POLYTECH.MONS

BELVAC/NEVAC Symposium

Monte-Carlo simulation of ionization in Self-Induced Ion Plating (SIP)

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Outline

- Self-induced Ion Plating (SIP)
- SIP modelling
  - Magnetic model
  - Heat transfer model
    - Monte-Carlo method
    - Heat transfer model
  - Evaporation model
- Conclusions

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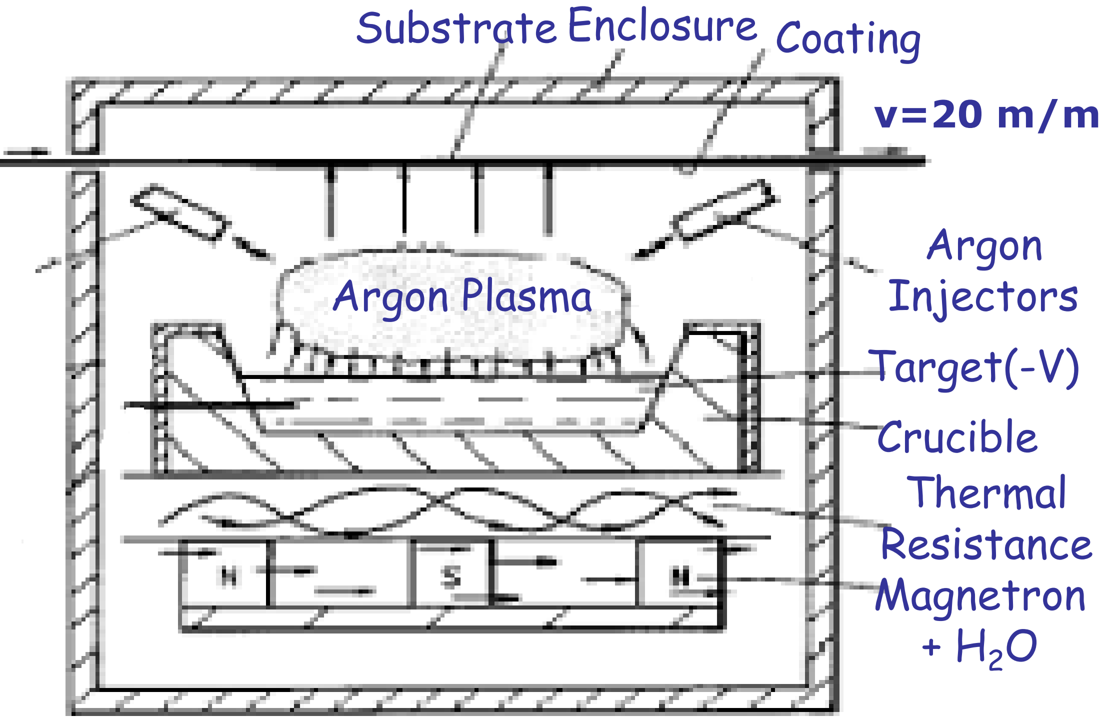
Self-induced ion plating



v=20 m/min

European Patent N°0780489

p=6,75 10^{-4} Torr=0,09 Pa ;

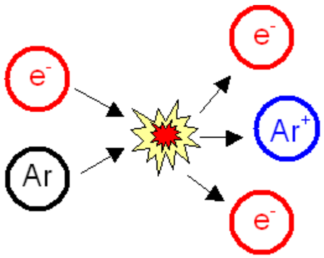
Target mean power density : 21,5 W/cm^2

Tin target at low voltage : -900V

↓

Electron displacement between the cathode and the anode

↓



⇒ Creation of Argon plasma

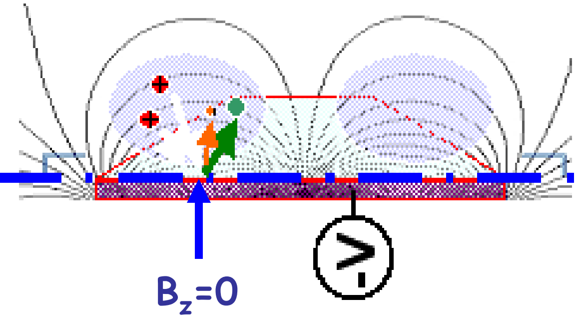
$Ar^+$and target at low voltage→Ion bombardment of the target

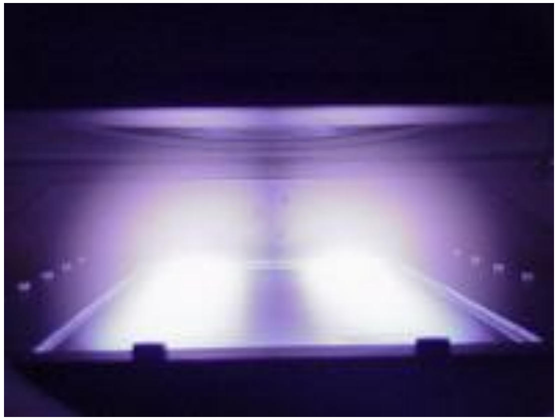
Thermal resistance under the crucible→ Target evaporation

Self-induced ion plating

→ **SIP = evaporation due to magnetron sputtering system**

- **Magnetron sputtering:Maximal erosion where the magnetic field is tangential to the target surface (B_z=0)**





- **SIP:Maximal heat flux where the magnetic field is tangential to the target surface (B_z=0)**

→ **Link between magnetic field and distribution of the ion bombardment heat flux : Monte-Carlo method**

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SIP modelling

Magnetic Model

Magnetic field
⇓
Ion bombardment heat flux

Heat transfer model

Temperature field at
the target level

Evaporation and coating model

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Magnetic Model

Magnetic field - FEMLAB® 3.0a

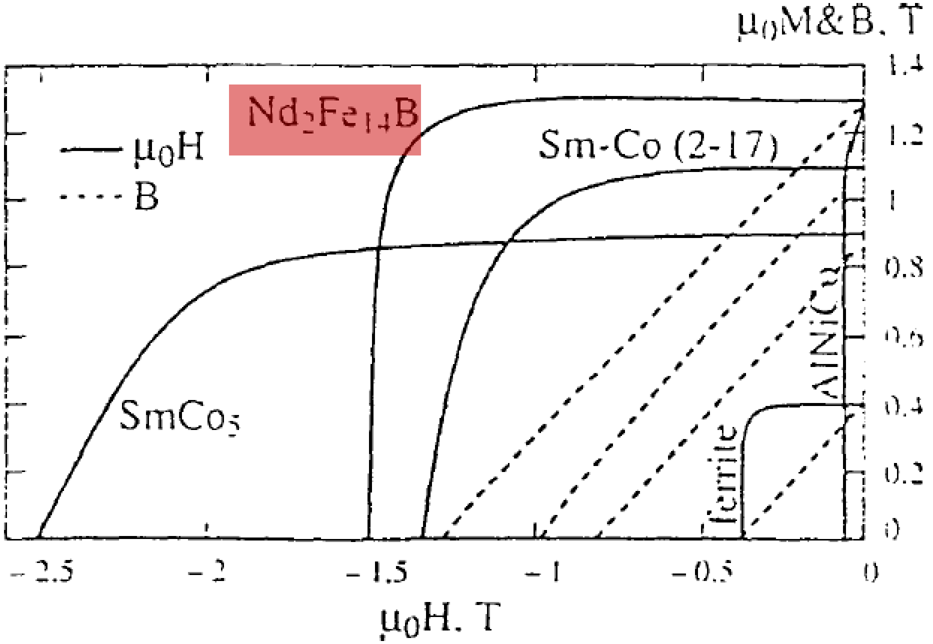
Magnetostatic laws

Neodymium magnets (NdFeB)

