Numerical analysis of the e-beam/sputter/liftoff process

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Outline

Topics:

- Facilities
- Liftoff process
- EBL mask fabrication
- Pattern transfer by liftoff
- Sputtering process
- Monte Carlo sputtering
- Computational results

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Facilities

- Lithography
  - Optical
  - Electron beam
- Deposition (mainly sputtering)
  - 2 x UHV Magnetron sputtering (S/F)
  - High pressure reactive sputtering (Oxides)
  - RF diode sputtering (Z-400)
  - Evaporation (K-cell)
- Etching
  - Wet etching
  - Ion beam etching / Ion milling

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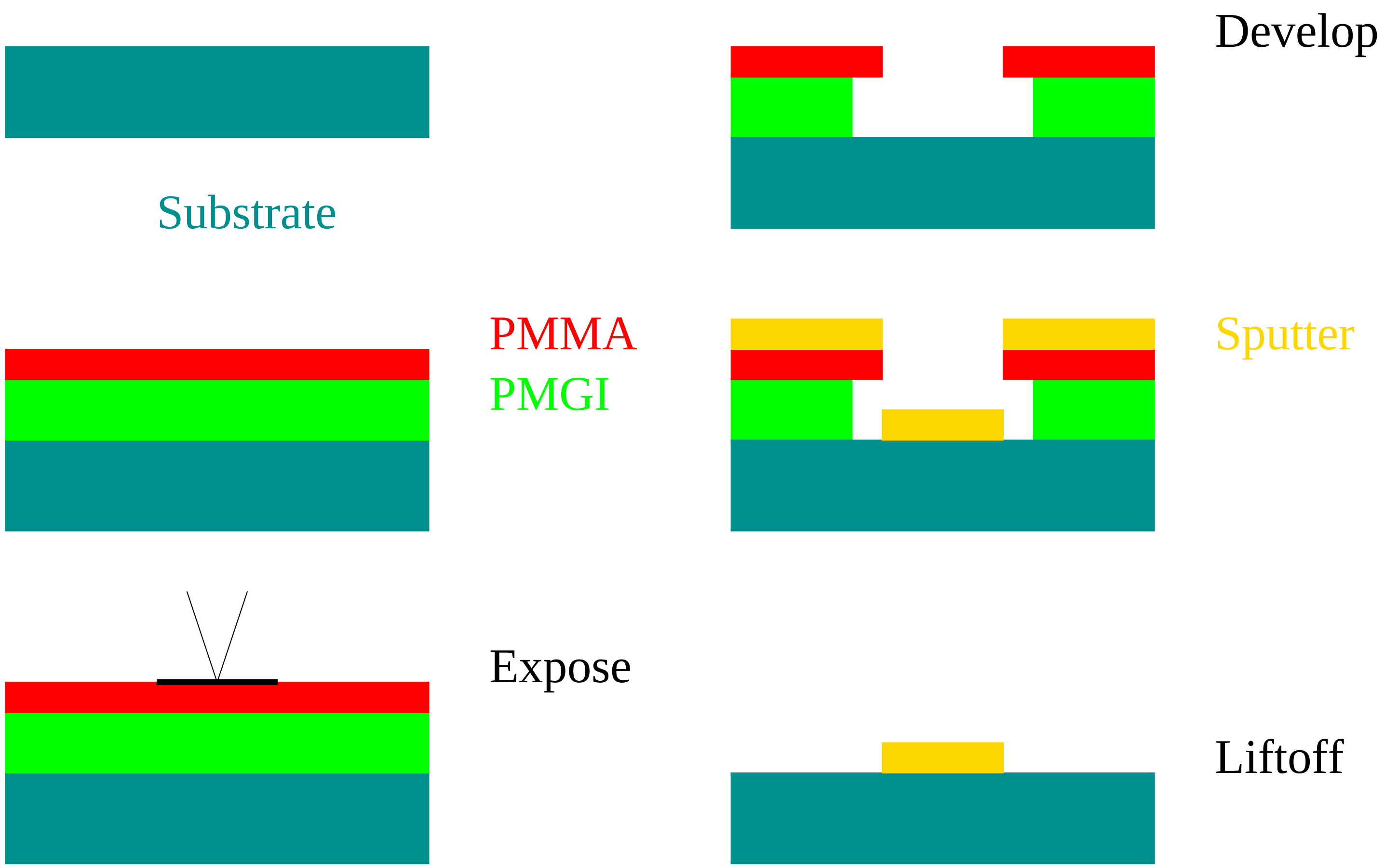
Lift-off process



Substrate

PMMA
PMGI

Expose

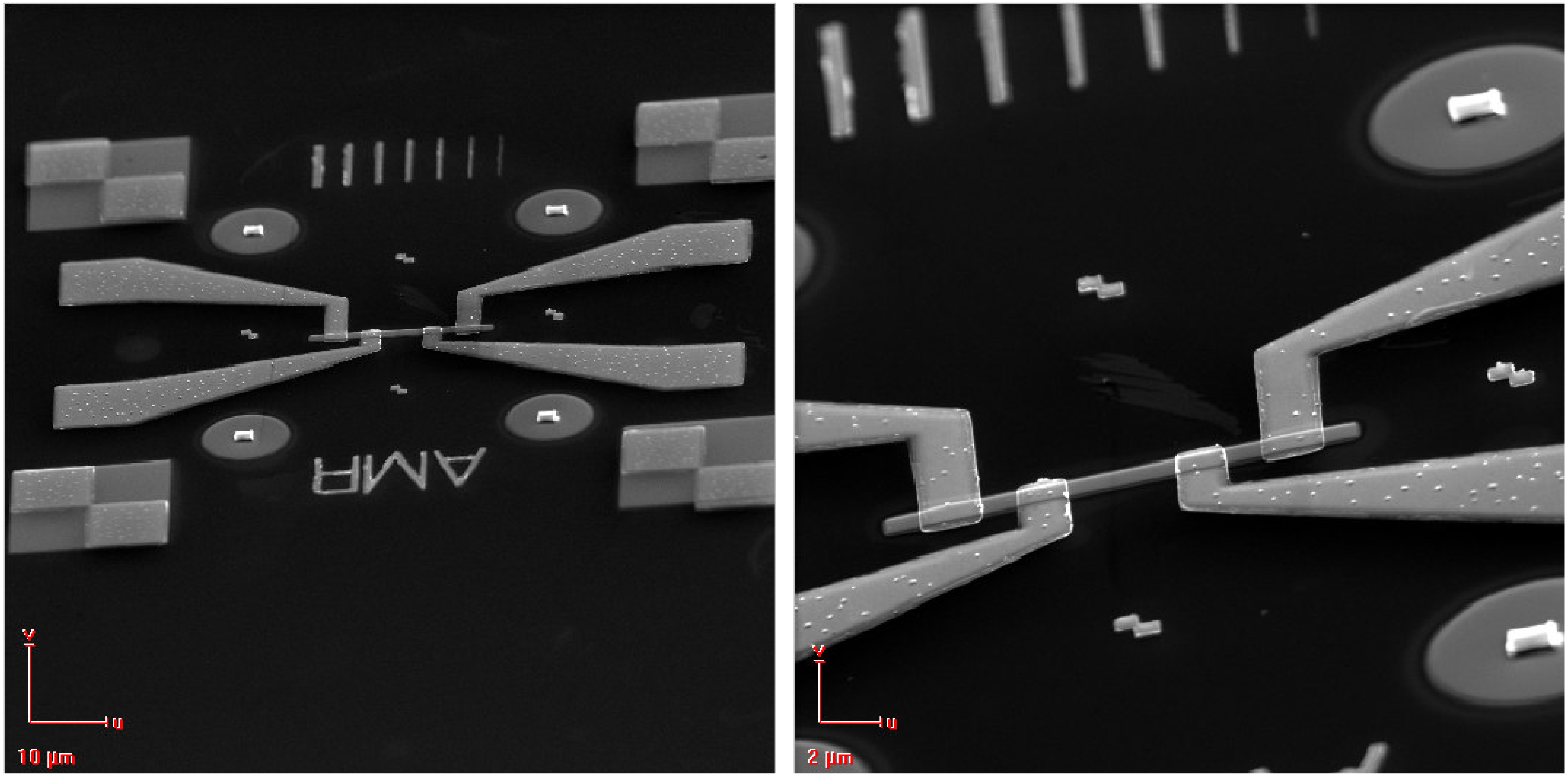
Develop

Sputter

Liftoff

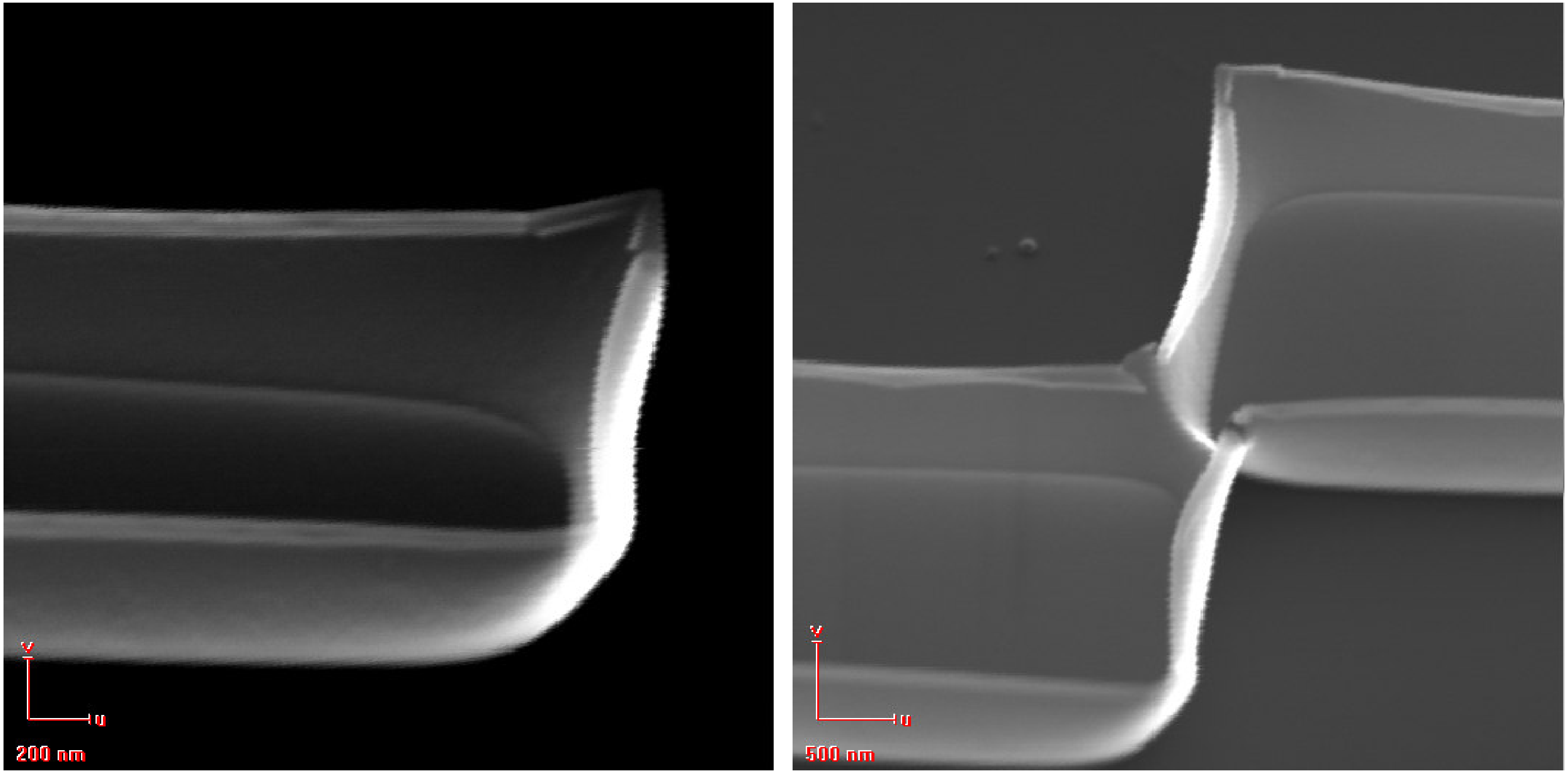
We can do this with sputtering!

Lift-off: a typical structure



Well-defined sharp edges

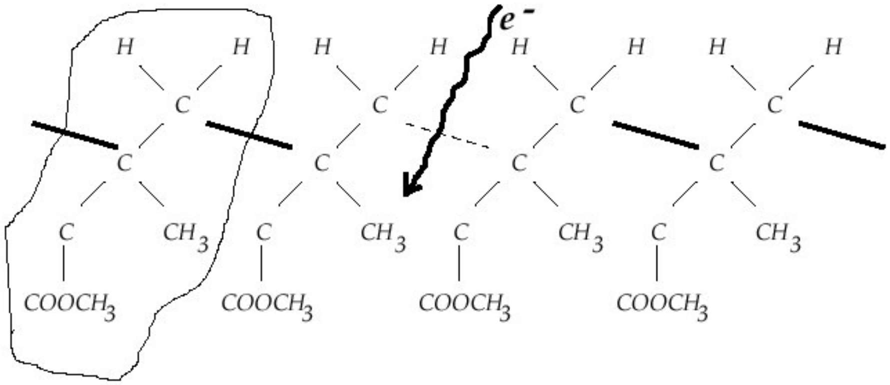
Liftoff: Oops

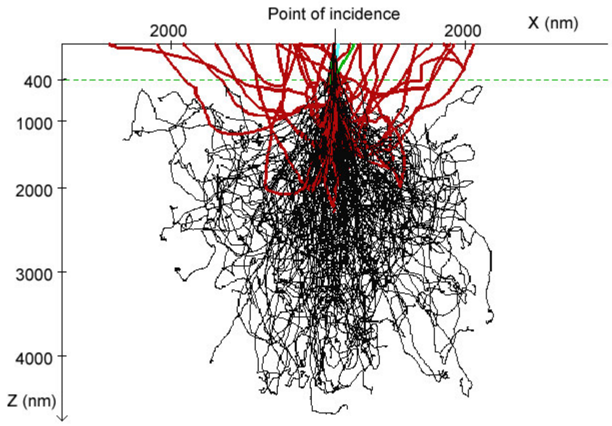


Failure: Several nm thick, 600 nm high edges!

E-beam lithography

EBL: modify a *resist* locally by electron bombardment so that the solubility in a *developer* is changed.





Acc. voltage = 30keV, beam diam. = 25nm, 400nm thick PMMA on Si

- secondary electrons
- forward scattering
- backscattering

2-gaussian model

1D proximity effect:
$dose(x) = pattern(x) * scatter(x)$

where $*$ is the infinite convolution
$f * g = \int_{-\infty}^{\infty} f(\xi) g(x - \xi) d\xi$

and
$scatter(x) = \frac{1}{\sqrt{\pi}(1+\eta)} \left(\frac{1}{\alpha} e^{\frac{-x^2}{\alpha^2}} + \frac{\eta}{\beta} e^{\frac{-x^2}{\beta^2}} \right)$

$scatter(x)$ is normalized: $\int_{-\infty}^{\infty} scatter(x) dx = 1$

Typical values for 500 nm PMMA on Si:
$\alpha = 75$nm, $\beta = 3000$nm, $\eta = 0.7$ (Casino, test patterns etc.)

