Process simulation

Front End of Line Process Models

Ion Implantation, Diffusion

Epitaxy, Oxidation,

Device simulation

Equipment simulation

Equipment Modeling, Transport Simulation

PVD (Monte Carlo, MD (*))

Feature scale, Topography (line of sight))

Lithography

CMP

CVD (*)

ECD

Etching (*)

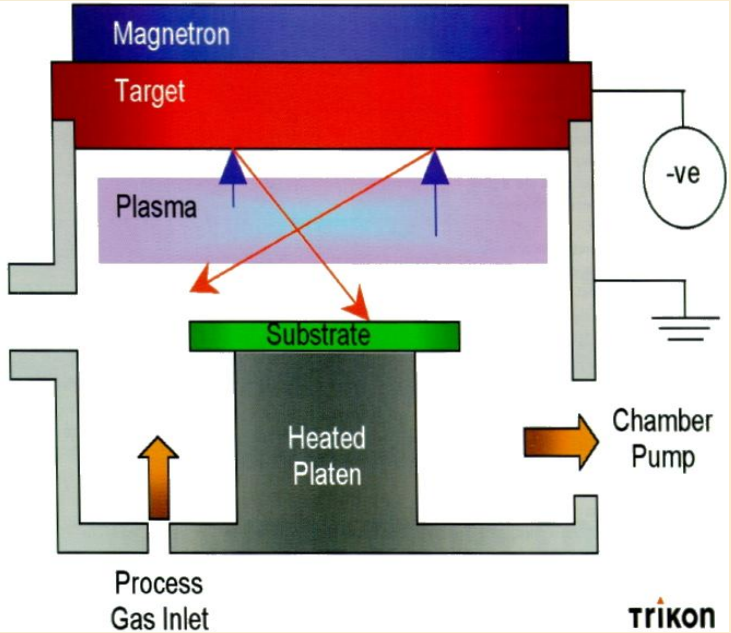
ALD

CVD Chemical Vapour Deposition / Epitaxy
ALD Atomic Layer Deposition
PVD Physical Vapour Deposition
ECD Electro Chemical Deposition
MBE Molecular beam epitaxy
spin on

...Modeling and Simulation

Transport Simulation

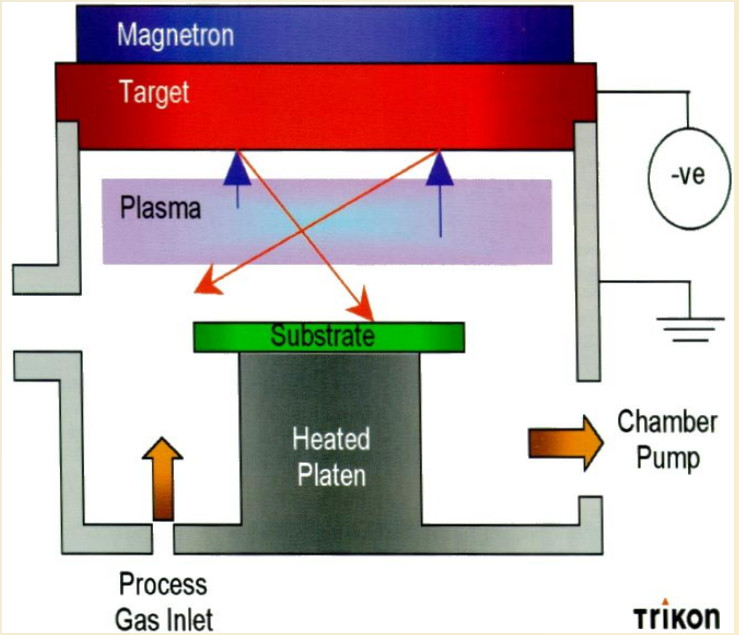
1. Particles to wafer



Sputtering Process

Principle:

The target consists of the material, which should be deposited on the wafer.



→ Area of ionization will not be separated from the area of deposition !

→ The pressure will be defined by the plasma.