$$B=\mu_0(H+M);H=-\nabla V_m$$

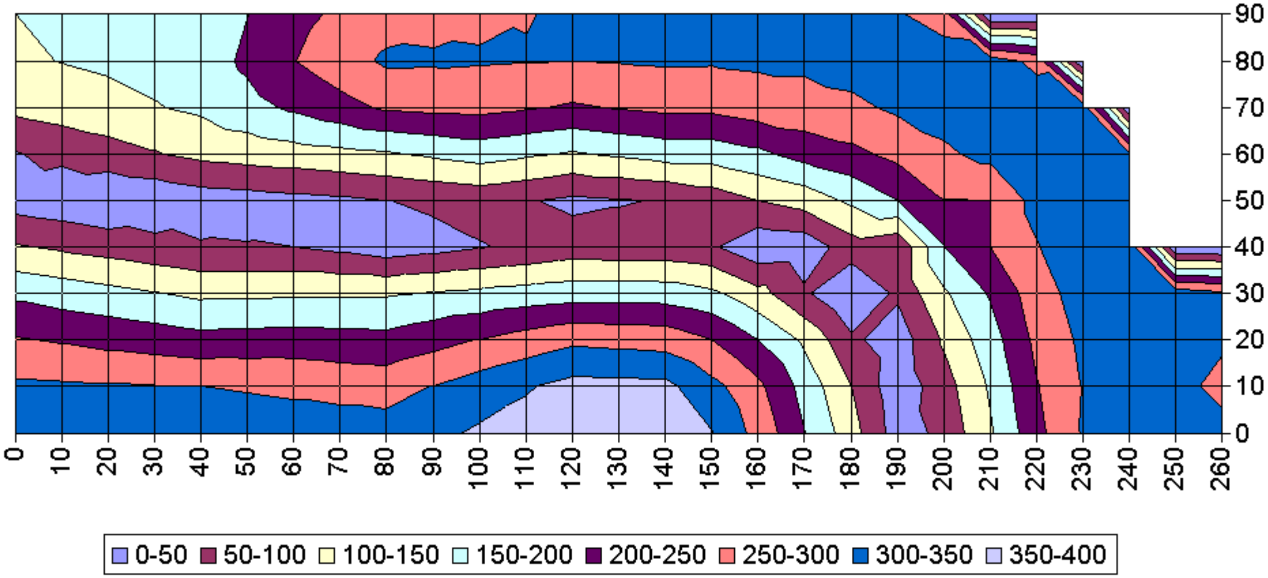
$$M=M_0+(\mu_r-1)H\Rightarrow B=\mu_0\mu_r H+B_r$$

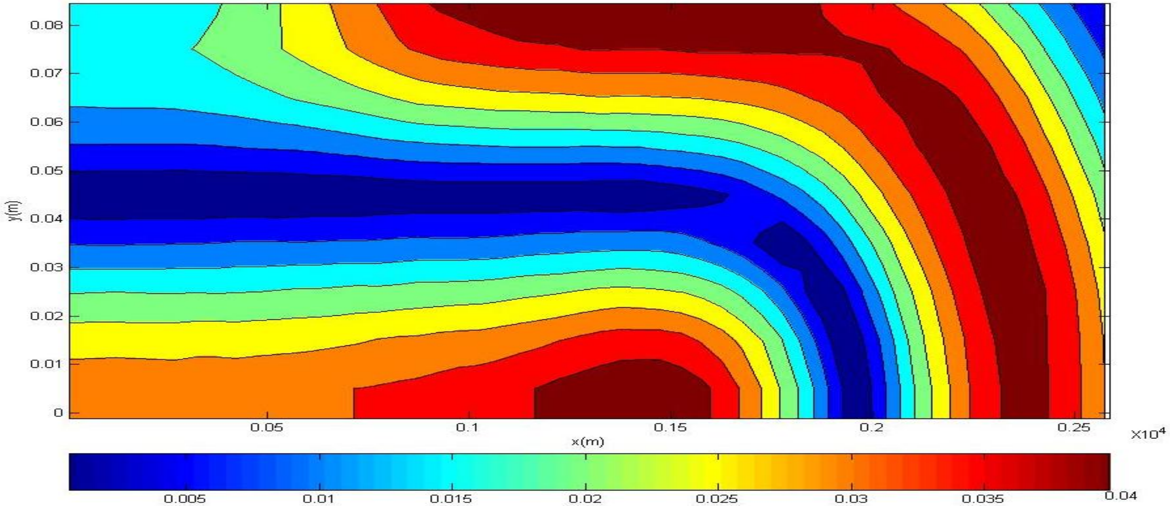
$$\nabla B=0\Rightarrow-\nabla(\mu_0\mu_r\nabla V_m-B_r)=0$$