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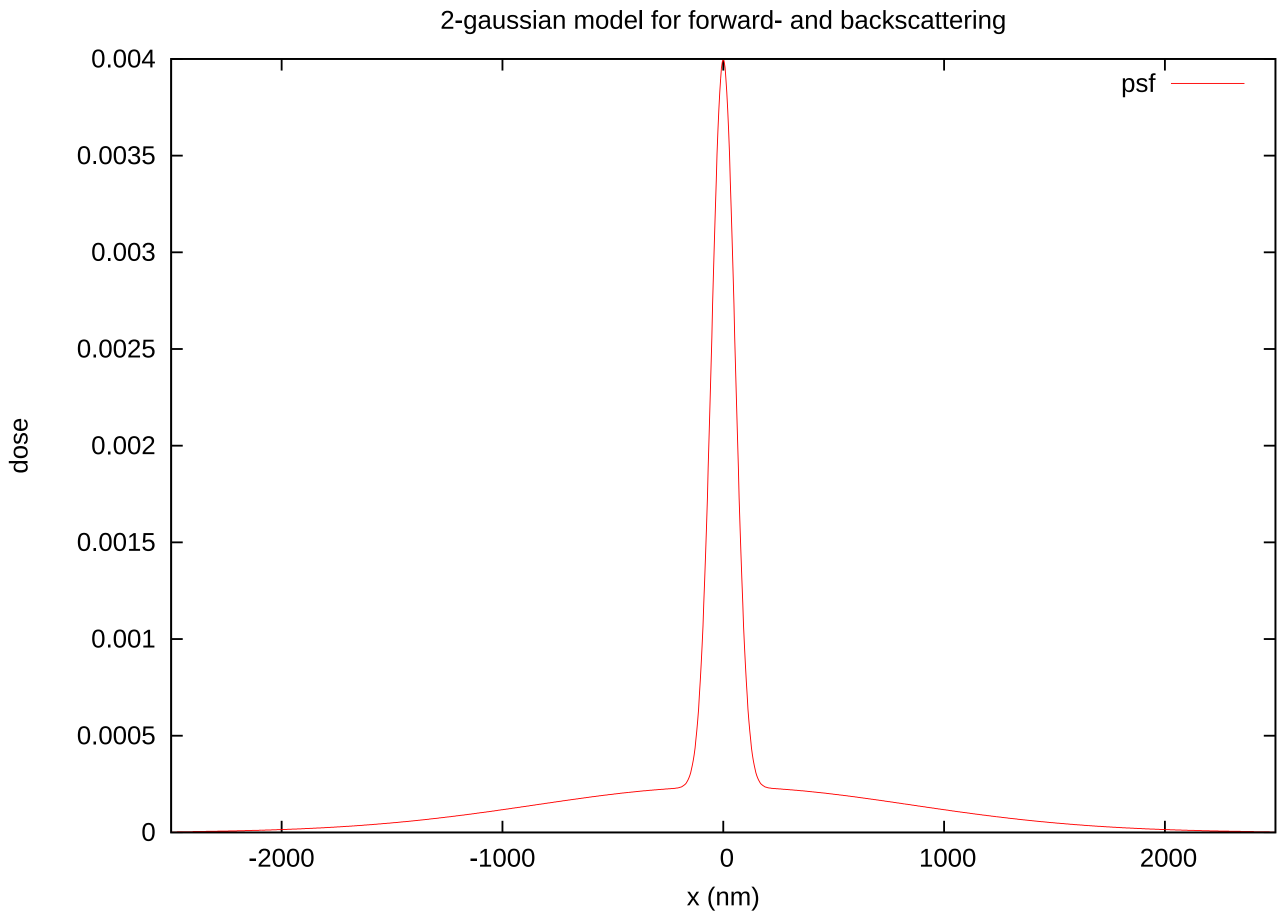
EBL example: PMGI/PMMA bilayer



Scatter distribution

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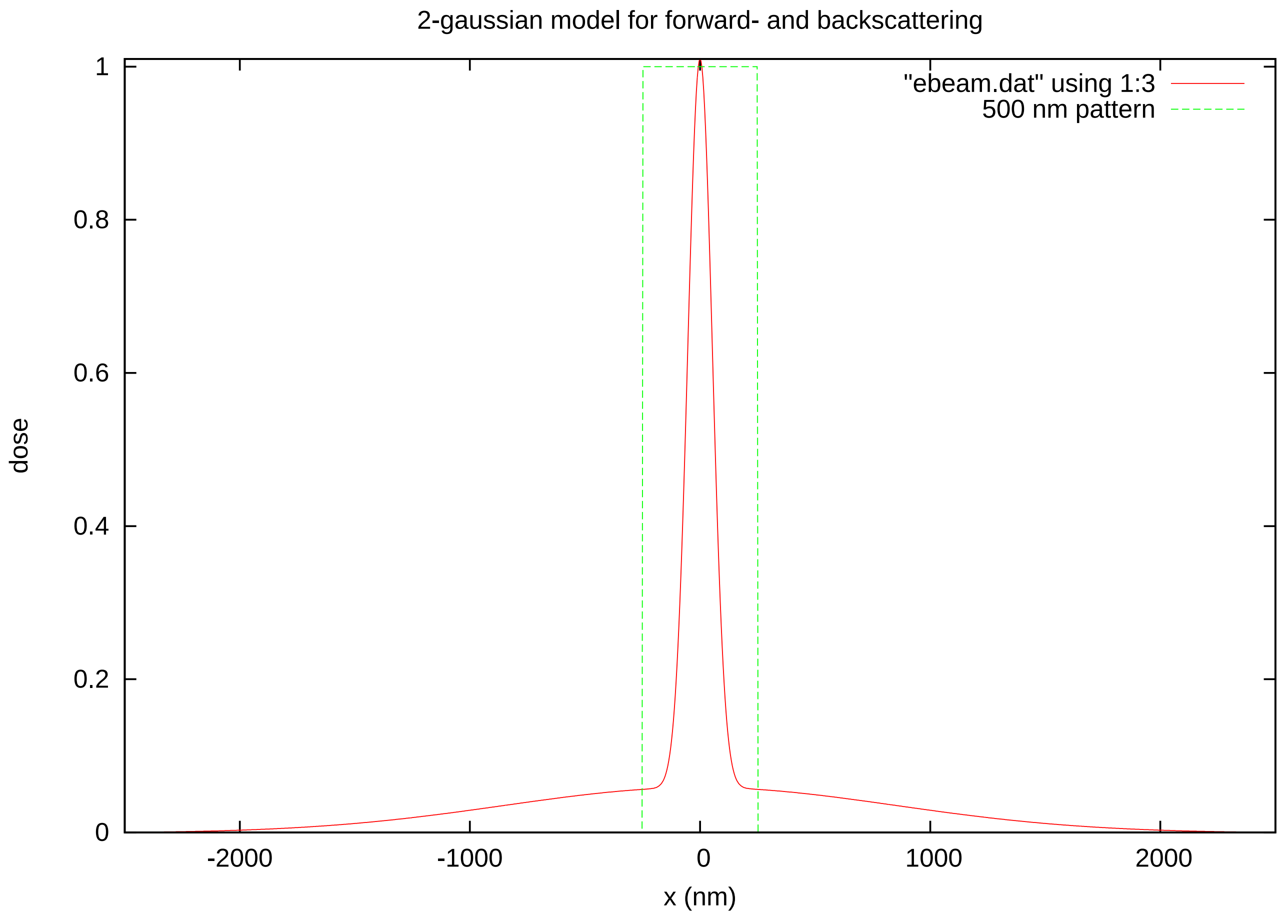
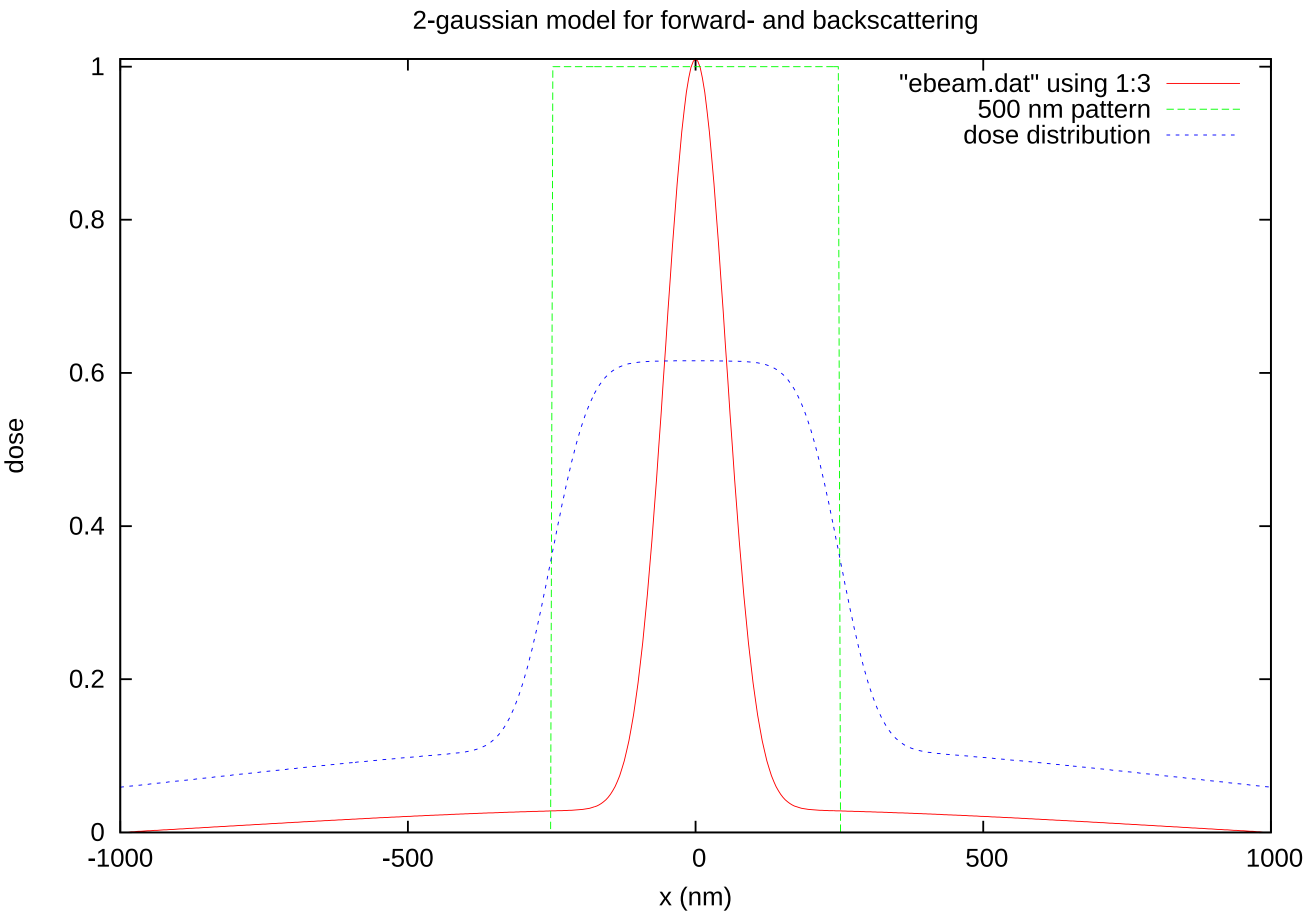
EBL example: PMGI/PMMA bilayer



500 nm Pattern

EBL example: PMGI/PMMA bilayer



Dose profile

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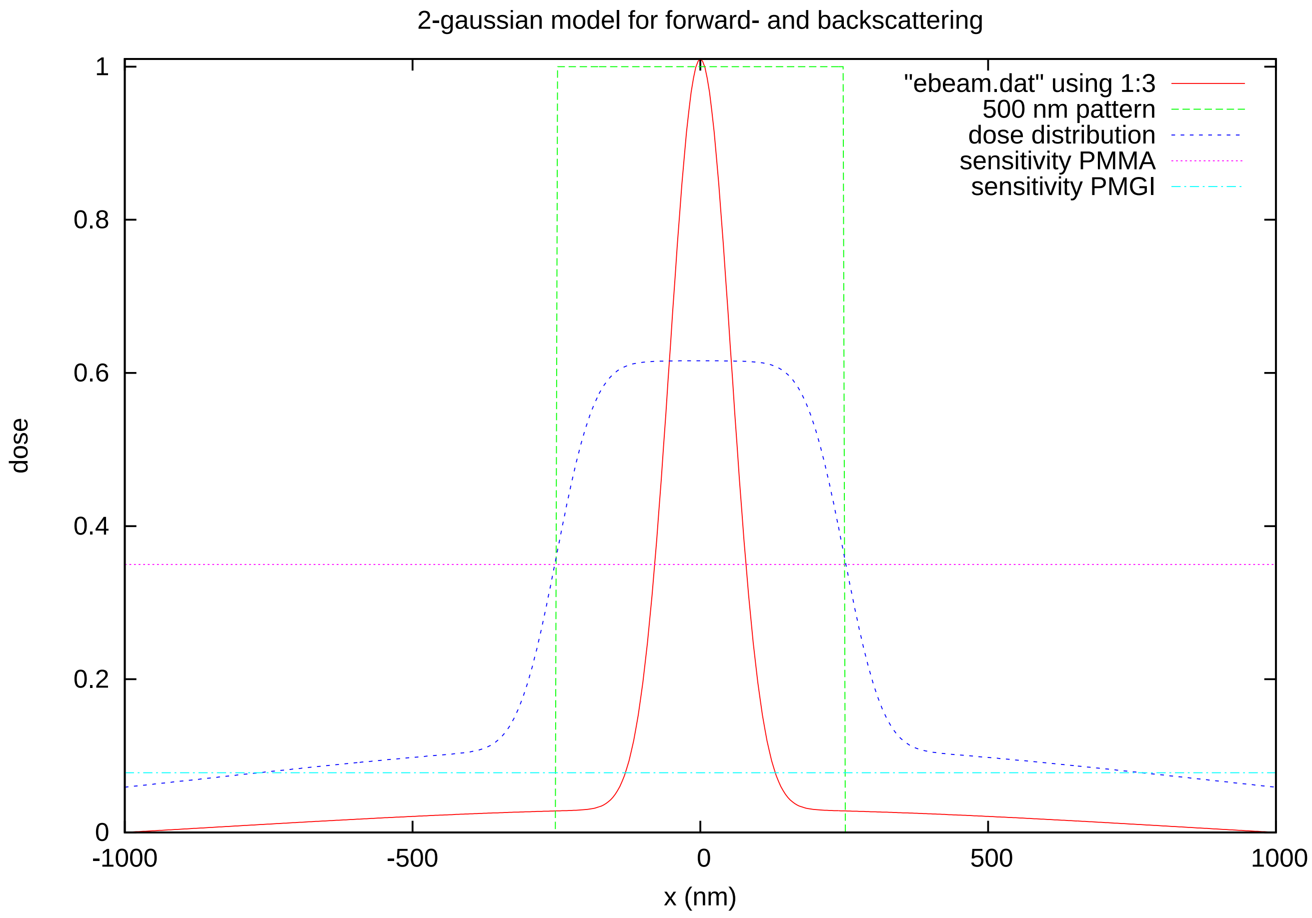
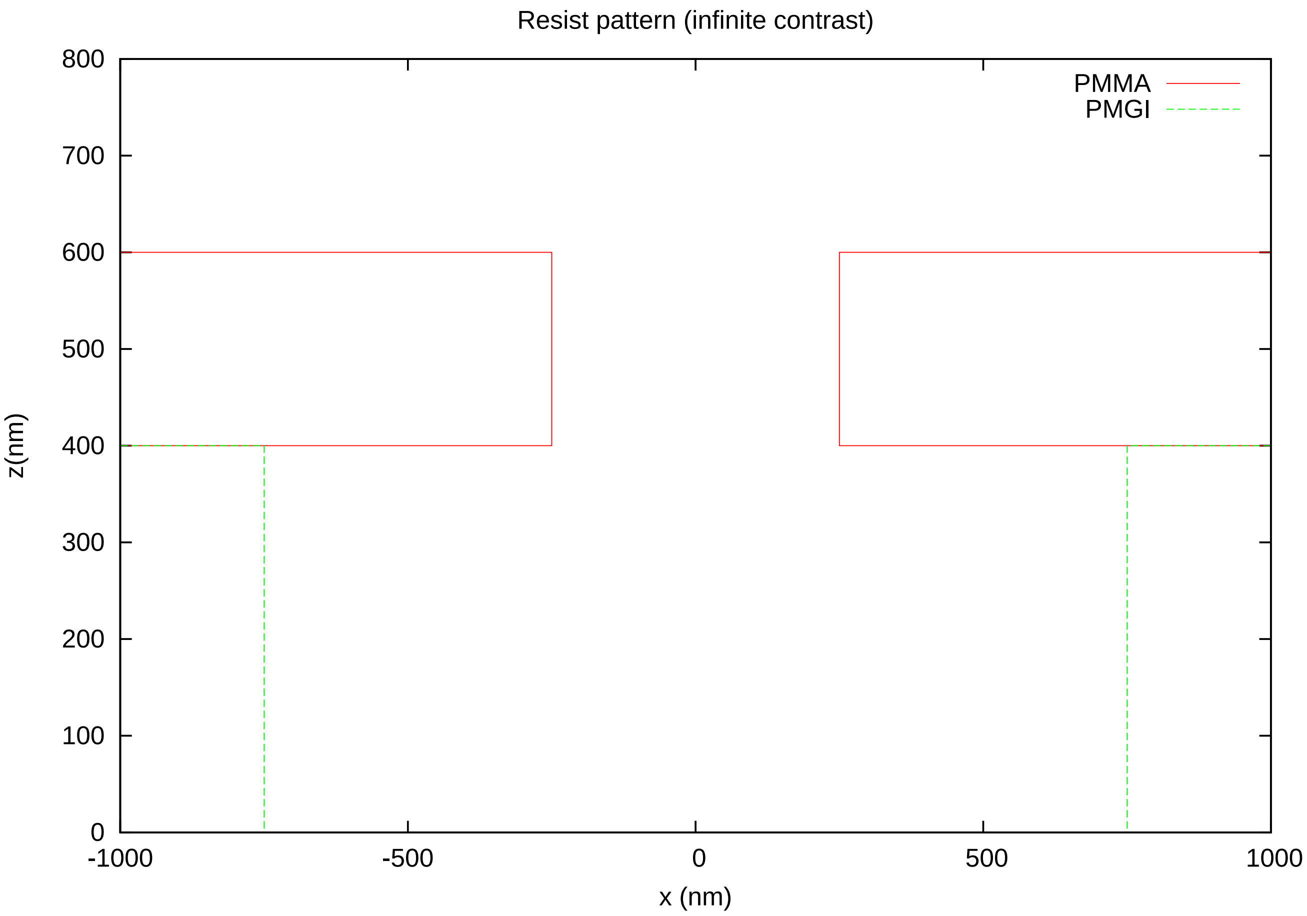
EBL example: PMGI/PMMA bilayer