→ Ballistic transport of the target atoms to the wafer (few collisions on the way to to the substrate)

→ Main field of application today in the microelectronic technology and technology of MEMS

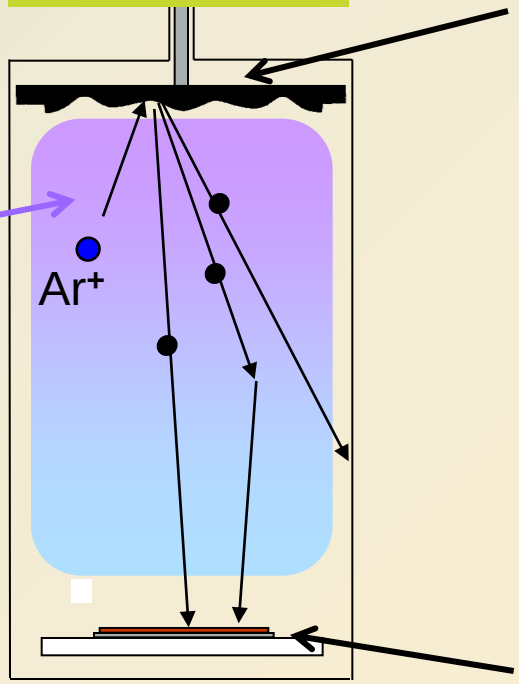
reason: productivity and purity of the targets *e.g.: 99.9995 %* ***[5N5]***

- ...Modeling and Simulation

Transport Simulation on different length scales

- Reactor - Monte Carlo Transport Simulation
- Feature - Monte Carlo Surface Kinematics Simulation
- Surface - Molecular Dynamics Approach

Reactor with a long target-to-substrate distance



Metal target, negative voltage (~ 500 V)

Sputtering of metal atoms by Ar+ bombardment

Angular and energy distributions of sputtered metal atoms

Molecular Dynamics

Transport in the argon plasma (scattering simulation)

IPVD: with additional ionization (e.g. a coil)
→ more metal ions

Transport of metal atoms – low pressure – few collisions

Monte Carlo Transport and Scattering

Deposition of metal atoms on the substrate in the feature (topography simulation)

PVD

Each atom that has reached the substrate is adsorbed (sticking coefficient 100%)

IPVD

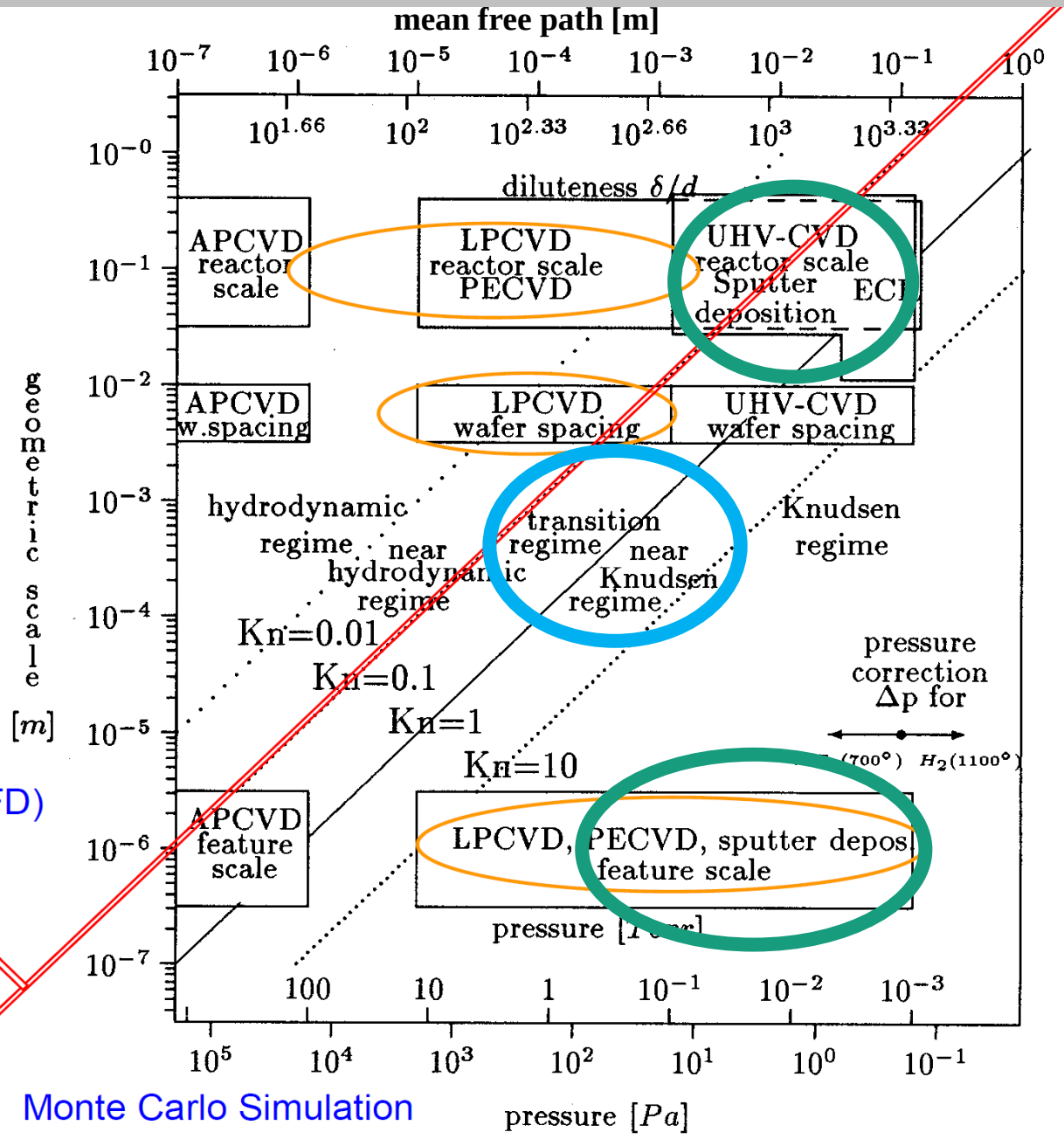
IPVD: Negative voltage on the substrate (~ 100 V)