Magnetic model

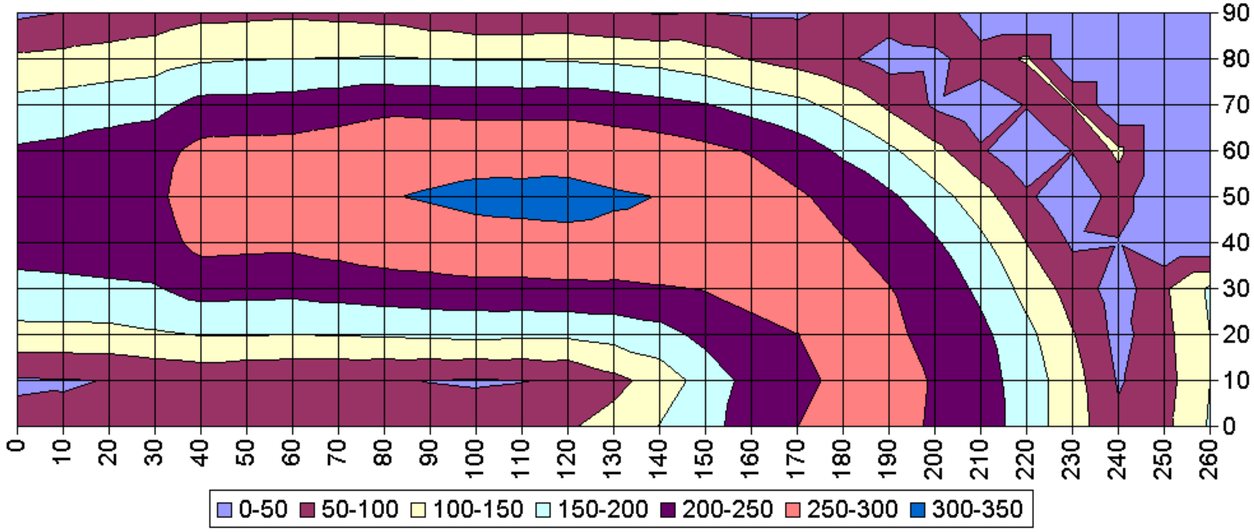
$|B_z|$(Gauss) at the target level

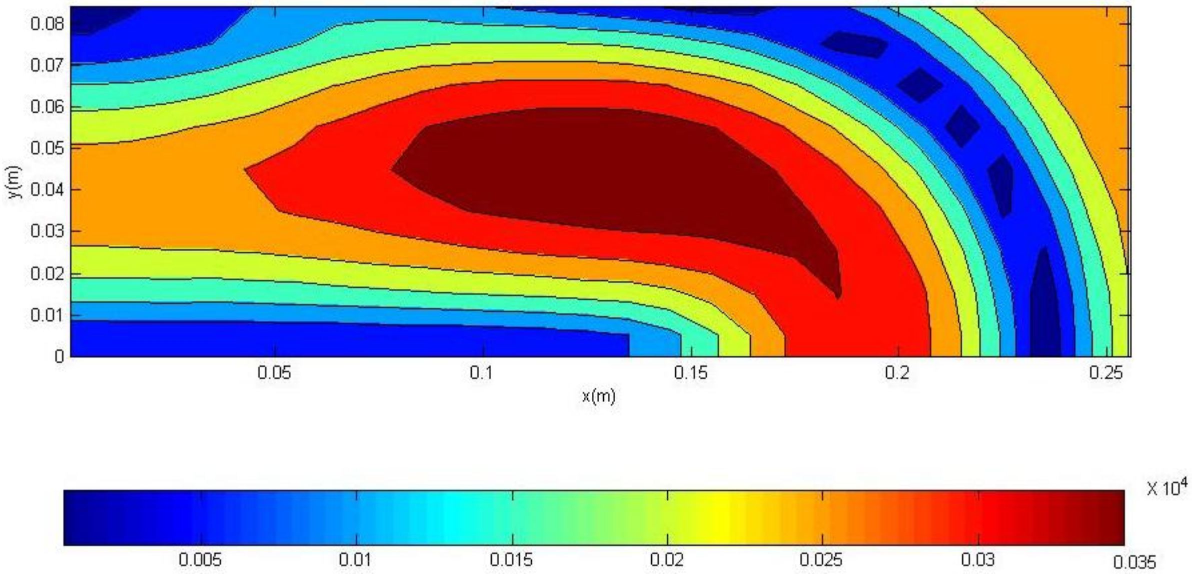




Magnetic model

$|B_{xy}|$(Gauss) at the target level





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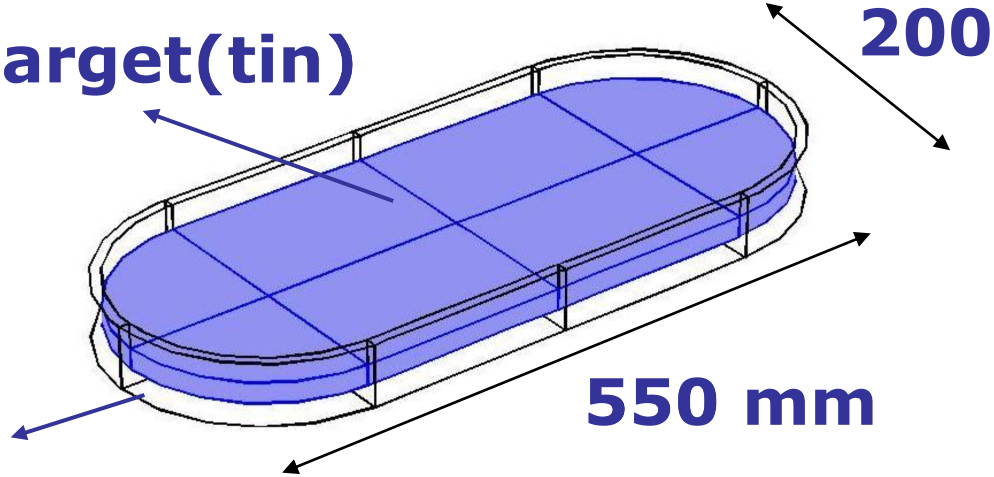
Heat transfer model

Geometry



Target(tin)

200 mm

Crucible (graphite)

550 mm

Distribution of ion bombardment heat flux unknown

→ **Monte-Carlo method**

→ **Distribution of bombardment heat flux = Distribution of ionisation points (ions not influenced by magnetic field)**

Monte-Carlo method

Step 1. Secondary electrons trajectories

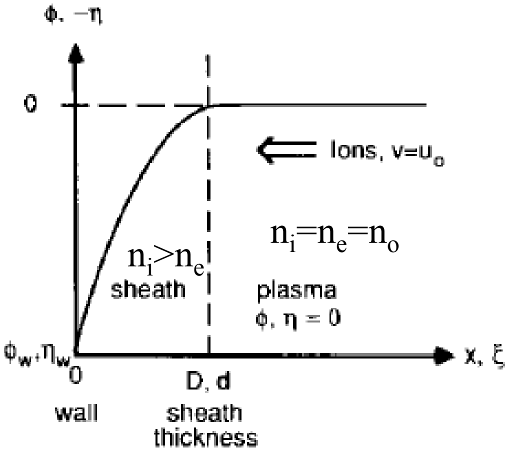
$$\vec{F}=q(\vec{E}+\vec{v}\times\vec{B})\Rightarrow\frac{\partial\vec{v}}{\partial t}=\frac{q}{m}(\vec{E}+\vec{v}\times\vec{B})$$ **(Lorentz law)**

Numerical integration – Runge-Kutta (4th order)

Magnetic field - Magnetostatic laws

Electric field - Analytical model : Sheridan & Goree*

*T. Sheridan, J. Goree, « Analytic expression for the electric potential in the plasma sheath »,IEEE Transactions on plasma science 17(6) (1989) p. 884



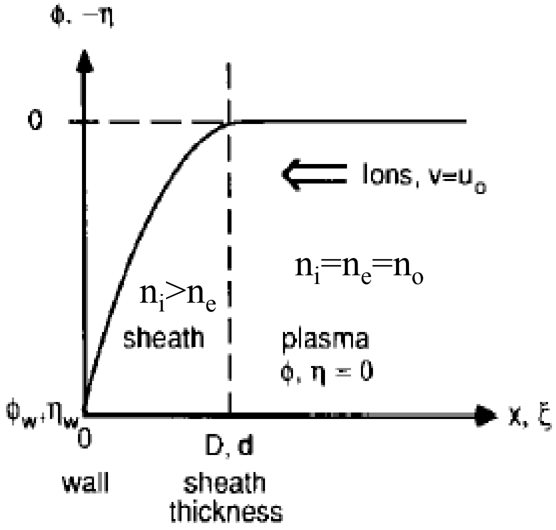
Sheath is source free→continuity

$$n_i v = n_0 v_0$$

Sheath is collisionless→energy conservation

$$\frac{Mv^2}{2}=\frac{Mu_0{}^2}{2}+e\phi$$

Monte-Carlo method



→ $n_i = n_0 (1 - \frac{2e\phi}{M u_0^2})^{\frac{-1}{2}}$

Boltzmann relation → $n_e = n_0 e^{\frac{e\phi}{kT_e}}$

Poisson 's relation → $\frac{d^2\phi}{dx^2} = -\frac{e}{\varepsilon_0}(n_i - n_e)$

$$\rightarrow \frac{d^2\phi}{dx^2} = -\frac{e n_0}{\varepsilon_0}\left[\left(1 - \frac{2e\phi}{M u_0^2}\right)^{\frac{-1}{2}} - e^{\frac{e\phi}{kT_e}}\right]$$

Dimensionless parameters : $\eta = \frac{-e\phi}{kT_e}; \xi = \frac{x}{\lambda_D}; M_a = \frac{u_0}{\left(\frac{kT_e}{M}\right)^{\frac{1}{2}}}$

→ if $\eta_c > 10^4$ (Child's law)

