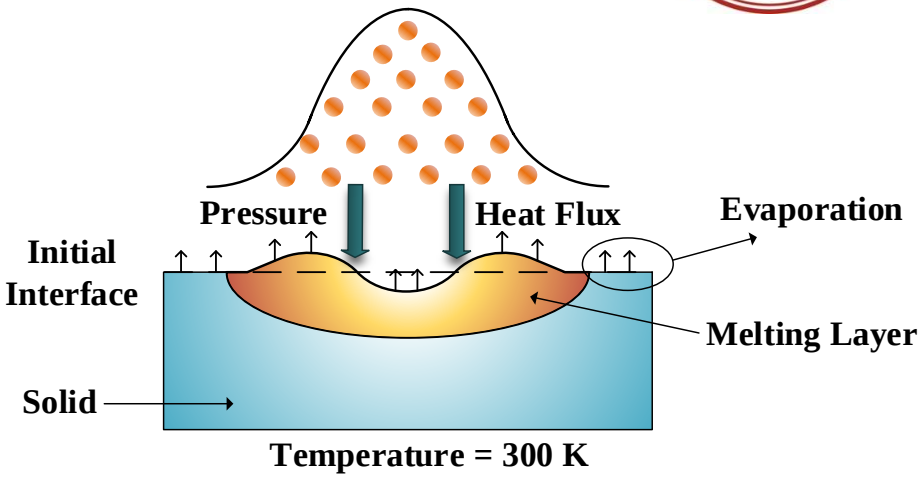
Momentum Applied On The Surface

- **The bottom atoms are movable .**
- **The momentums vary with time linearly, and the total forces F are derived from the slopes of the curves.**
- **The surface is S=10nm*10nm, and pressures (F/S) for two fluxes are 8.51e7Pa and 6.48e7 Pa.**

FEM Model Description

Model

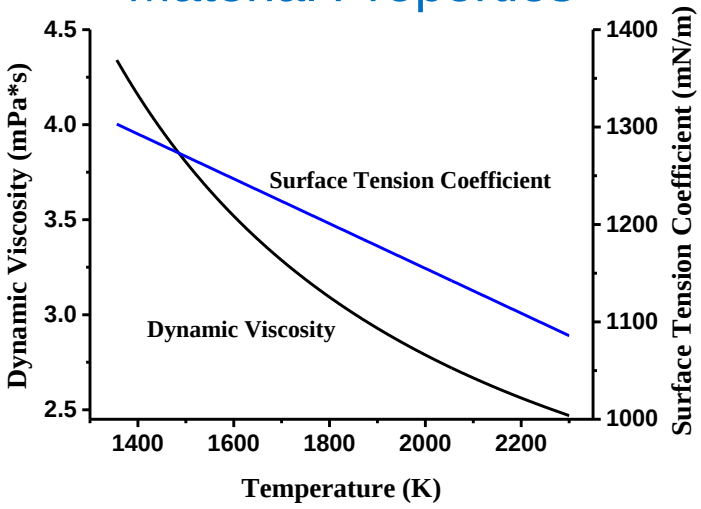
- Free surface
- Heat transfer and fluid dynamics
- Phase changes
- The pressure and heat flux are applied upon the free surface with Gaussian distribution along the X-direction, having a peak value at zero position



Boundary Condition

- **Heat transfer:**
  - ✓ Bottom: Fixed to 300K
  - ✓ Top: Outflow
  - ✓ Sides: Thermal Insulation
- **Fluid:**
  - ✓ Top: Outlet
  - ✓ Others: Walls

Material Properties



Detailed Equations

Fluid Dynamics

$$\rho\frac{\partial\vec{u}}{\partial t}+\rho(\vec{u}\cdot\nabla)\vec{u}=\nabla\cdot[-p\mathbf{I}+\eta(\nabla\vec{u}+(\nabla\vec{u})^{\mathrm{T}})]+\mathrm{G}\nabla\phi+\vec{F}_{\mathrm{st}}+\vec{F}\delta(\phi)+K\vec{u}$$

$$\nabla\cdot(\vec{u})=\dot{m}\delta(\phi)(\frac{1}{\rho_{\mathrm{V}}}-\frac{1}{\rho_{\mathrm{L}}})\qquad p_{\mathrm{sat}}(\mathrm{T})=p_{atm}\exp[\frac{mL_{\mathrm{v}}}{k_{\mathrm{b}}}(\frac{1}{T_{\mathrm{vap}}}-\frac{1}{T})]\qquad \dot{m}=\sqrt{\frac{m}{2\pi k_b T}}p_{\mathrm{sat}}(\mathrm{T})$$