Increase of the normal component of velocity for charged particles: not 100% absorption,

also reflection, and sputtering of film particles

→ Molecular Dynamics Calculation

Tansport Simulation in Relation to geometric Scale



Computational Fluid Dynamics (CFD)

Navier-Stokes Equation

Monte Carlo Simulation

Boltzmann Transport Equation

A. Kersch, W. J. Morokoff, „Transport Simulation in Microelectronics“ Birkhäuser Verlag, Basel, 1995

Mathematical methods:

numerical treatment of differential equations describing particle flow

- simulation of continuum flow

condition: Knudsen number Kn << 1

Physical methods:

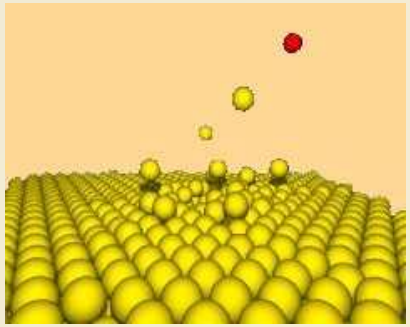
Simulation of particle flow by tracking of particle trajectories and interactions of the particles among themselves and with interfaces

Each simulated particle represents a huge number of physical particles

Molecular-Dynamics (MD)

The MD-method emulates trajectories of particles and collision interactions accordingly given interaction potentials

(particularly solids, liquids)



Direct simulation Monte Carlo (DSMC)

No exact emulation of particle trajectories and interactions

Particle movement and interaction independent

Collisions not exact, but random

Calculation of

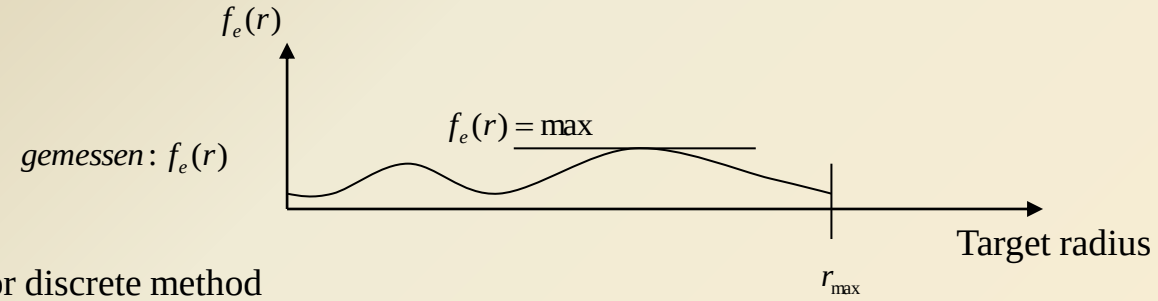
energy distribution

angular distribution

of particles impinge at wafer surface

1. Start particle at target (Modelling of target emission)
2. Modelling of particle flight through from target to wafer taking collisions into consideration
3. Store particle properties at wafer (position, species, energy, angle)
4. Repeat (10 000 000 and more)

1. Emission position



e. g. acceptance-rejection or discrete method

Or measured distribution (Jones))