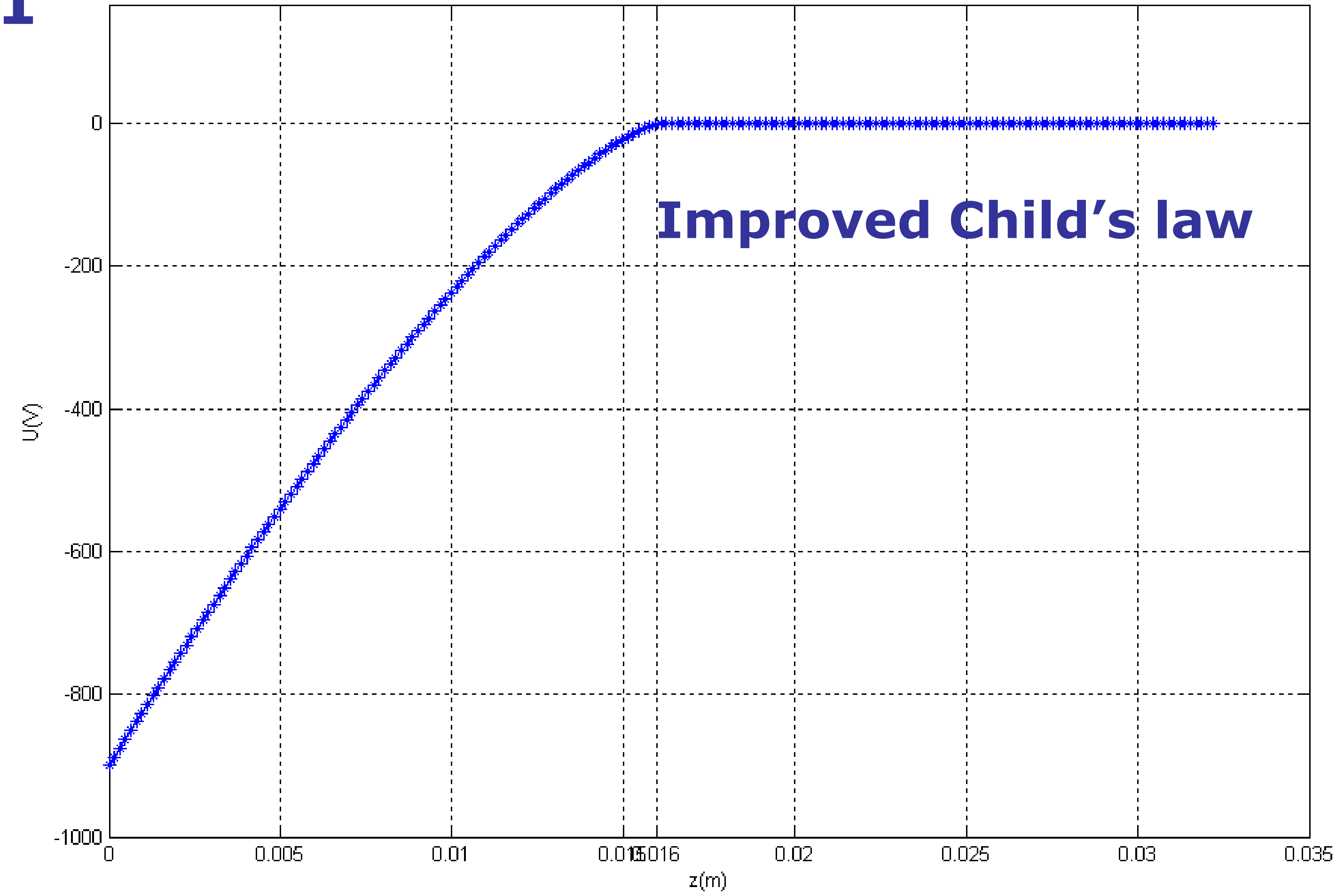
$$\eta(\xi) \cong 1.36284 (d - \xi)^{\frac{4}{3}}; d \cong 0.7928 \eta_c^{\frac{3}{4}}$$

→ if $10^4 > \eta_c > 10$ (Improved Child's law)

$$\eta(\xi) = a(d - \xi)^b; a = \frac{\eta_c}{d^b}; d = \frac{\eta'_c \eta_c}{\eta''_c \eta_c - {\eta'_c}^2}; b = \frac{1}{1 - \frac{\eta''_c \eta_c}{{\eta'_c}^2}}$$

Monte-Carlo method

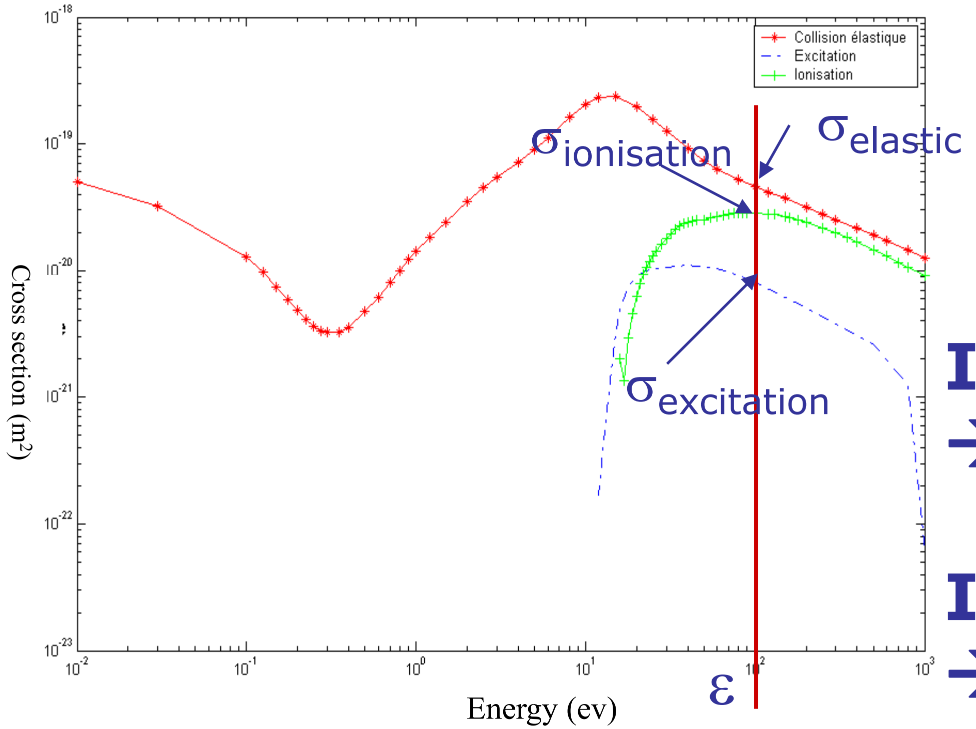
Improved Child's law for SIP : T_e=4ev; Φ=-900V; η_c=261



Width of the sheath : 16 mm

Monte-Carlo method

Step 2. At each time step : collision or not ?



Probability of a collision

$$P = 1 - e^{-v \Delta t \sigma_{tot}(\varepsilon) n_g}$$

$$\sigma_{tot}(\varepsilon) = \sigma_{elast}(\varepsilon) + \sigma_{excit}(\varepsilon) + \sigma_{ionis}(\varepsilon)$$