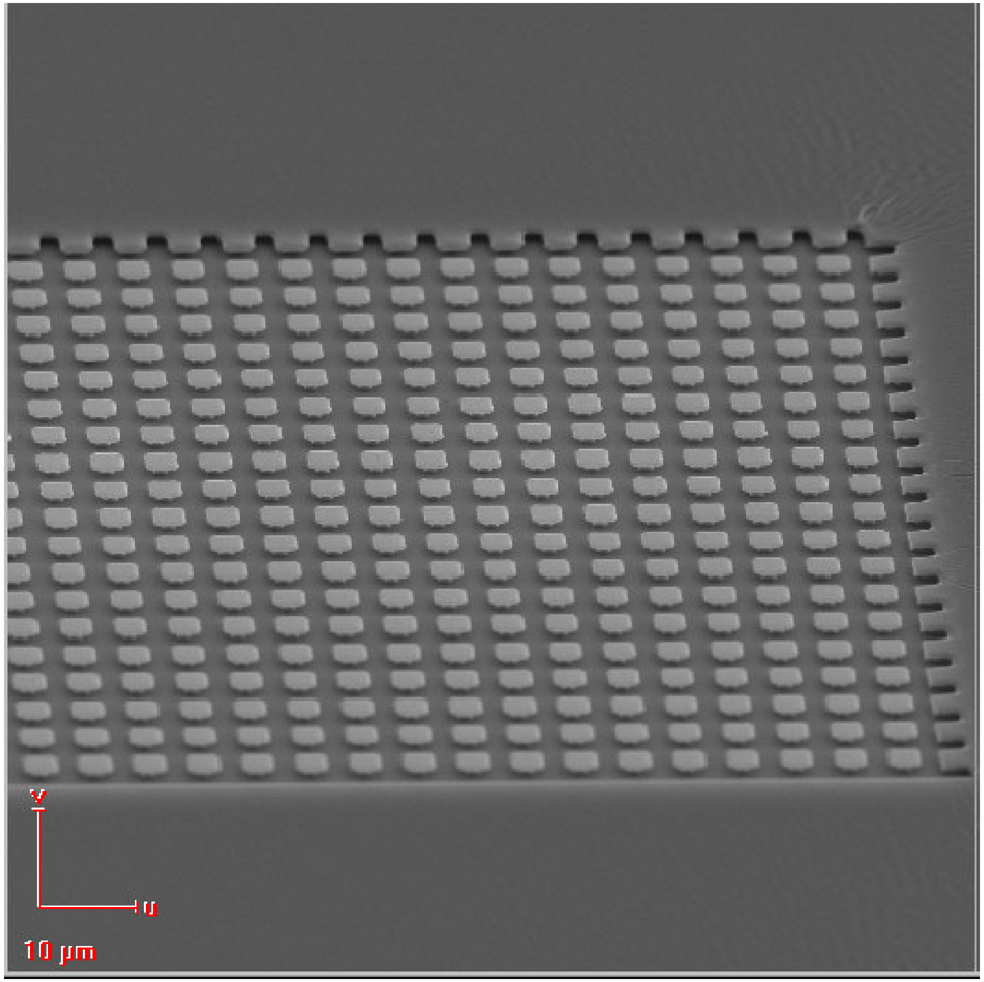
Clearing criterion: $dose(x) \geq d_{c_{resist}}$

EBL example: PMGI/PMMA bilayer



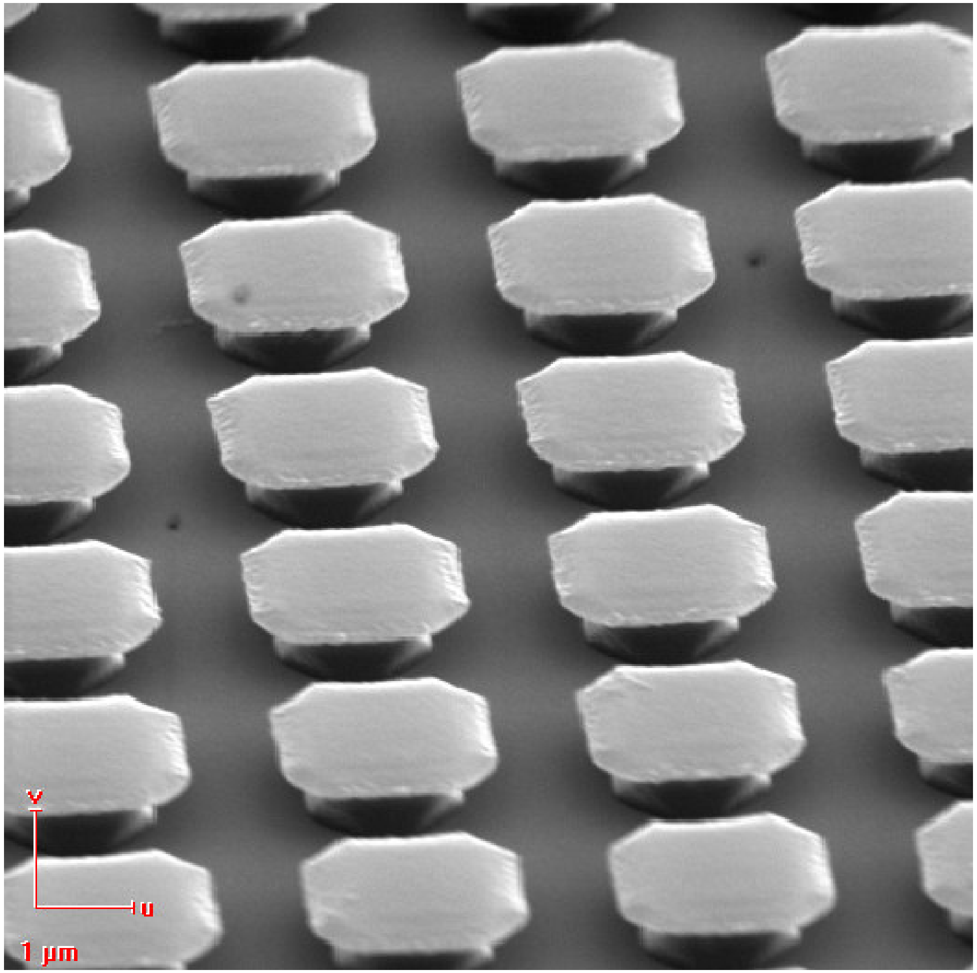
Resist after development (infinite contrast)

PMGI/PMMA bilayer: undercut pattern



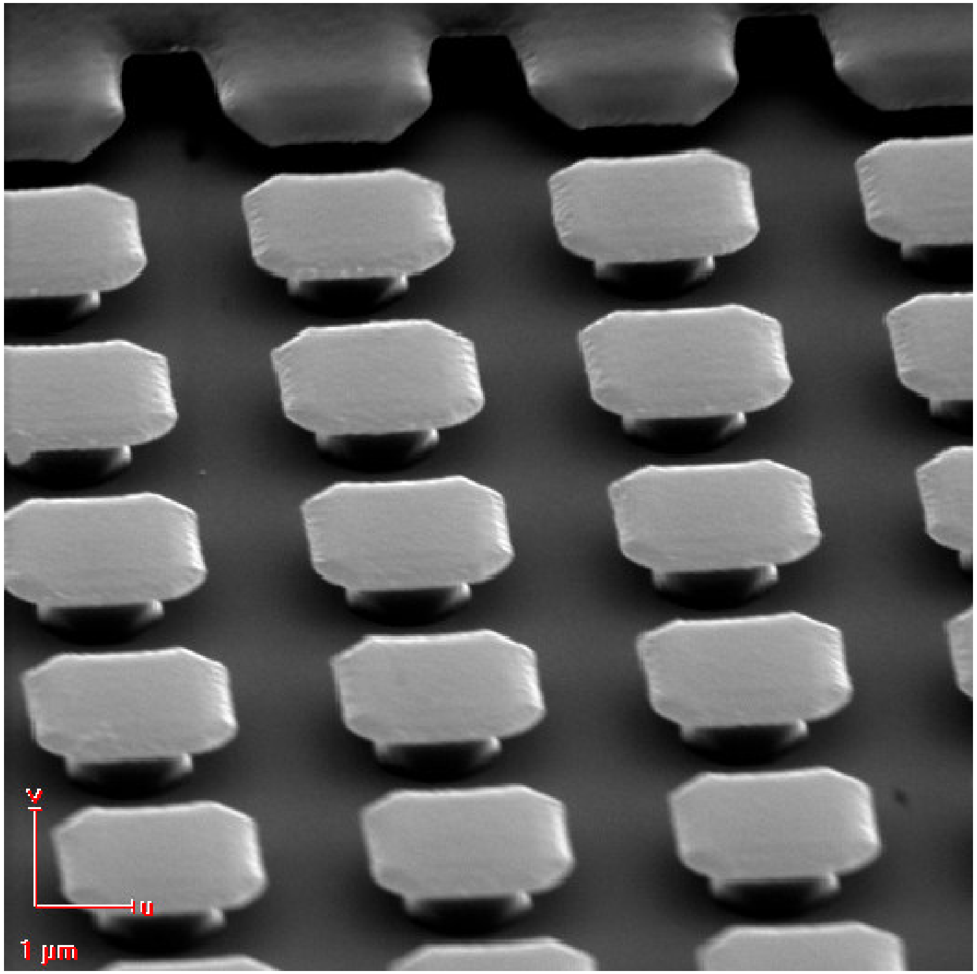
100 x 100 μm test field

PMGI/PMMA bilayer: dose scan



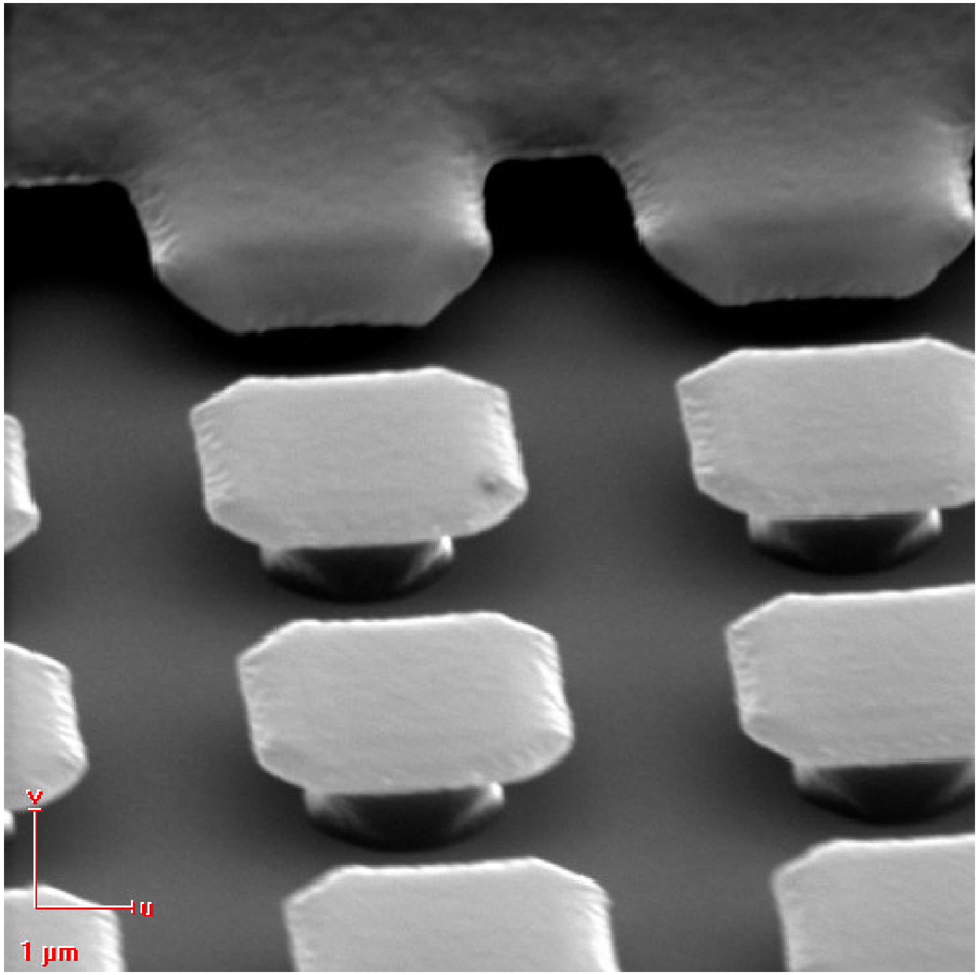
$80\mu C/cm^2$

PMGI/PMMA bilayer: dose scan



$88\mu C/cm^2$

PMGI/PMMA bilayer: dose scan



$96\mu C/cm^2$

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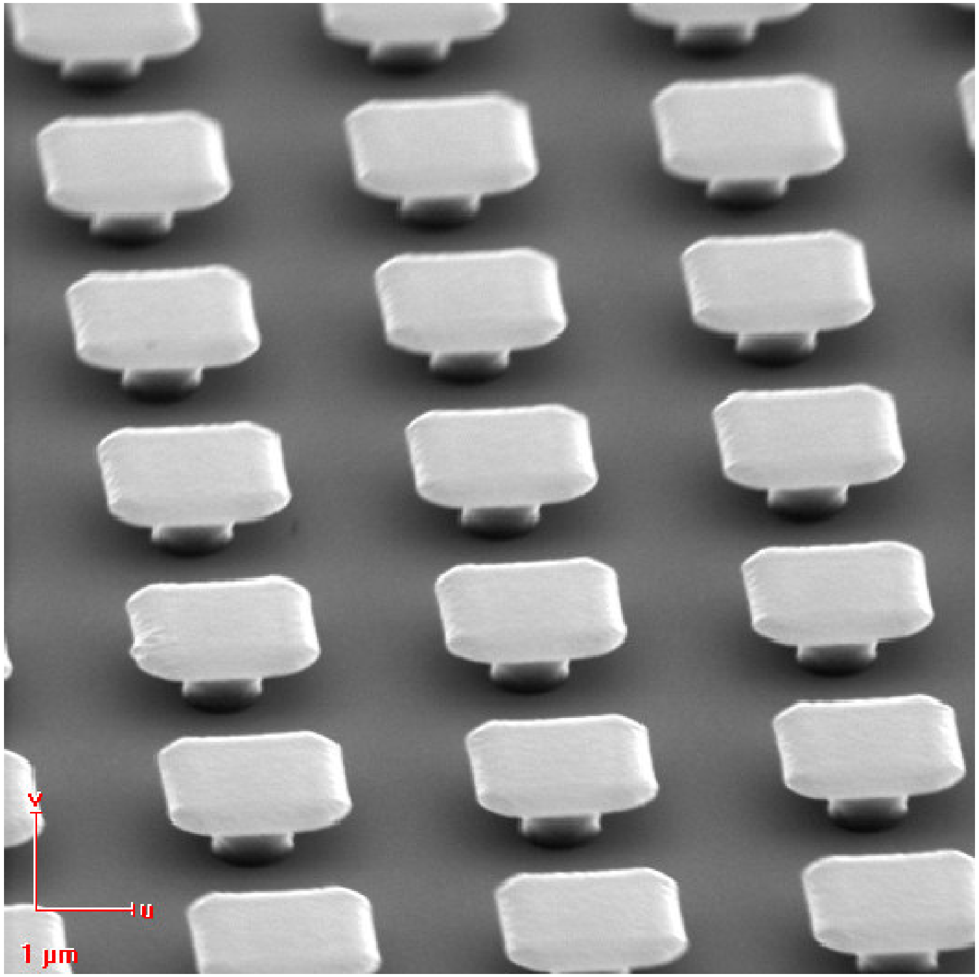
PMGI/PMMA bilayer: dose scan