Heat Transfer

$$\rho C_{\mathrm{p}}[\frac{\partial T}{\partial t}+\nabla\cdot(\vec{u}T)]=\nabla\cdot(\lambda\nabla T)+\mathrm{S}_{\mathrm{ion}}+Q_{\mathrm{vap}}$$

$$C_{\mathrm{p}}^{\mathrm{eq}}=C_{\mathrm{p\text{-}s}}+L_{\mathrm{f}}\frac{\exp[-(\frac{T-T_f}{T_{\mathrm{l}}-T_{\mathrm{s}}})^2]}{\sqrt{\pi(T_{\mathrm{l}}-T_{\mathrm{s}})}}\qquad Q_{\mathrm{vap}}=-L_{\mathrm{v}}\dot{m}\delta(\phi)$$

$$K=-C(\frac{(1-f)^2}{f^3+b})$$

$$f=\begin{cases}0 & T<Ts\\ \dfrac{T-T_l}{T_l-T_s} & T_s<T<T_l\\ 1 & T>T_l\end{cases}$$

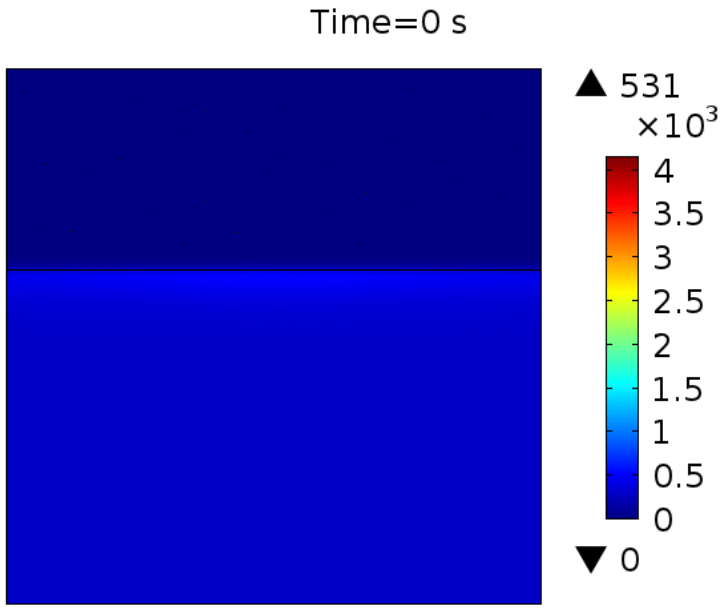
Phase Field-Tracking Free Surface

$$\frac{\partial\phi}{\partial t}+\vec{u}\cdot\nabla\phi-\dot{m}\delta(\phi)(\frac{V_{\mathrm{f,V}}}{\rho_{\mathrm{V}}}+\frac{V_{\mathrm{f,L}}}{\rho_{\mathrm{L}}})=\nabla\cdot(\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi)$$

$$\psi=-\nabla\cdot\varepsilon^2\nabla\phi+(\phi^2-1)\phi$$

$$\delta(\phi)=3V_{\mathrm{f,L}}(1-V_{\mathrm{f,L}})\left|\nabla\phi\right|$$

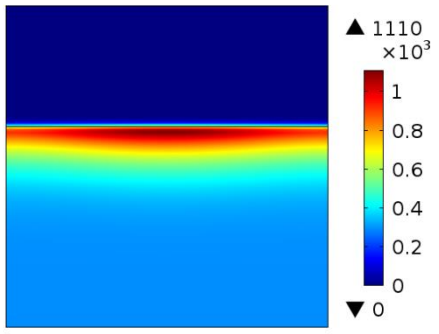
Result-With Recoil Force



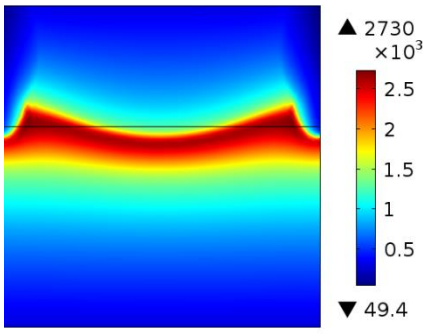
Ion Energy: 55 eV
Ion Flux: 8e24 ions/cm^2/s

- **Instability of liquid is observed after the temperature achieving the boiling temperature.**
- **The droplets are generated at the end of the simulation.**
- **A crater is an accumulated result of time and energy.**