If R>P→ No collision
→ integration in t+Δt

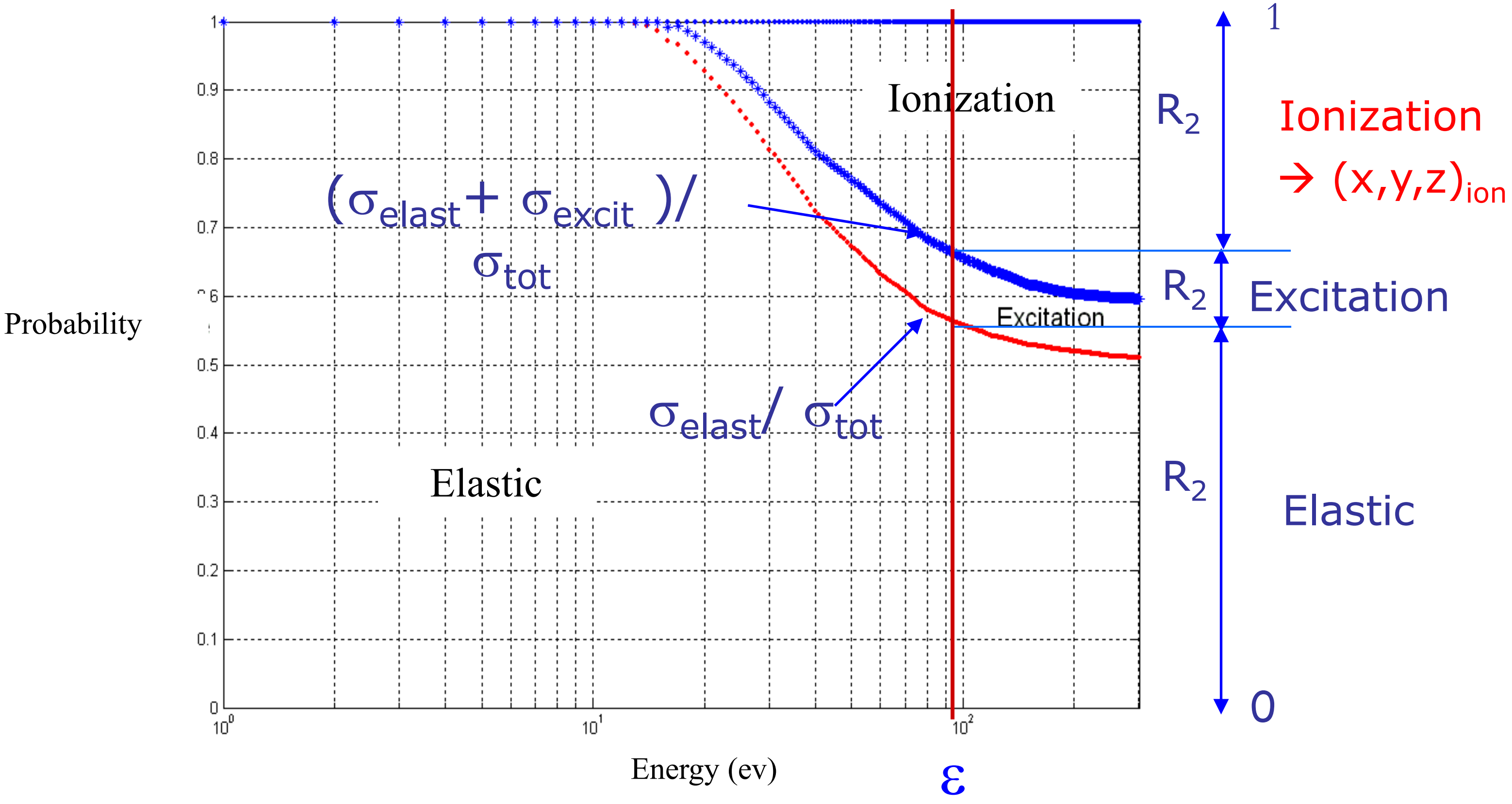
If R<P→ Collision
→ Definition of the collision type

R, random number uniformly distributed in the interval (0,1)

Monte-Carlo method

Step 3. Definition of the collision type and consequences on the incident electron orbit

R_2, random number uniformly distributed in the interval (0,1)



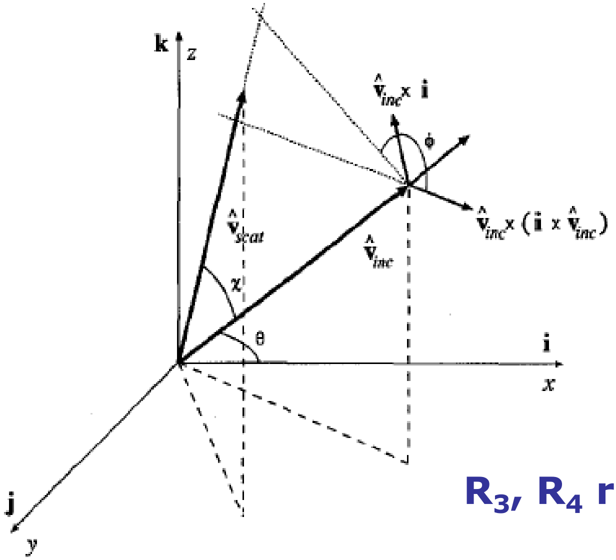
Monte-Carlo method

Consequences :

- **Decreasing of the incident electron energy**

Collision	Energy decreasing (eV)
Elastic	0
Excitation	11,6 (Excitation pot.)
Ionization	15,8 (Ionization pot.)

- **Scattering of the incident electron velocity**

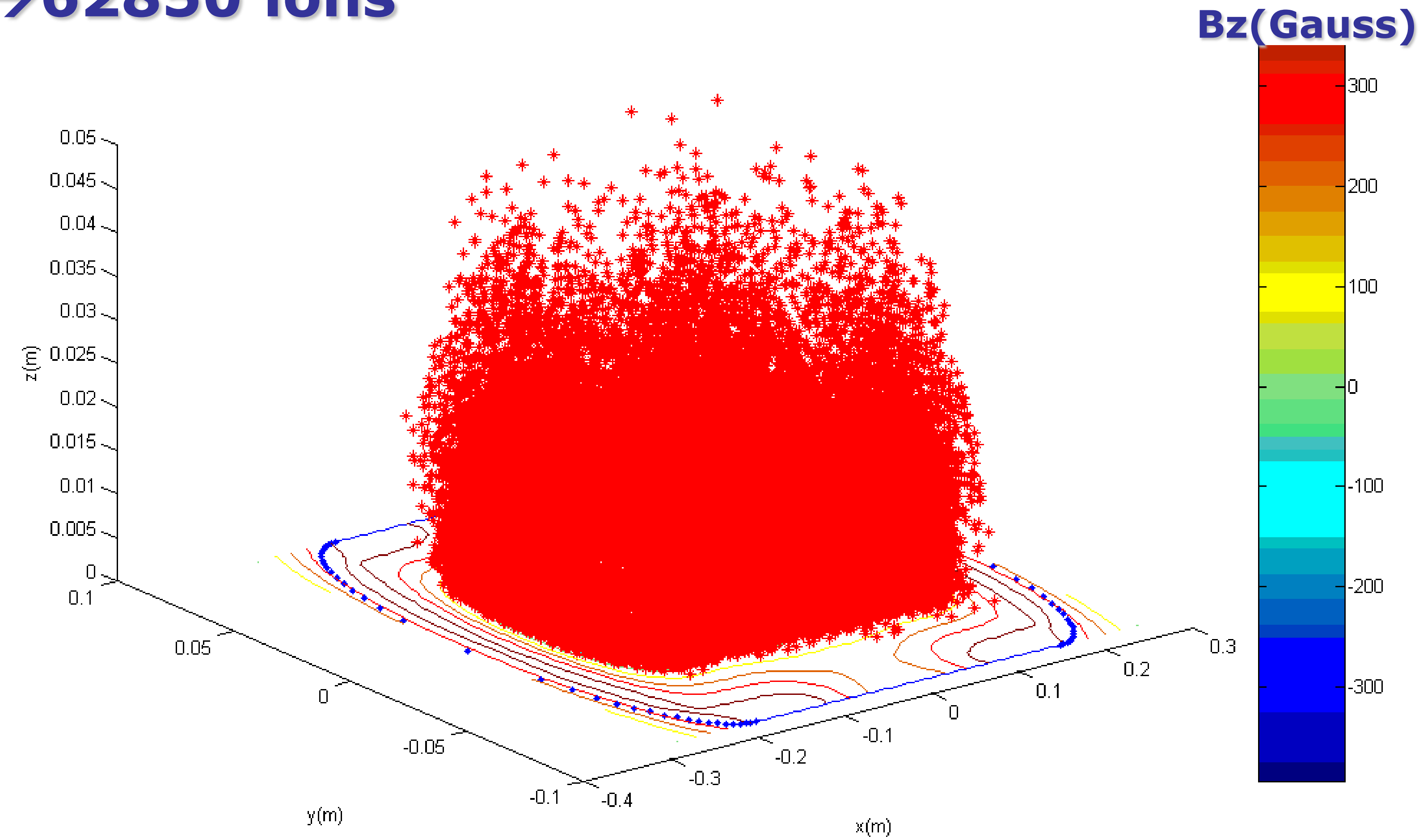


Scattering angles
$\chi = \frac{2+\varepsilon-2(1+\varepsilon)^{R_3}}{\varepsilon}$ $\phi = 2\pi R_4$