$104\mu C/cm^2$

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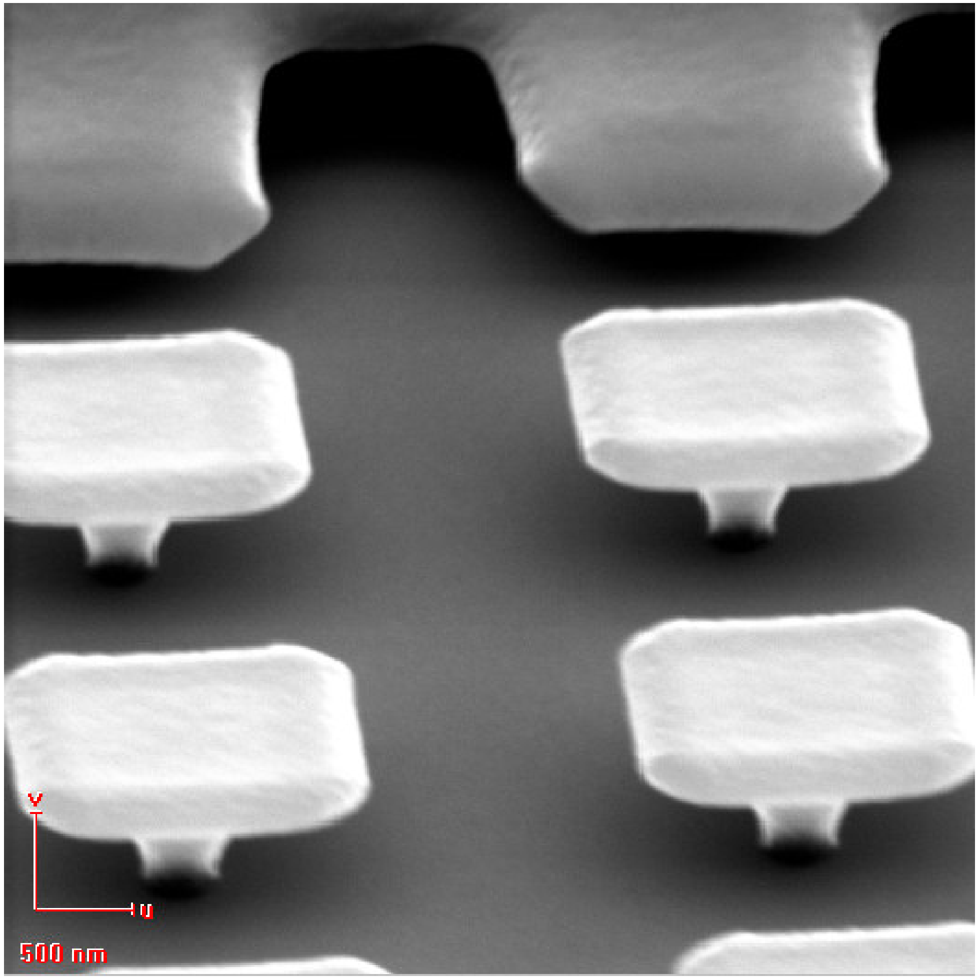
PMGI/PMMA bilayer: dose scan



$112\mu C/cm^2$

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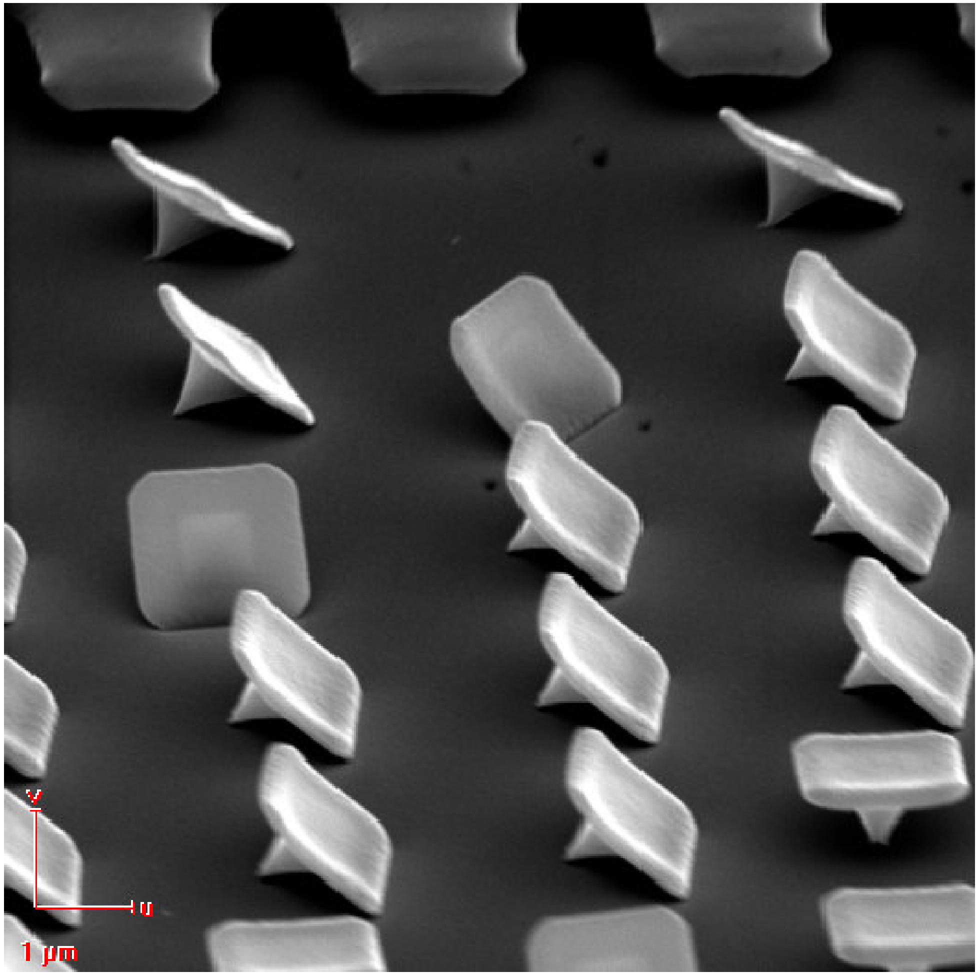
PMGI/PMMA bilayer: dose scan



$120\mu C/cm^2$

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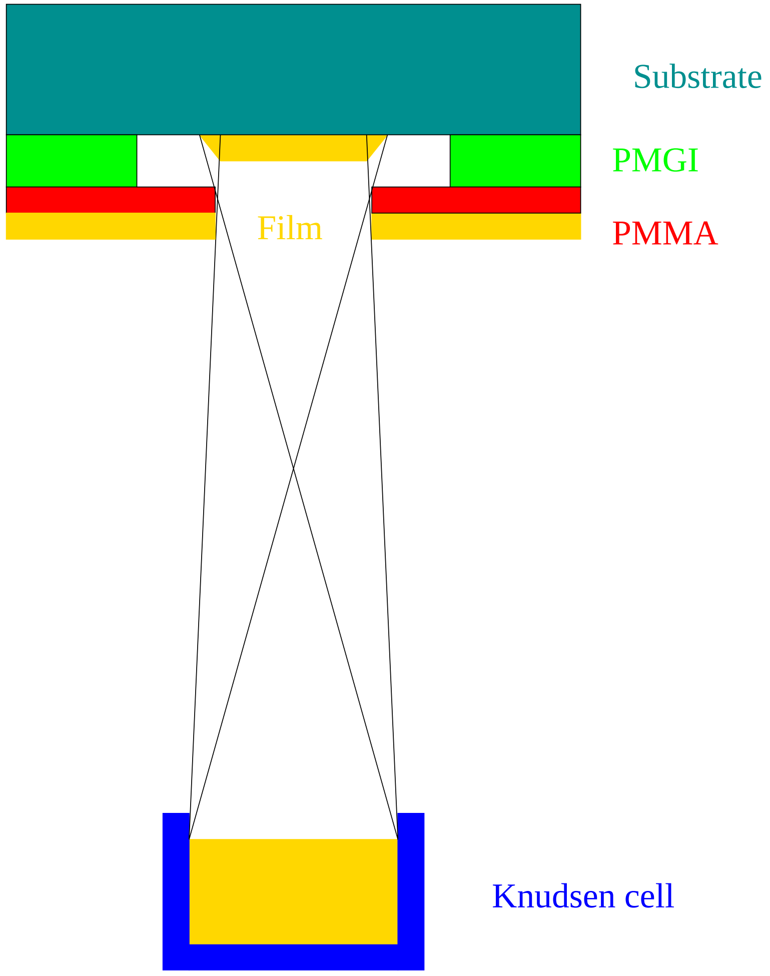
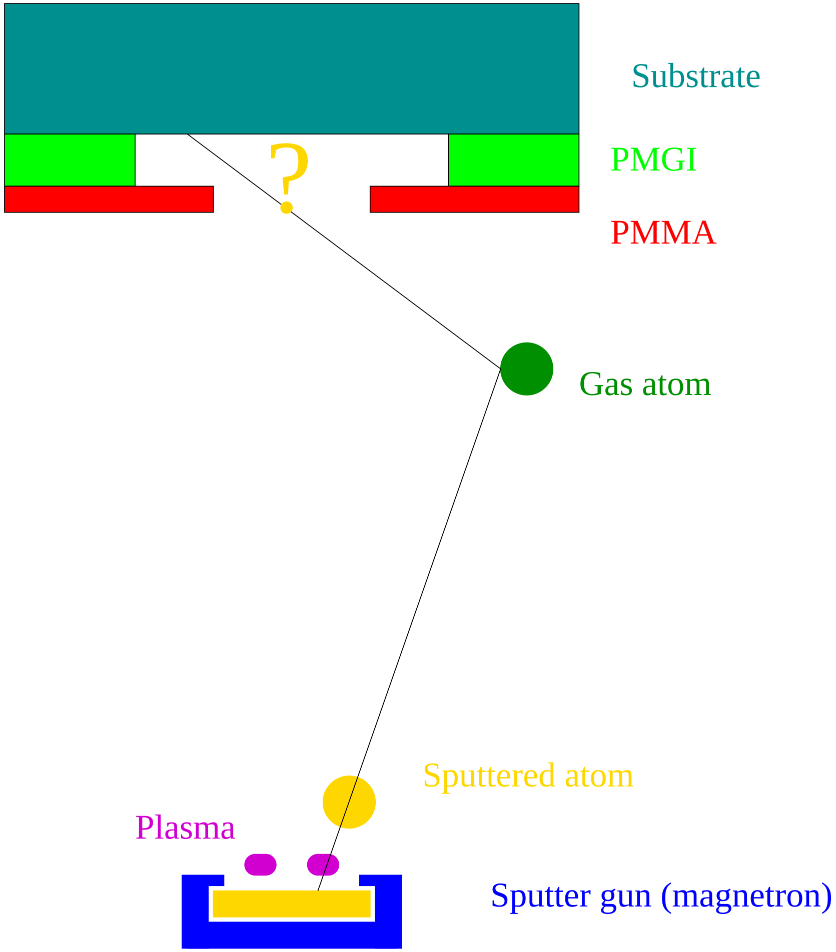
Pattern transfer: K-cell



$flux \sim \cos\phi$ (effusion)

Pattern transfer: Magnetron



What does the strip cross-section look like?

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Monte Carlo simulation of sputtering

Statelessness of MC is justified: collisions between sputtered atoms are rare and the effect of the collisions with the sputtering gas can be described by a (not so relevant) steady state temperature of the gas ($\approx$ 450 K)

We need a statistically accurate description of the sputtering process for a realistic geometry

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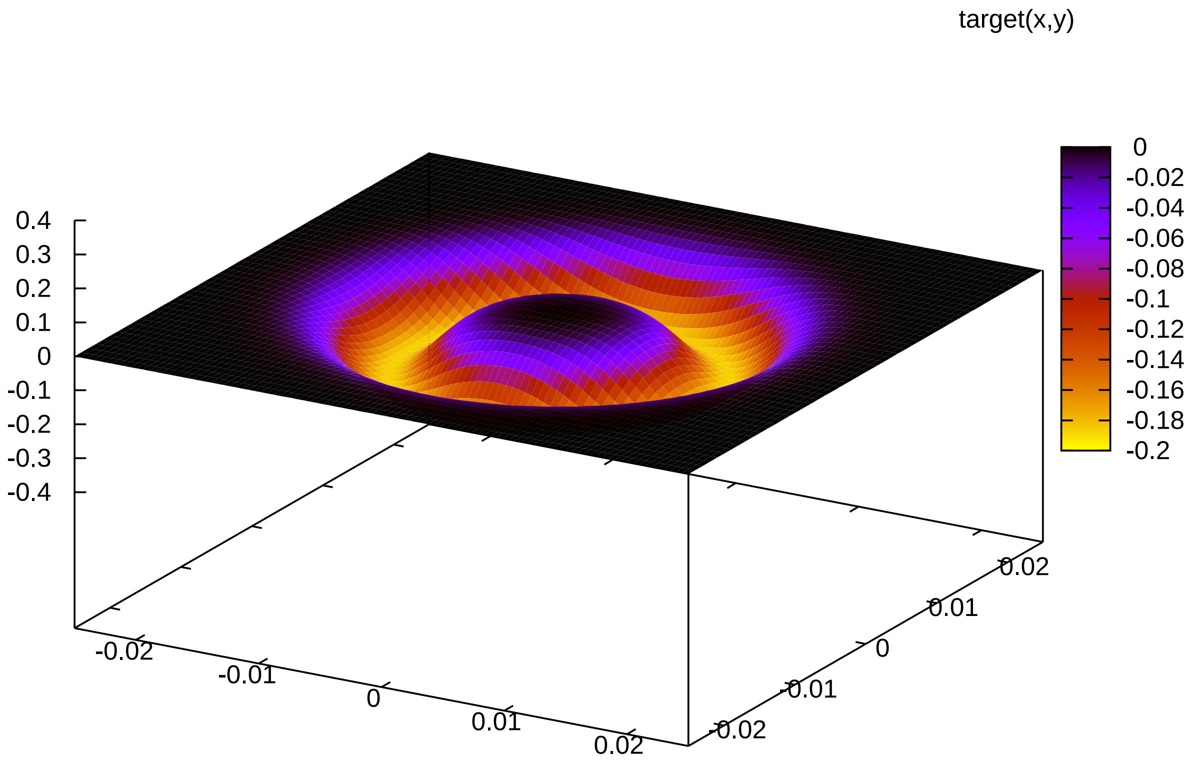
Sputtering: ion impact

- plasma: constant (low) potential region
- ionization fraction varies because B inhomogenous
- ions accelerate in Crooke’s dark space ⊥ target