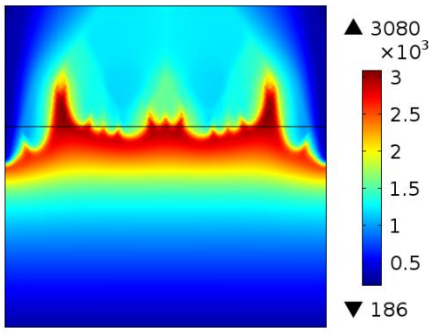
1ns



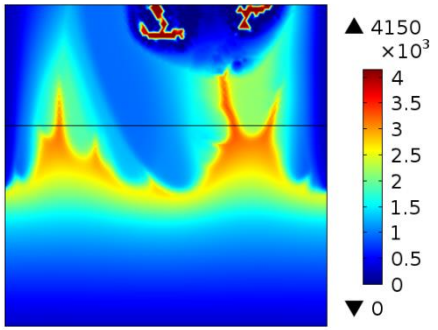
10ns



15ns

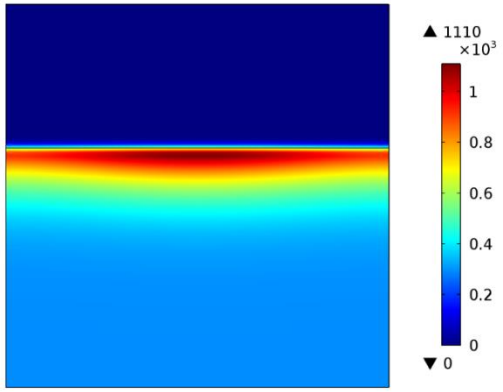


21.6ns

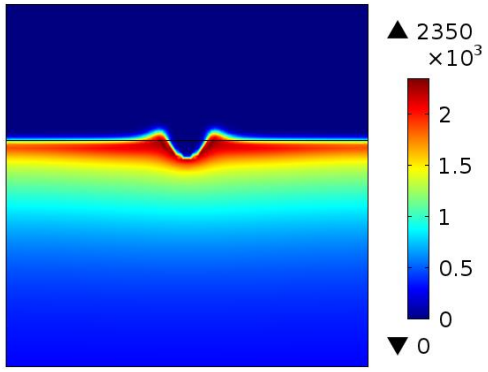


Result-Without Recoil Force

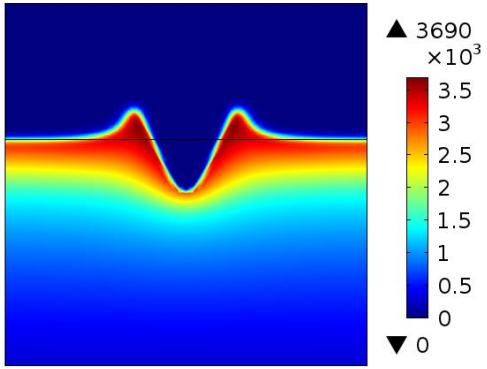
1ns



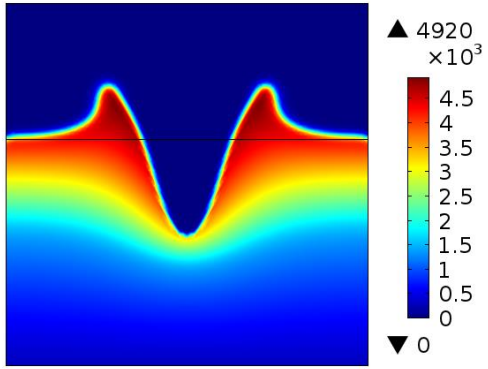
5ns



10ns



16ns

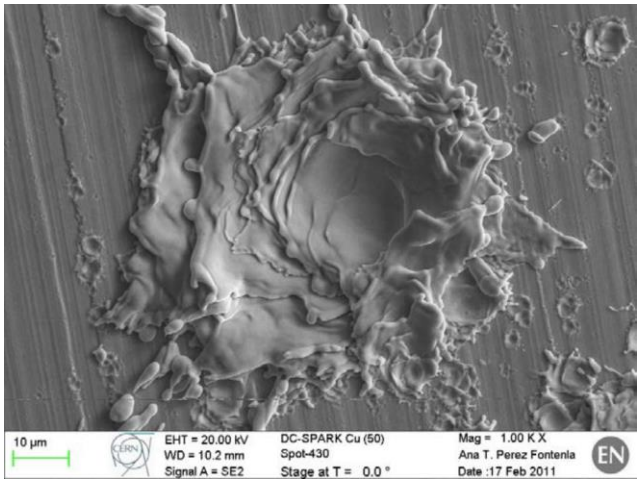


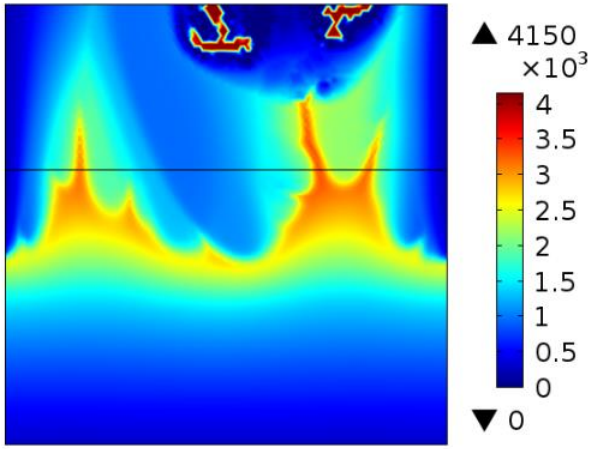
Ion Energy: 55 eV
Ion Flux: 8e24 ions/cm^2/s

- **The depth of the crater becomes deeper and deeper with time.**
- **No instability is observed.**
- **The recoil force from evaporations may be the main reason to lead to a instability.**
- **The pressure from the ion shower gives a basic pattern of a crater – the crown-shape crater.**

Conclusions

- It is possible to obtain a crown-shape by bombarding a surface with low energy (lower than 200 eV) ion shower.
- A crater is an accumulated result of time and energy.
- The pressure from the ion shower gives a basic shape of the crater.
- The instability comes from strong evaporations after the surface temperature is above the boiling point.





Thanks for your attention!