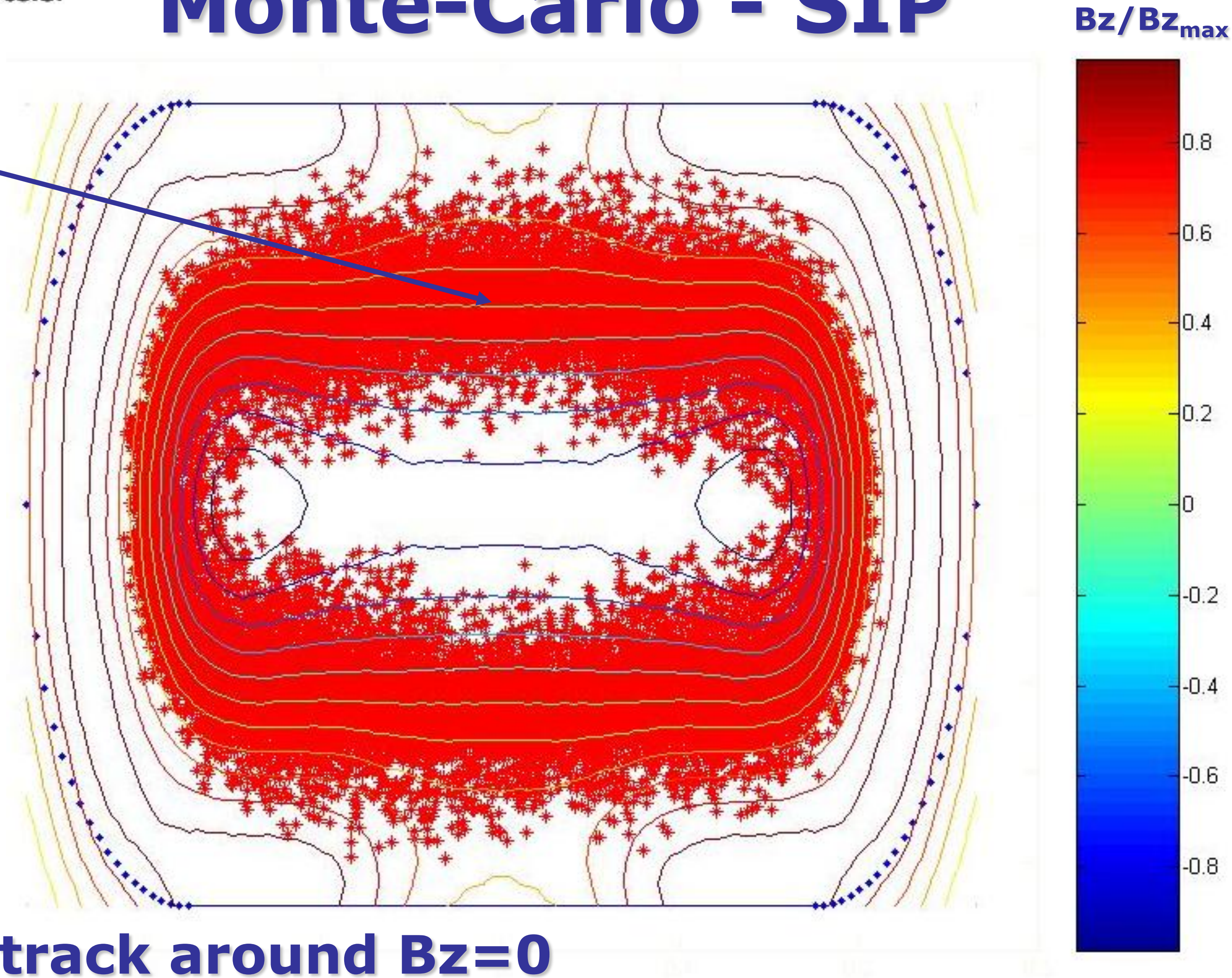
R_3, R_4 random numbers uniformly distributed in the interval (0,1)

Monte-Carlo - SIP

Distribution of ionization points : 34000 secondary electrons from the projections of ionization sites on target →62850 ions



Monte-Carlo - SIP



Bz=0

→ race-track around Bz=0

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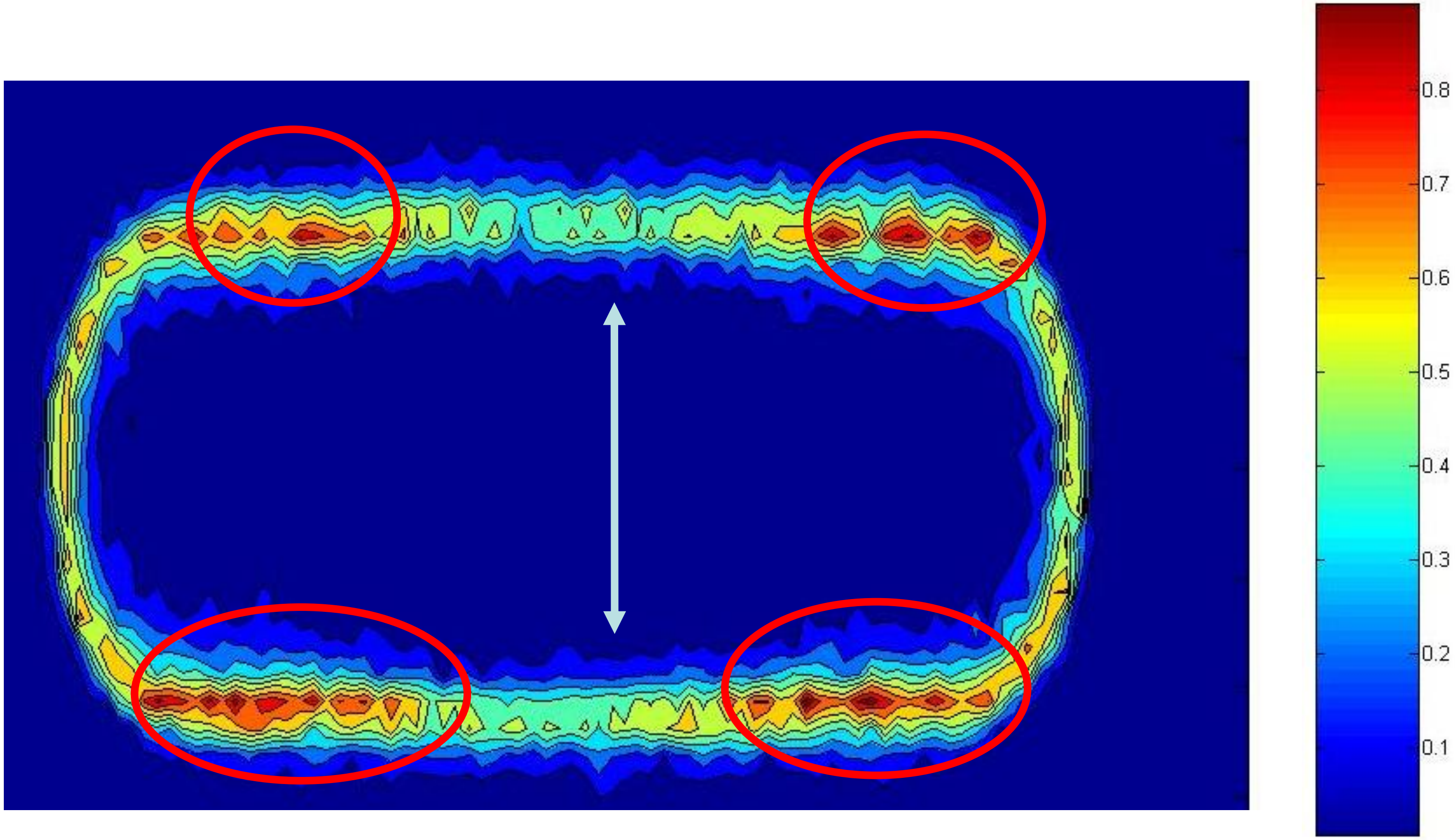
Monte-Carlo - SIP