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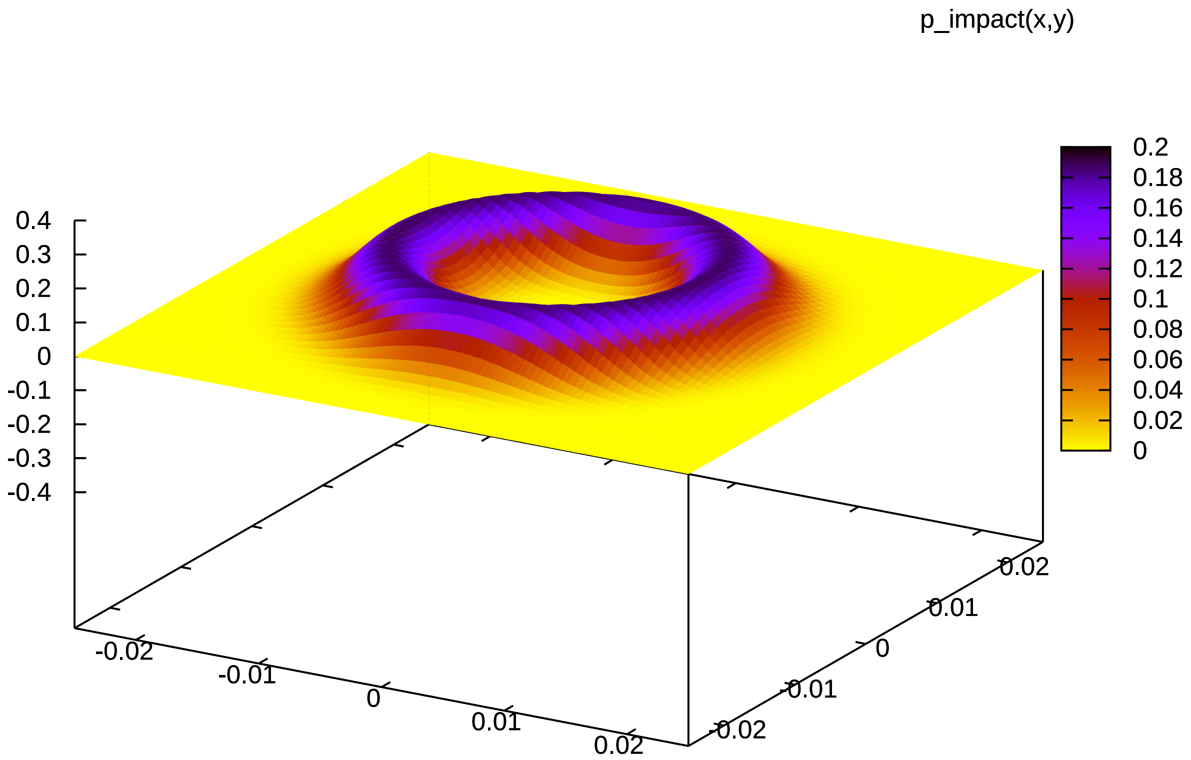

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Sputtering: ion impact

- plasma: constant (low) potential region
- ionization fraction varies because B inhomogenous
- ions accelerate in Crooke's dark space $\perp$ target

$P_{impact}(r, \theta) = N_{\mu,\sigma}(r) U_{[0,2\pi>}(\theta)$

Sample a normal distribution for r:

$r = \mu + \sigma N(\rho_1)$

and a uniform distribution for θ:

$\theta = 2\pi\rho_2$

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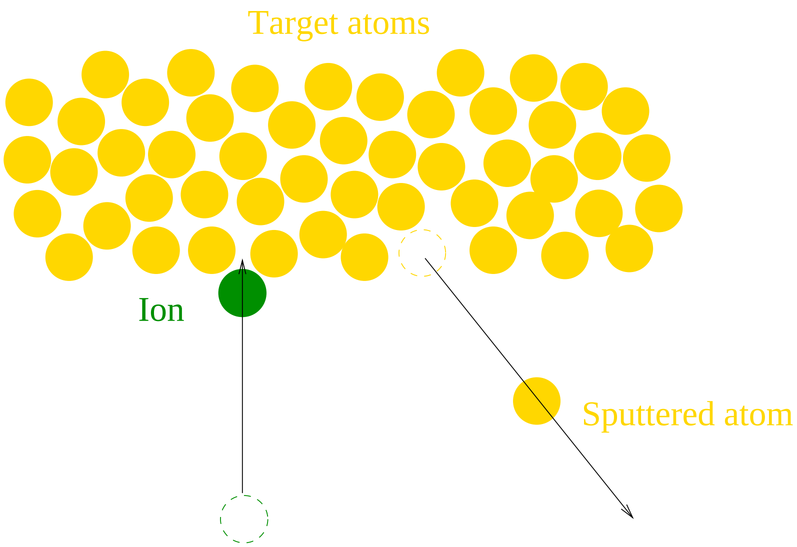
Sputtering: Nascent distribution



Thompson theory (accurate for amorphous targets)
Flux:

$$\Phi(E,\phi)d\Omega dE = \frac{\pi a^2 \Lambda E_a \eta D \Phi_1}{16} \cos\phi \frac{1-[(E_{surf}+E)/(\Lambda E_{ion})]^{1/2}}{E^2(1+E_{surf}/E)^3} d\Omega dE$$

$$E_a = \frac{2E_R(Z1Z2)^{7/6}(m_t+m_g)}{em_g}, \; \Lambda = \frac{4m_t m_g}{(m_t+m_g)^2}$$

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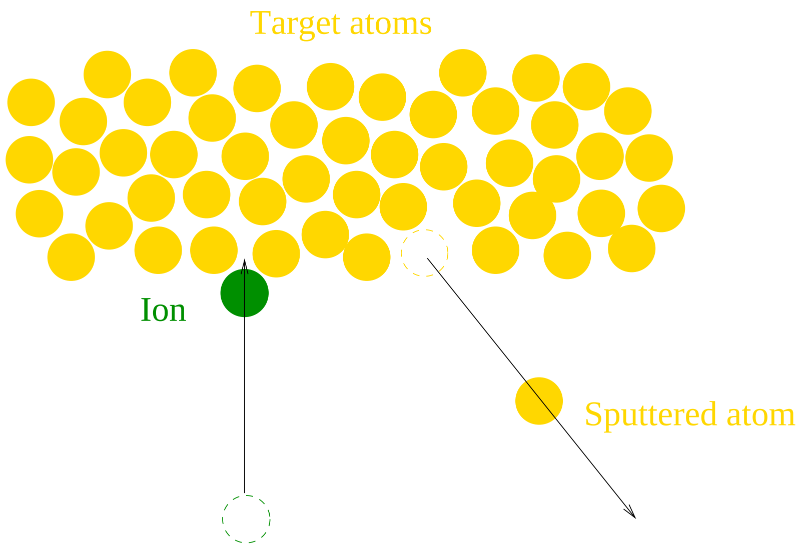
Sputtering: Thompson distribution



Thompson:

$$\Phi(E,\phi)d\Omega dE \sim \cos\phi \frac{1-[(E_{surf}+E)/(\Lambda E_{ion})]^{1/2}}{E^2(1+E_{surf}/E)^3} d\Omega dE$$

$\Lambda = \frac{4m_t m_g}{(m_t+m_g)^2}$, $E_{ion} = V_{source}$, E_{surf} = surface binding energy

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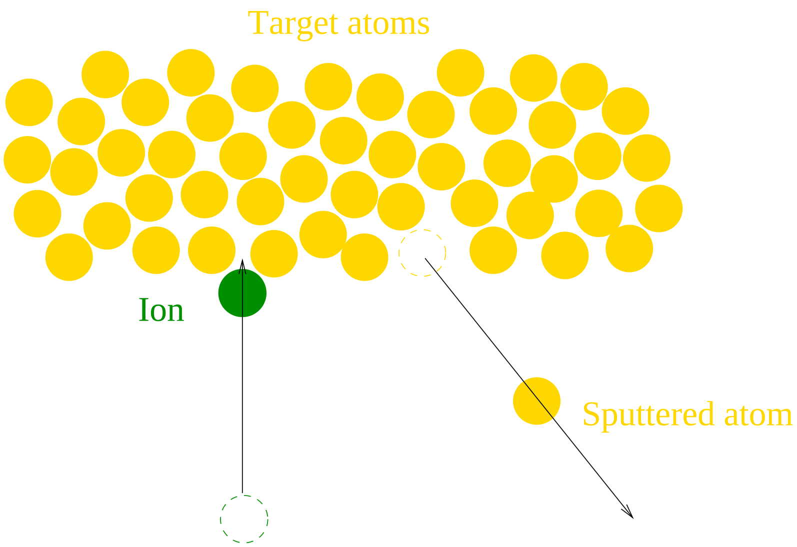
Sputtering probabilities



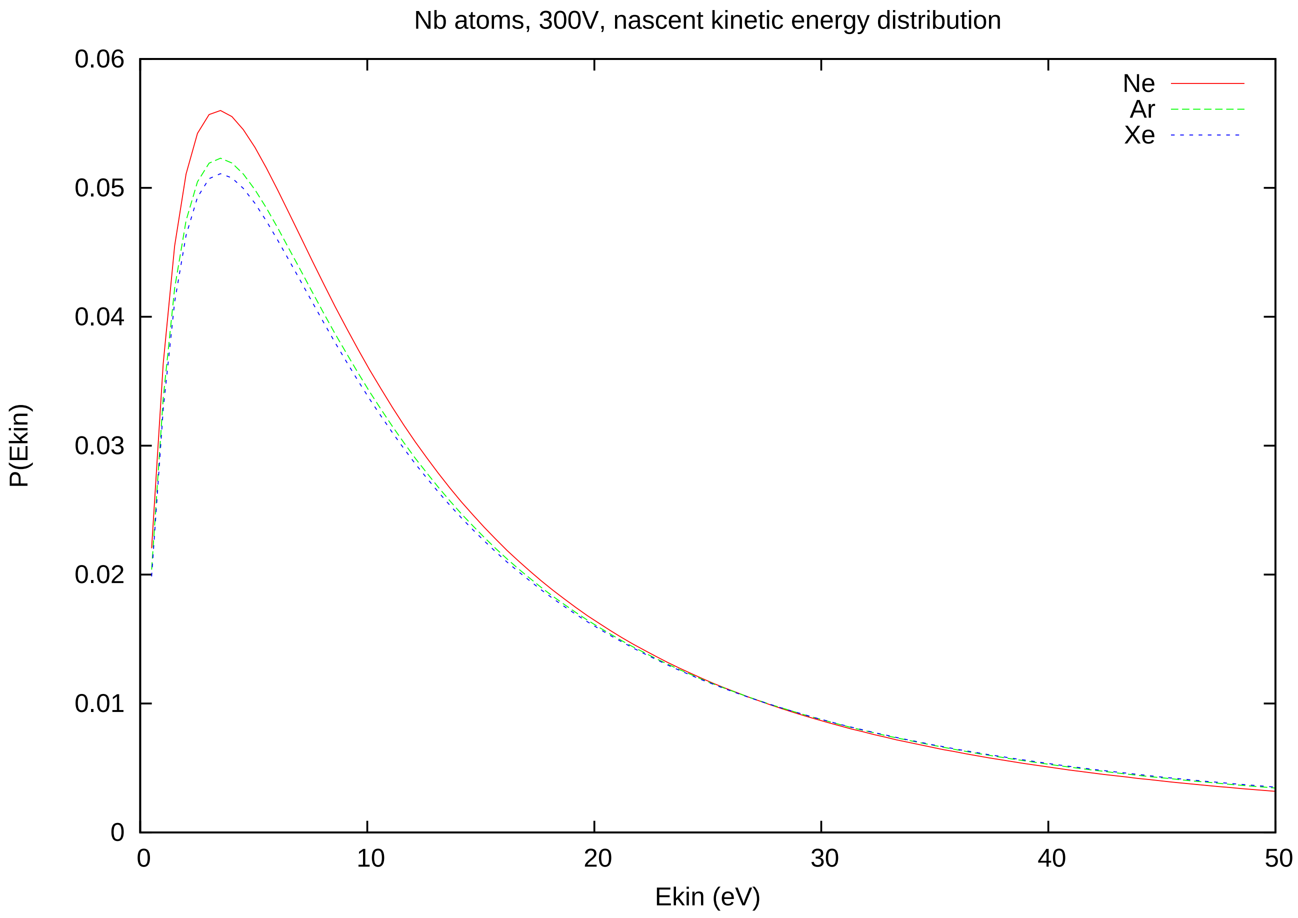
$$P(\phi)d\Omega \sim \cos\phi d\Omega$$

$$P(\phi)d\phi \sim \cos\phi 2\pi \sin\phi d\phi \sim sin(2\phi)d\phi,\ \phi = cos^{-1}\sqrt{\rho_3}$$

$$P(E) = \frac{1-[(E_{surf}+E)/(\Lambda E_{ion})]^{1/2}}{E^2(1+E_{surf}/E)^3},\ max(P)\rho_4 \leq P(E_{max}\rho_5)$$

$$\theta = 2\pi\rho_6$$

Nascent energy distribition for Nb



Sputtering: In-gas transport

Ballistic below 10^{-4} mbar, diffusive above 10^{-1} mbar
Sputtering done exactly in this range (Kn $\approx$ 1)

- Collision partner:

  $$P(E_{kin}) \sim e^{-E_{kin}/kT} = e^{\frac{-m_g v^2}{2kT}}$$

  $v_x = \sigma N(\rho_7)$, $\sigma = \sqrt{kT/m_g}$, T=450K

- Mean flight path: $\lambda(\mathbf{v_{rel}}) = \frac{m_g v_{rel}^2}{2\sqrt{\pi} P b_{max}^2 f(|\mathbf{v_{rel}}|)\sqrt{\frac{m_g}{2kT}}}$

  $$f(v) = ve^{-v^2} + (2v^2+1)\frac{\sqrt{\pi}}{2}\mathrm{erf}(v)$$

- Free flight path is exponentially distributed with mean $\lambda(\mathbf{v_{rel}})$: $\mathbf{p_{new}} = \mathbf{p} - \lambda(\mathbf{v_{rel}}) ln(\rho_8)\frac{\mathbf{v}}{|\mathbf{v}|}$

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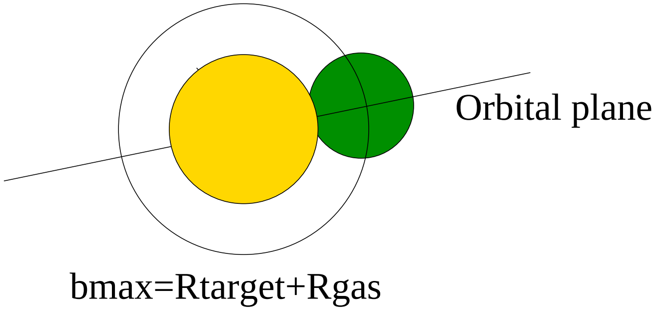
Sputtering: Collision



- impact parameter b: $P(b) \sim b$, $b = \sqrt{\rho_9}$
- orbital plane angle γ: $P(\gamma) = U_{[0,2\pi>}$, $\gamma = 2\pi\rho_{10}$
- Now: integrate equations of motion for some potential (LJ (6/12), Abrahamson) or assume hard sphere scattering (computationally more attractive).
- Hard sphere model deviates a couple of degrees at small angles and below 1 eV.