Normalised distribution of ionization points

→ Normalised distribution of ion bombardment heat flux



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Heat transfer model

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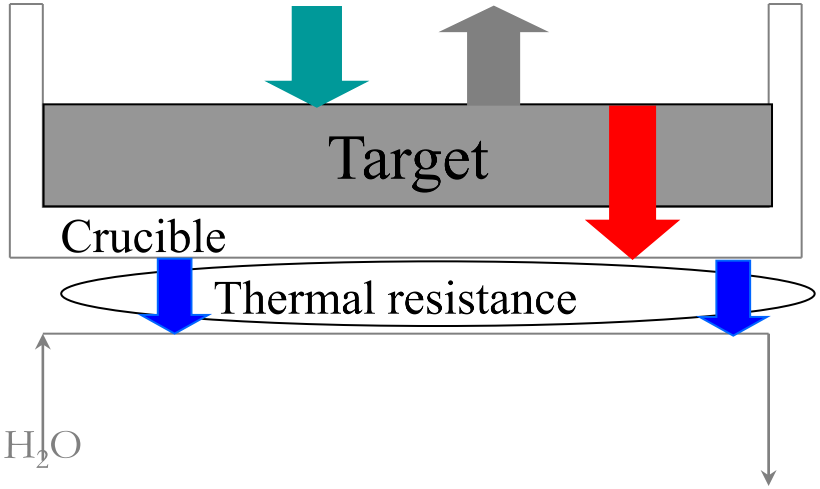


- Conduction through target and crucible

Lower crucible surface

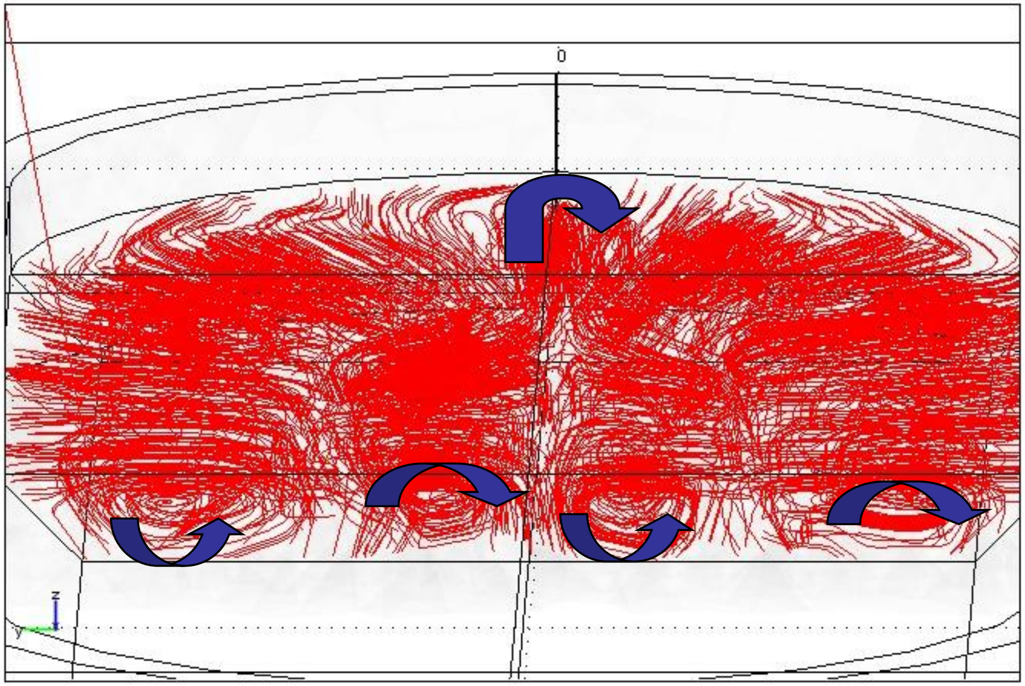
- Exchange between the lower crucible surface and the water flow through thermal resistance

Target Level

- Heat flux due to the ion bombardment (MC)
- Heat flux lost because of target evaporation

Heat transfer model

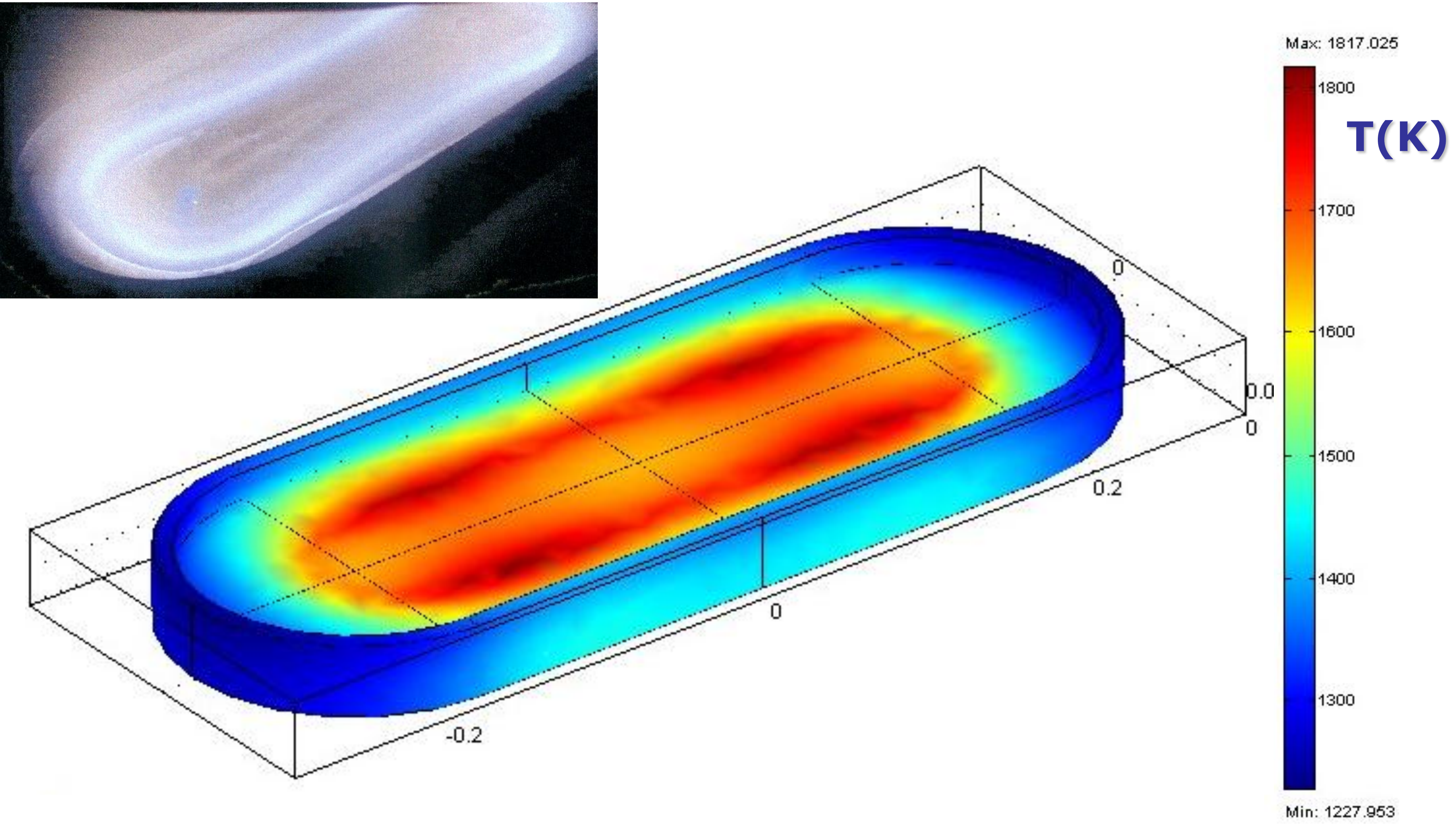
- **Free convection in the liquid target due to variation of the density with temperature**