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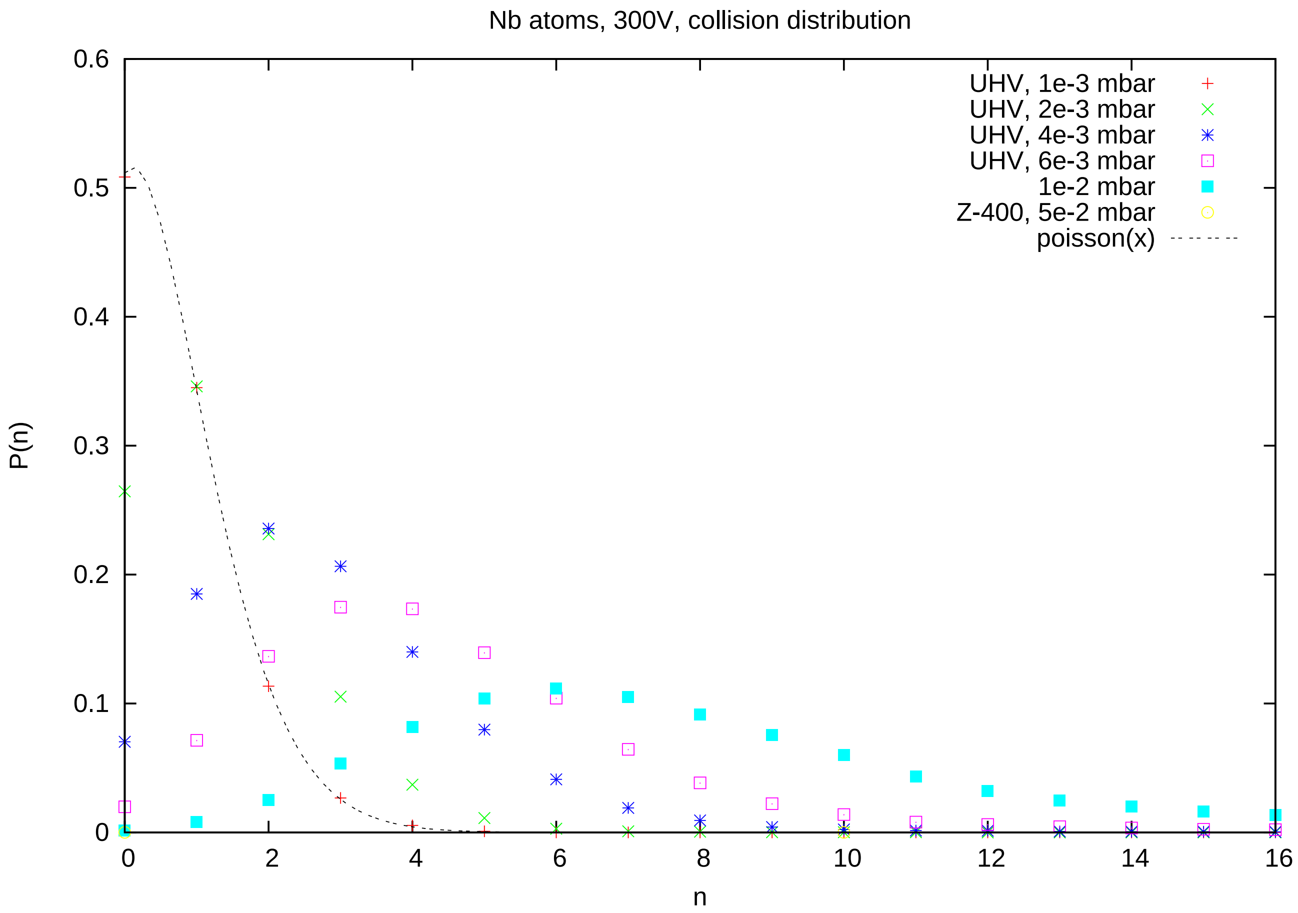
Monte Carlo algorithm

```
while (less than N atoms on substrate)
    sputter atom
    free-fly
    while (not wall collision)
        collide
        free-fly
    if (wall is substrate)
        save position, velocity etc.
```

- N=40000 for ‘good statistics’
- 10^9 atoms sputtered for a realistic geometry
- Simulation time: 5-30 minutes (depending mainly on the gas pressure)

Results: Collision histograms



Poisson process: $\frac{P(n) = \mu^n e^{-\mu}}{n!}$, $\mu \approx \frac{distance}{mean free path}$

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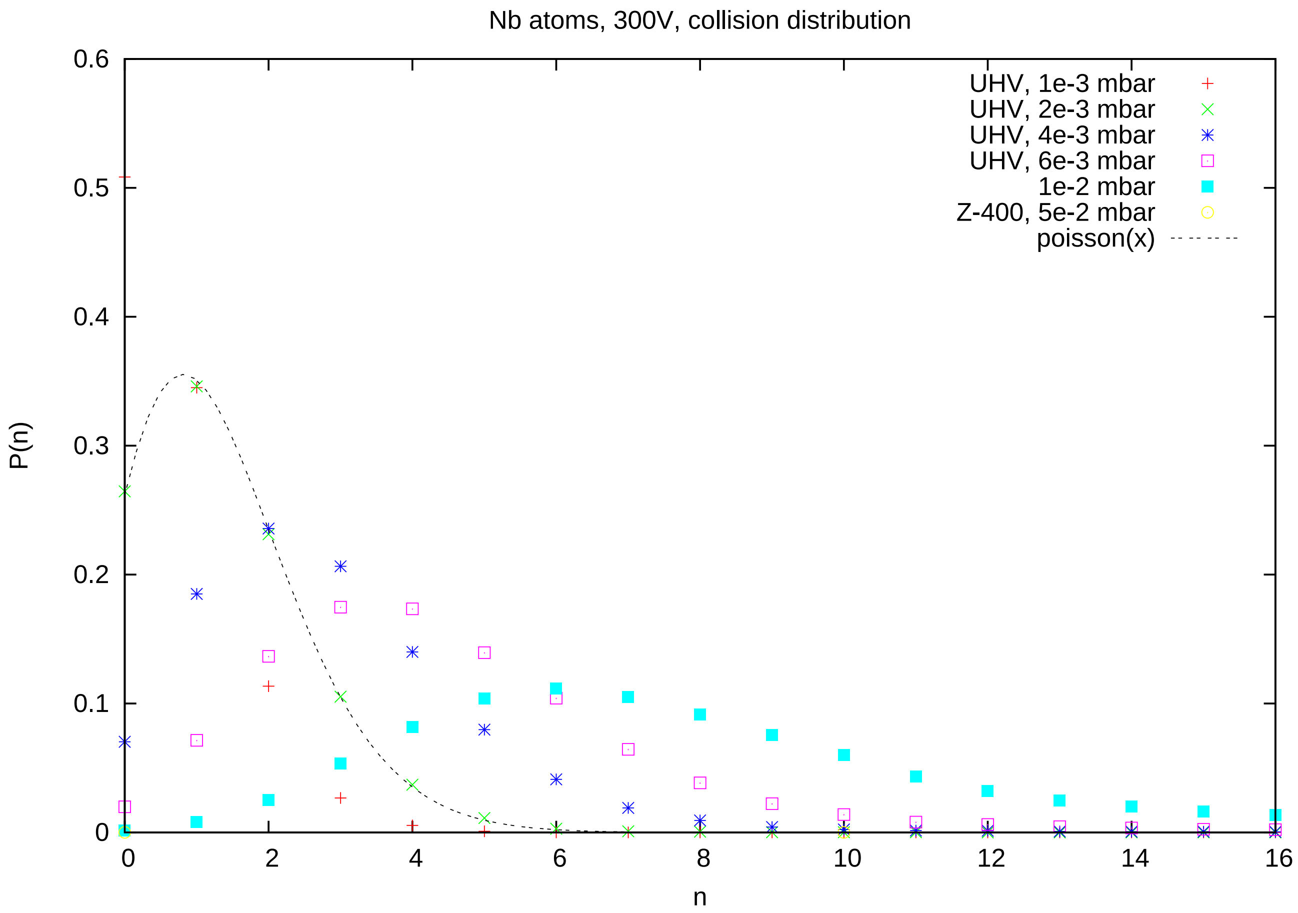
Results: Collision histograms



Poisson process

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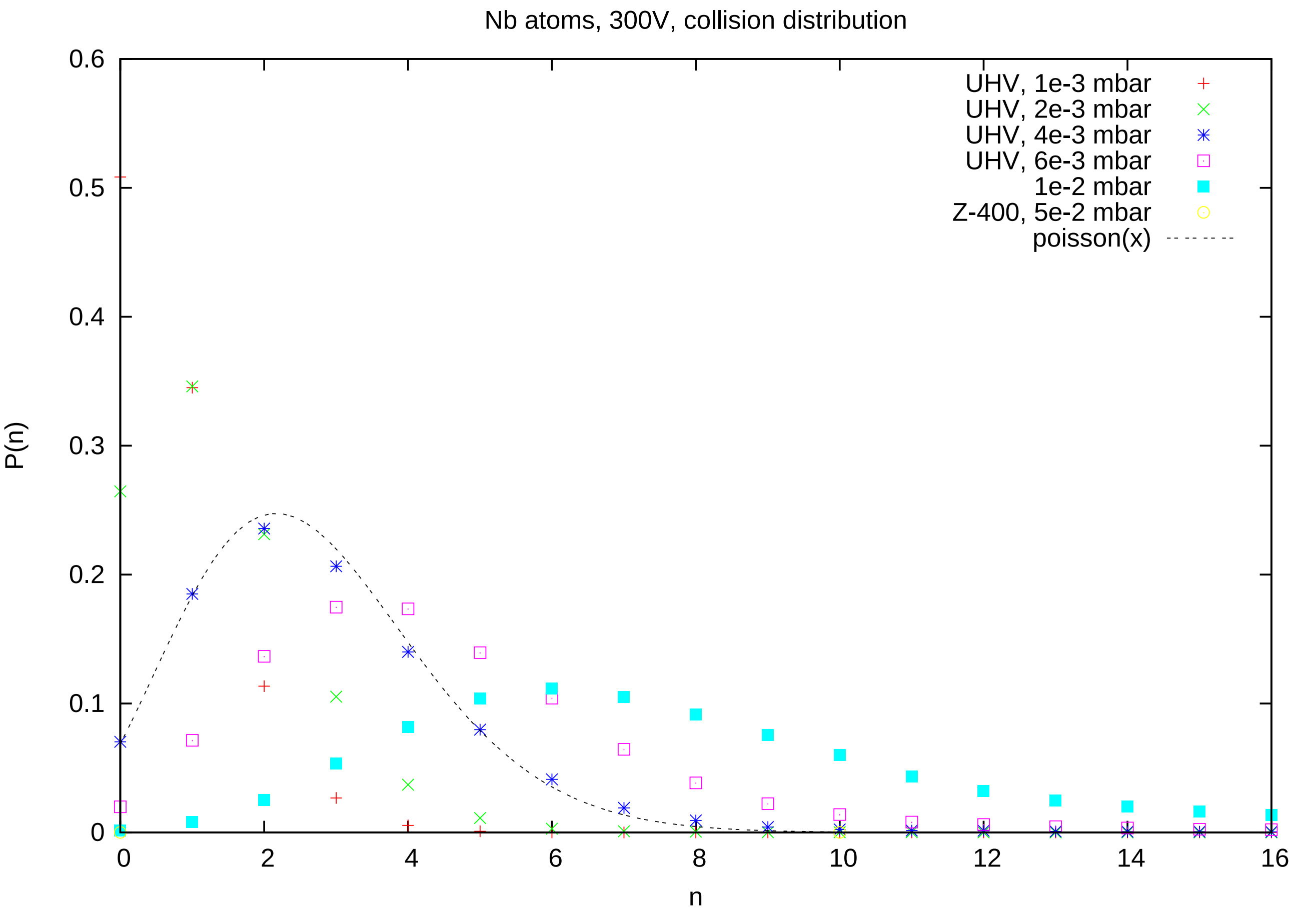
Results: Collision histograms



Poisson process

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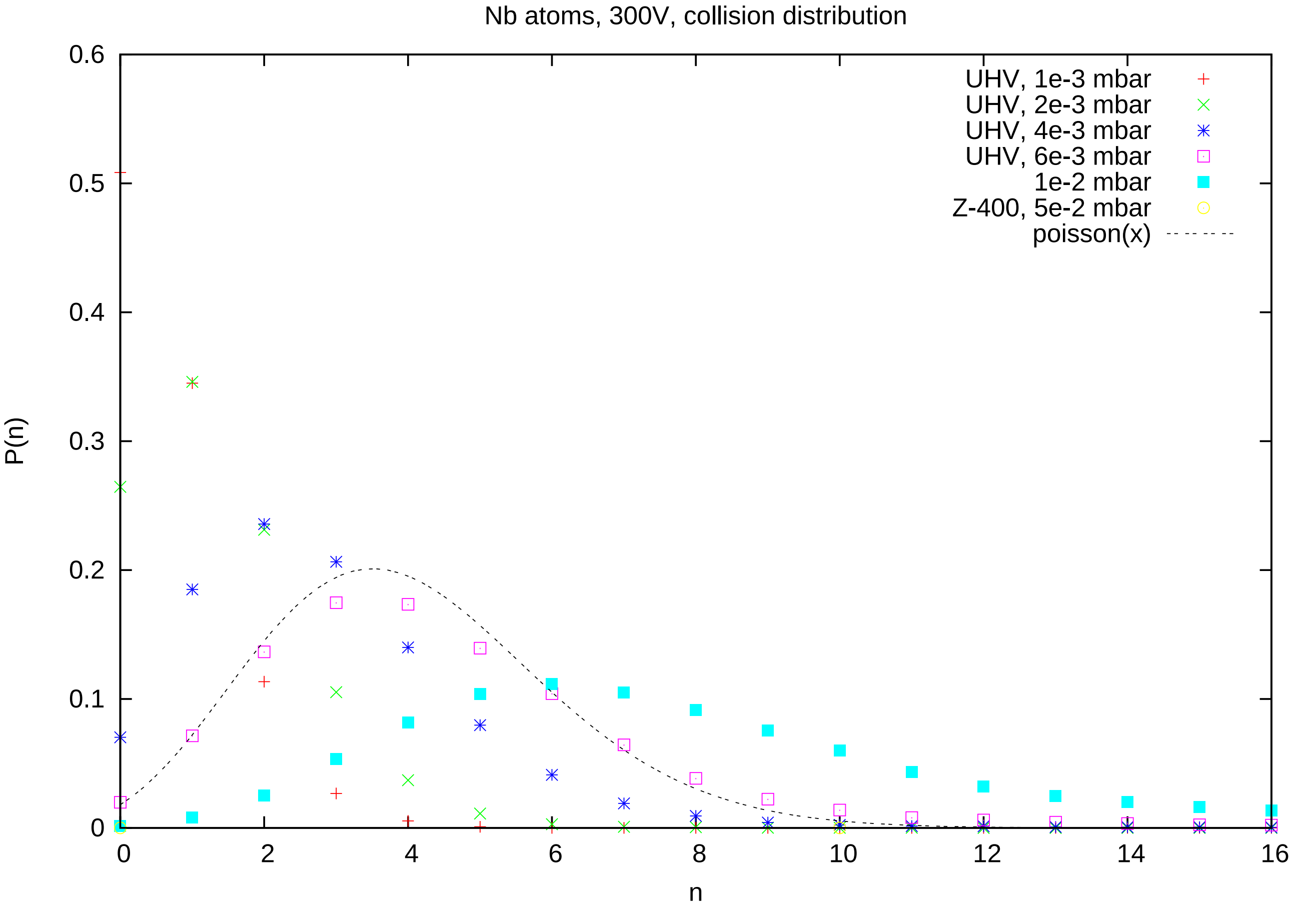
Results: Collision histograms



Deviation from Poisson process

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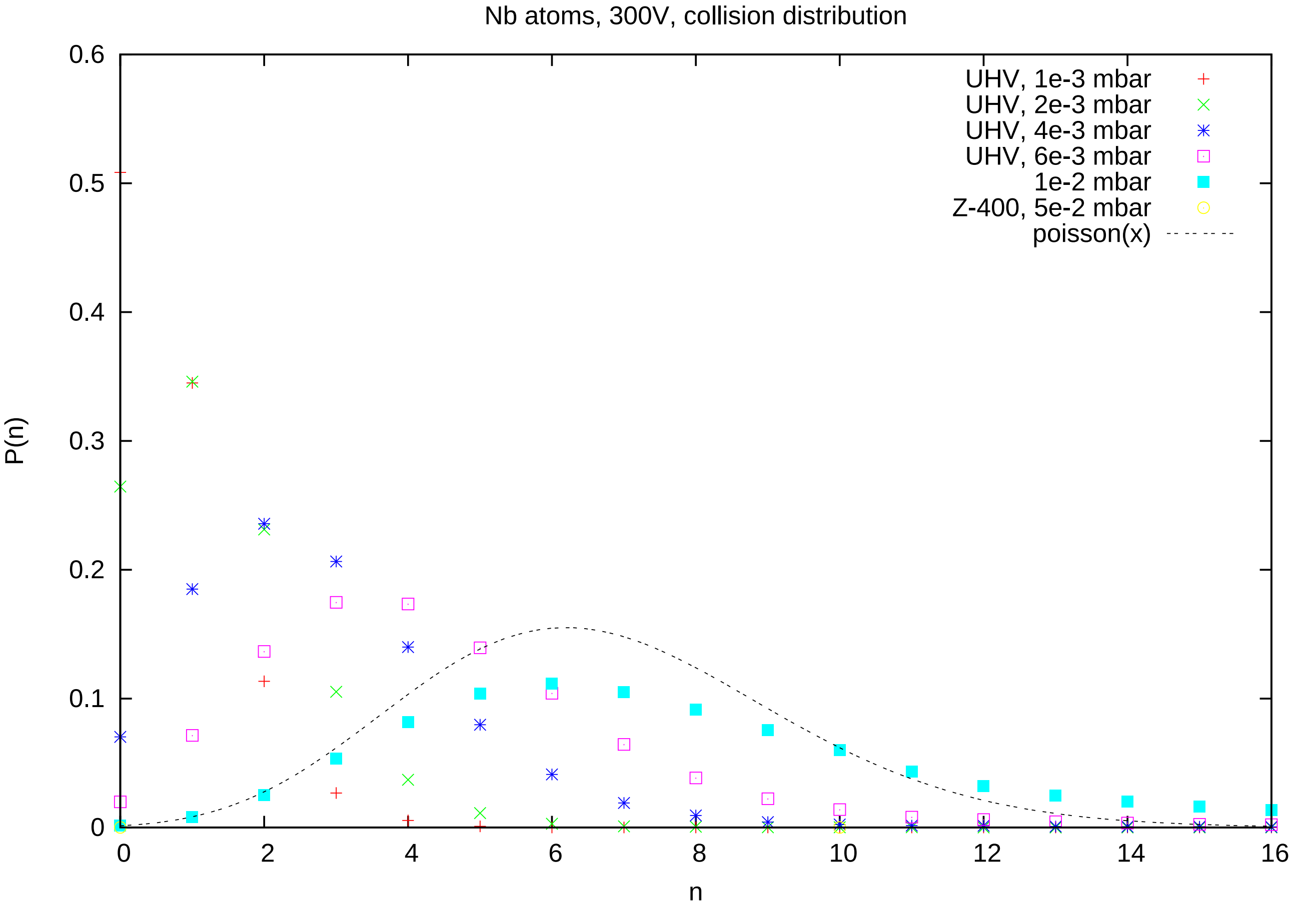
Results: Collision histograms



About to become diffusive...