- **Radiative heat transfer between target, crucible, substrate and enclosure not taken into account accurately with Femlab**

→ Need of improvement of the heat transfer model

Heat transfer model



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Evaporation model

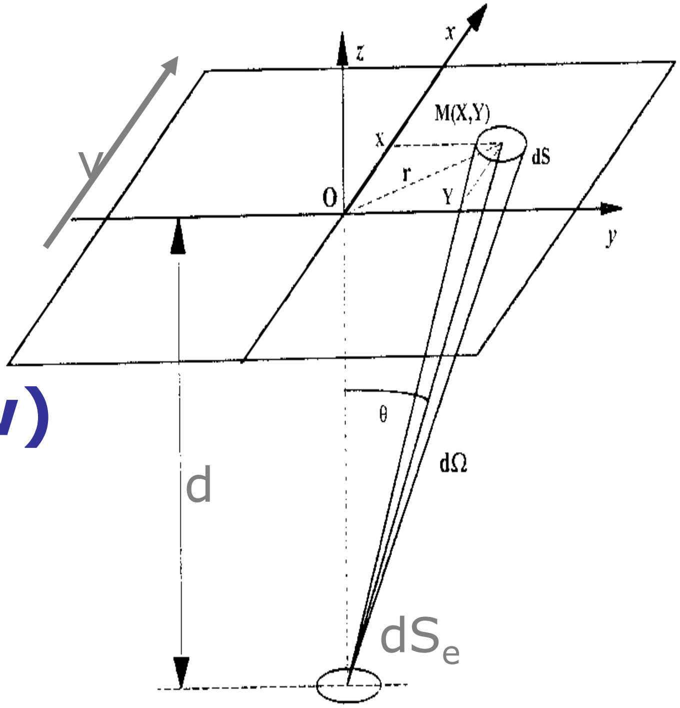
Temperature at the target level → thickness coating profile

Theory of evaporation from a point source

$$v_d = \sum_{i=1}^{i=nbr_{evap}} \frac{J_{ei} S_{ei} h^2}{\pi \rho ([(x_d - x_{ei})^2 + (y_d - y_{ei})^2] + h^2)^2}$$

$$J_{ei} = 0{,}5834 \sqrt{\frac{M}{T}} p_v$$ **(Knudsen's law)**

Tin: $p_v = 0.0075 * 10^{10.268 - \frac{15332}{T}}$



Displacement of the substrate taken into account

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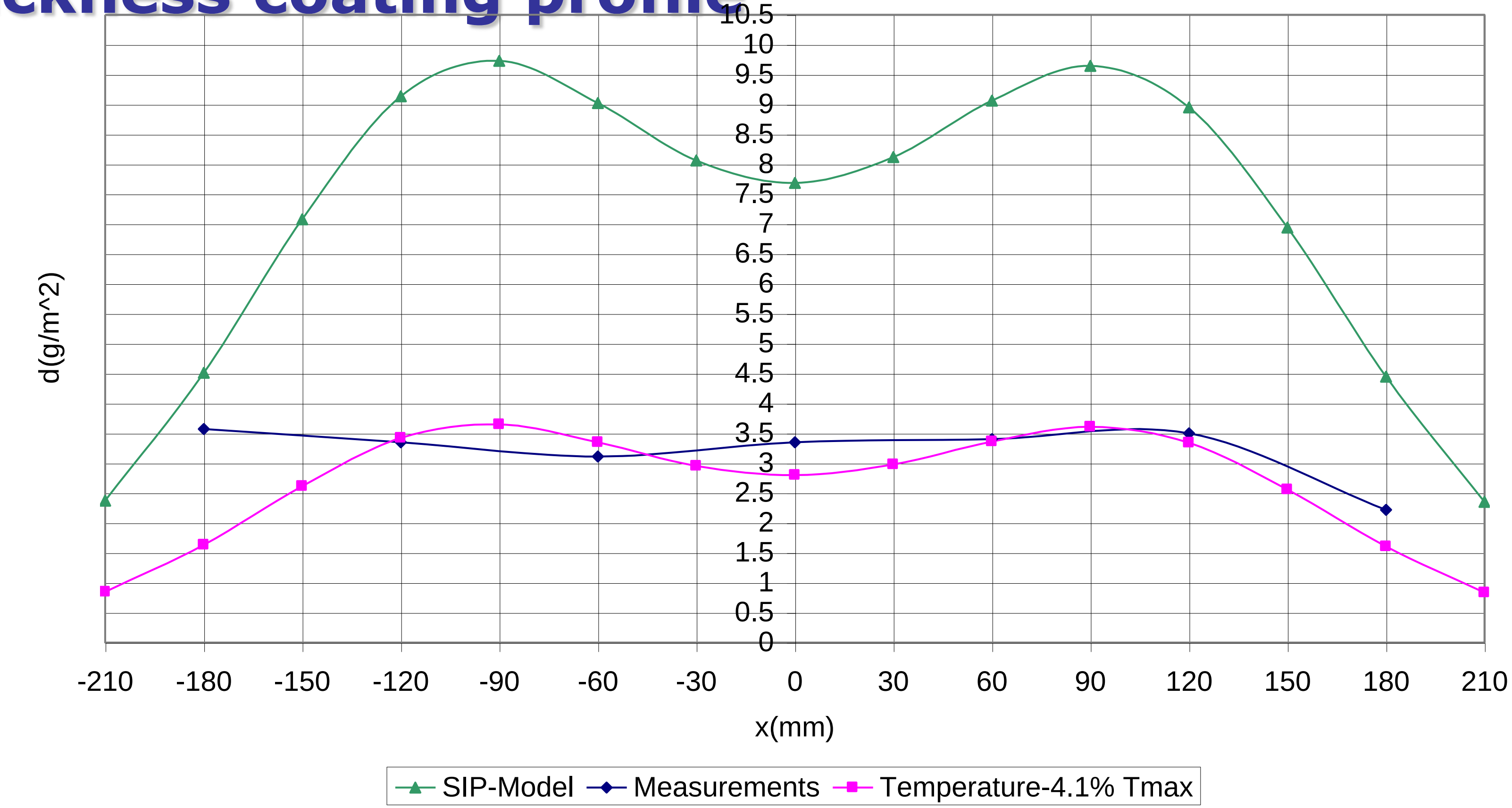
Evaporation model

Thickness coating profile



→ **Overestimation of the thickness measurements → radiation computation**

→ **No symetry of measurements → new tests planned**

→ **System very sensitive to temperature variation**

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Conclusions

- Modelling of the SIP

Magnetic model → Heat transfer model → Evaporation model

- Monte-Carlo method → ion bombardment heat flux distribution

- Improvements of the model :
  - Computation of radiative heat transfer
  - New tests are planned to validate model