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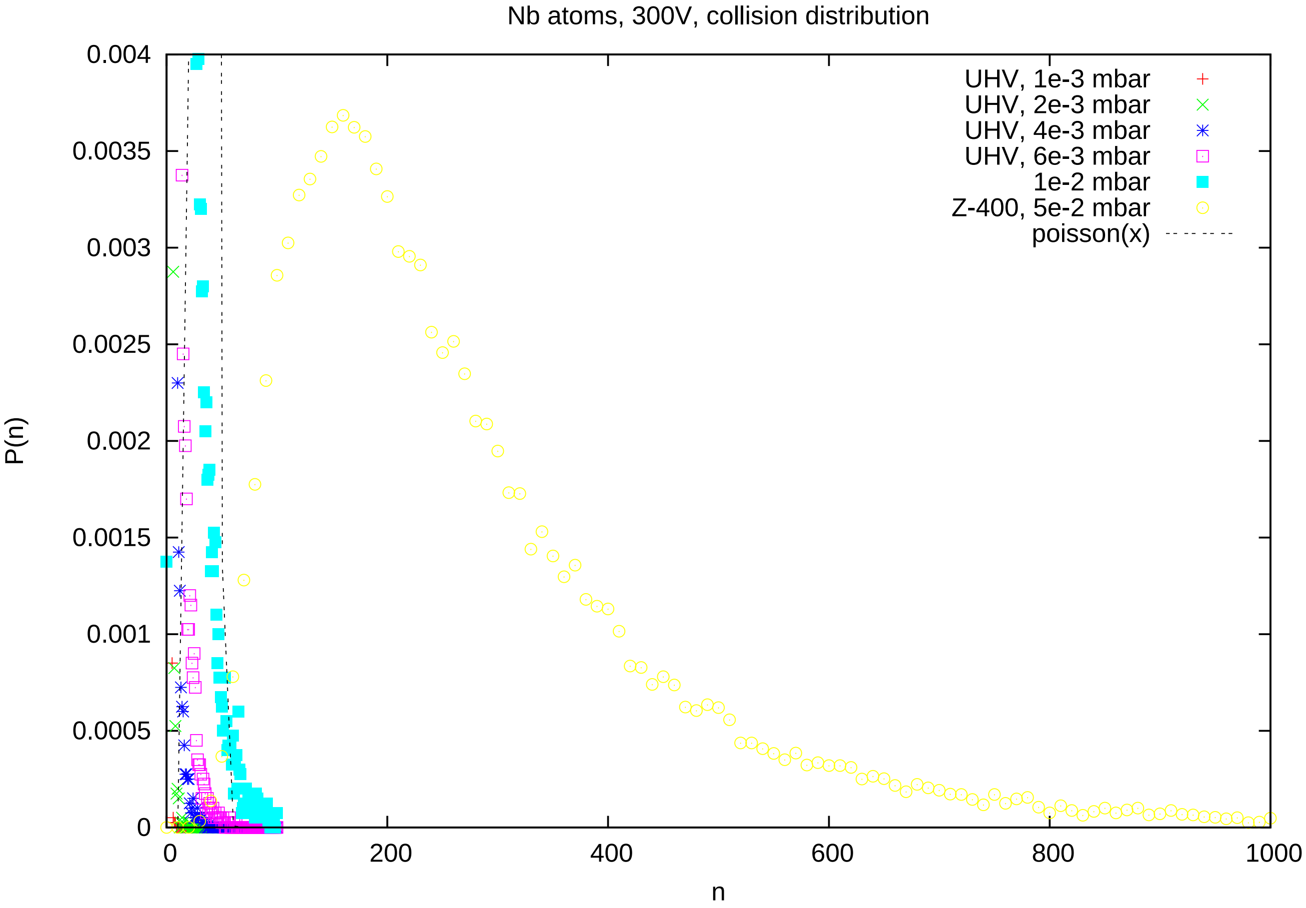
Results: Collision histograms



Diffusive (thermalized) transport

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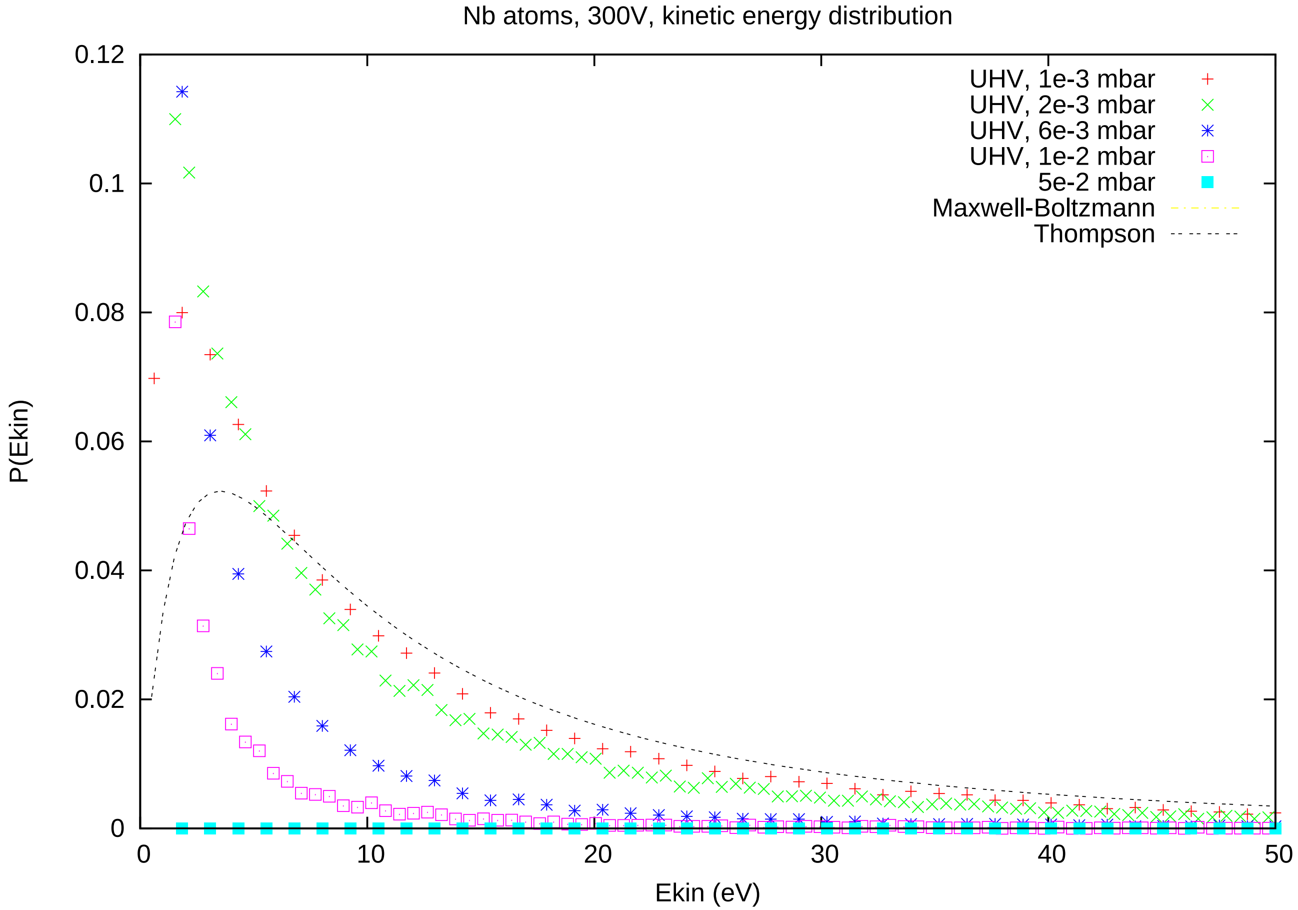
Results: Impact energy distribution



Low pressure (magnetron sputtering)

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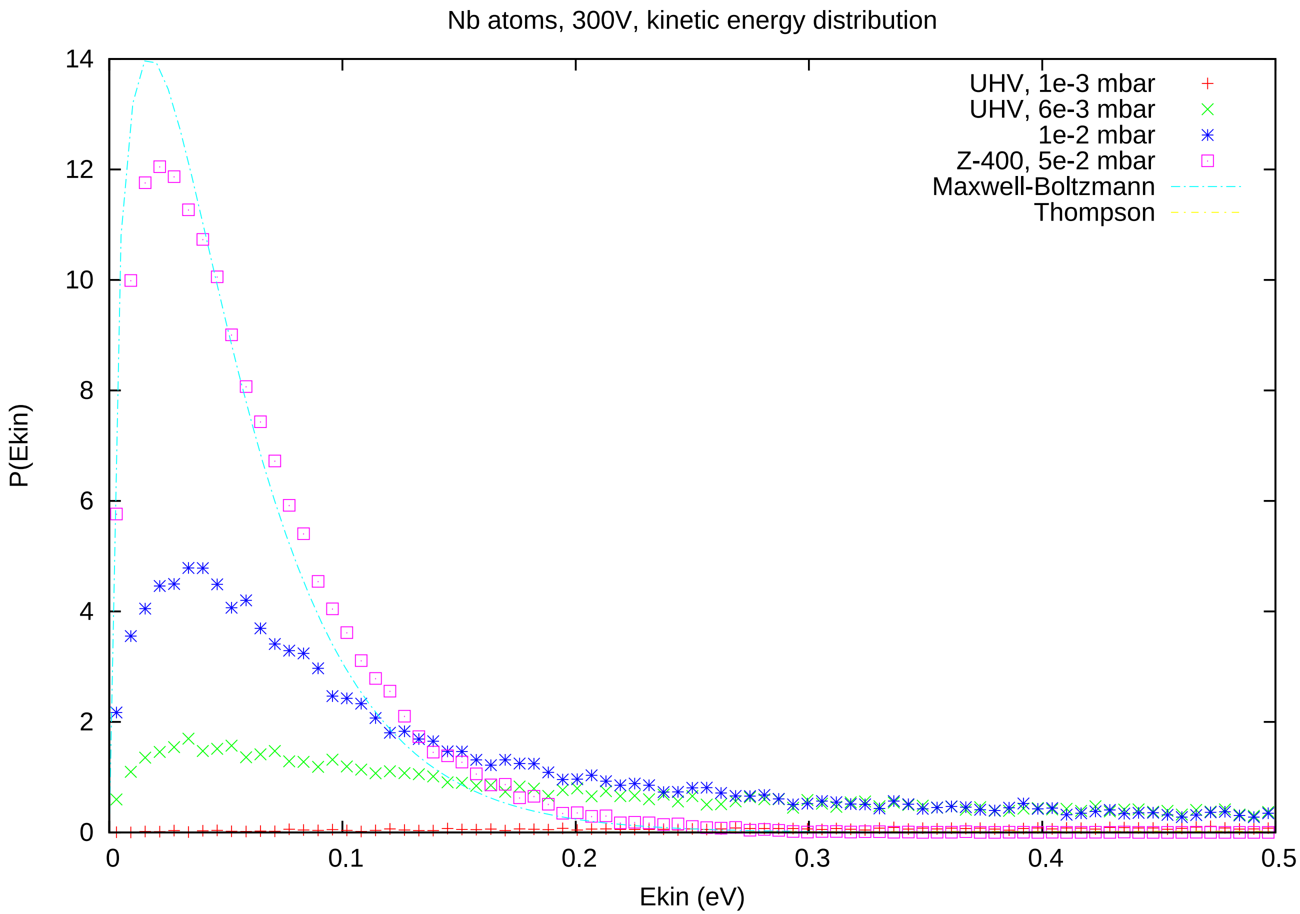
Results: Impact energy distribution



High pressure (diode sputtering)

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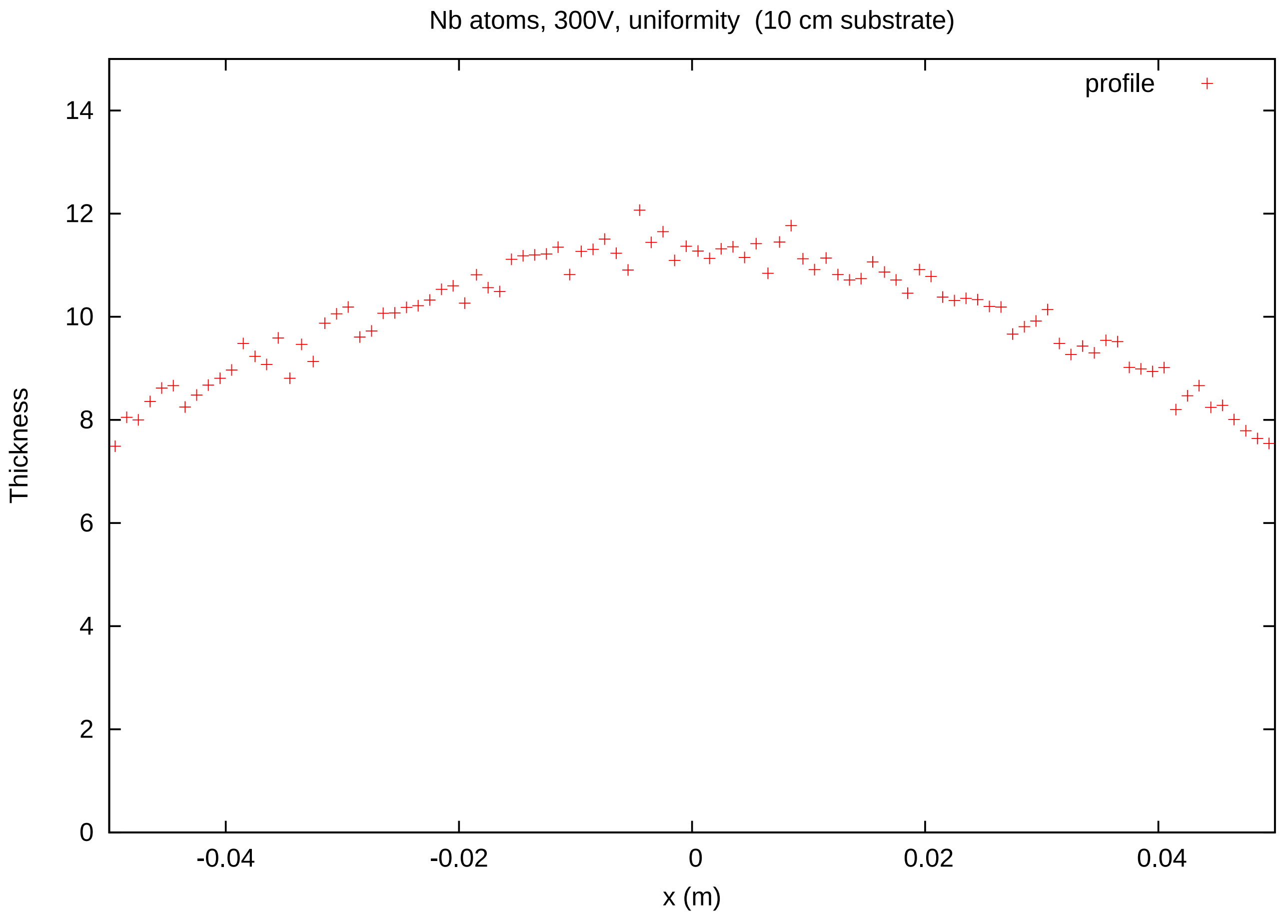
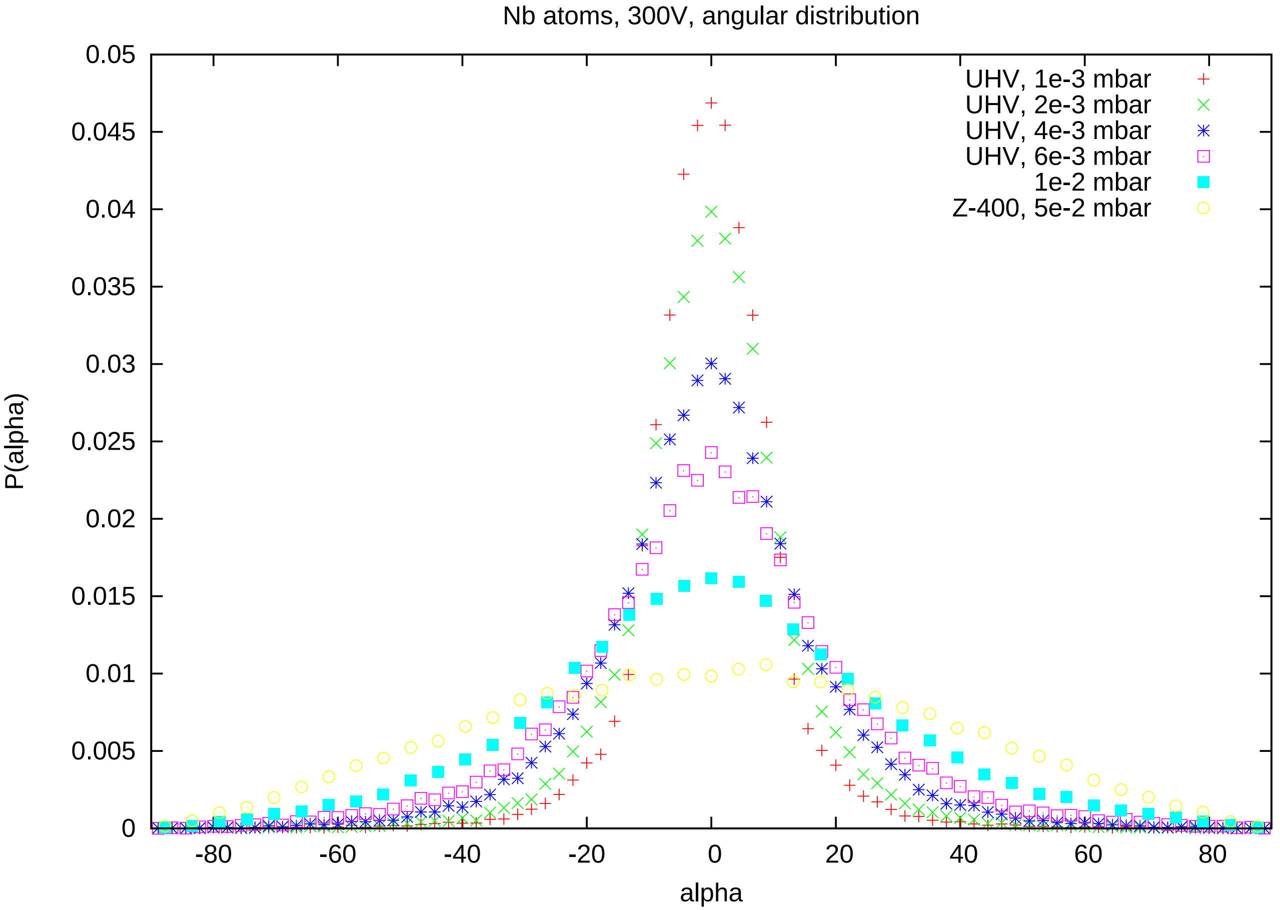
Results: uniformity



10 cm substrate

Results: Impact angle distribution



High pressure: $\cos\phi$ distribution (diffusive)

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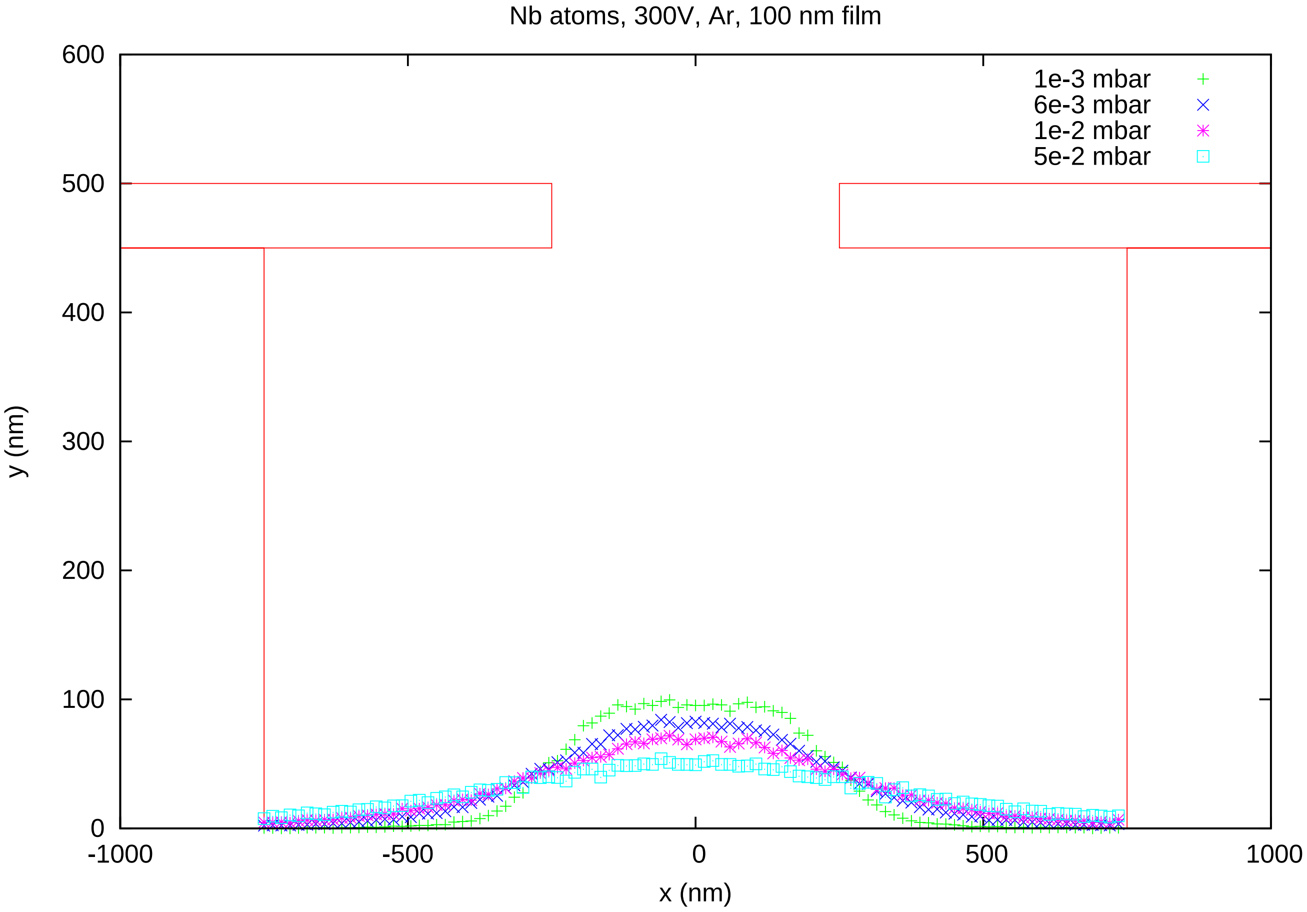
Results: Ray-tracing the cross section



Large-area thickness: 100 nm

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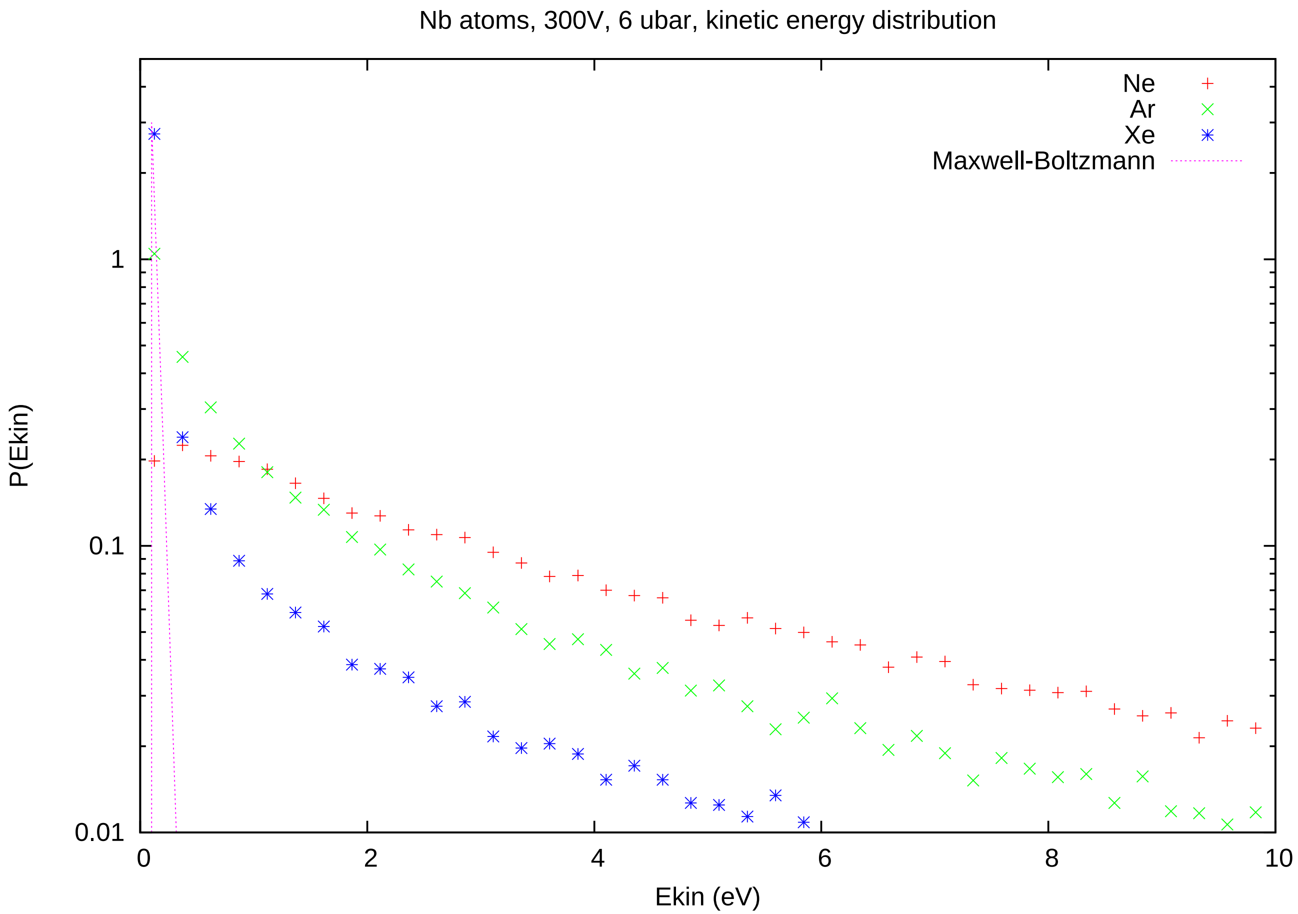
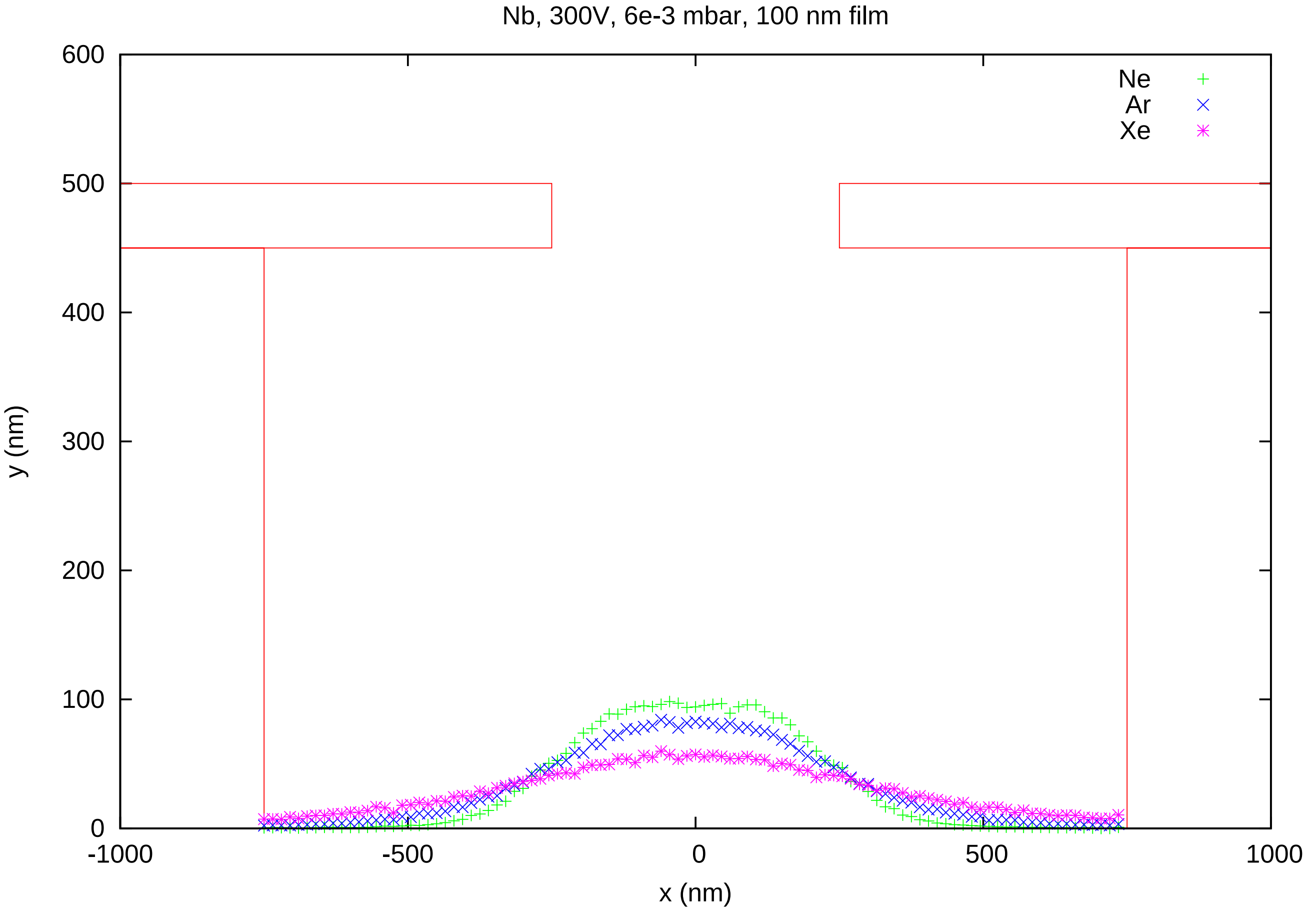
Results: Gas dependence



Very different growth conditions!

Results: Gas dependence 2



Gas choice can be important!

Conclusions

- Sputtering gas and pressure determine the growth conditions (the gas is a moderator)
- But at high pressures liftoff produces undesired results
- We can simulate this process
- The simulation results correspond with our findings
- We can calculate required sputtering conditions

The program is called `sputsim` and will be installed on the public PC in room 626

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