1. Emission angle (polar, azimuthal)

$$f_{polar}(\Theta) = \sin(\Theta)\cos(\Theta)$$

$$f_{azimuthal}(\varphi) = 2R\pi$$

2. Emission energy (Thompson)

$$f_{Tho}(E) = E\left(1 - \frac{\sqrt{\frac{E_b - E}{\lambda E_i}}}{\left(\frac{E_b - E}{eV}\right)^3}\right)$$

$$\lambda = \frac{4m_i m_t}{(m_i + m_t)^2}$$ max. energy transfer

E_b Surface binding energie

E_i Av. kinetic ion energy

mfp Mean free path

3. Mean free path

$$x = -mfp\ln(R)$$

If new collision position outside reaktor then goto **6.**

4. Collision

$S = 0$

$for(i = 0; i < numberOfSpecies; i++)\{$

$S = S + mole\_fraction_i$

$if\ (S > R) break;$ // i is index of collision partner

$\}$

5. Energy of collision partner (Maxwell distribution)

$$t = \sqrt{-2\ln(R/2)}$$

$$v = \sqrt{kT/m}\left(t - \frac{c_0 + c_1 t + c_1 t^2}{1 + d_1 t + d_2 t^2 + c_3 t^3}\right)$$

c, d empirical coefficients

5. Calculation of collision (model dependent)

result: new direction

new energy of collision parters

dependent on collision parameters, particle mass, energies

…goto **3.**

6. Calculation of surface interaction

rsc = 1… save particle (position, direction, energy)

or MD based calculation of adsorption/sputtering/reflexion probability f_{ads}, f_{reflex}, f_{sputt}

rsc: reactive sticking coefficient

$$f_{ads} + f_{reflex} + f_{sputt} = 1$$

$if\left(f_{ads} > R\right)$: Adsorption

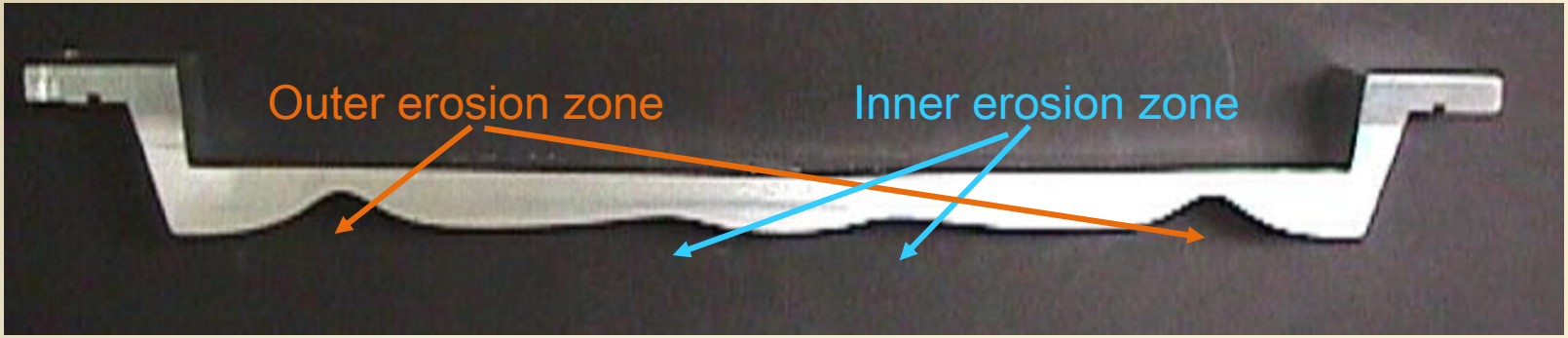
$if\left(f_{reflex} > R\right)$: Reflexion

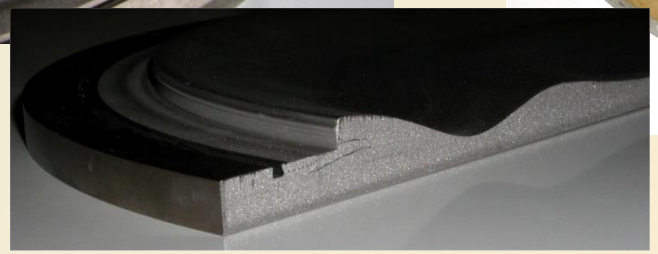
else Sputtering → Sputtering rate, emission angle, energy of sputtered particles

feature scale simulation

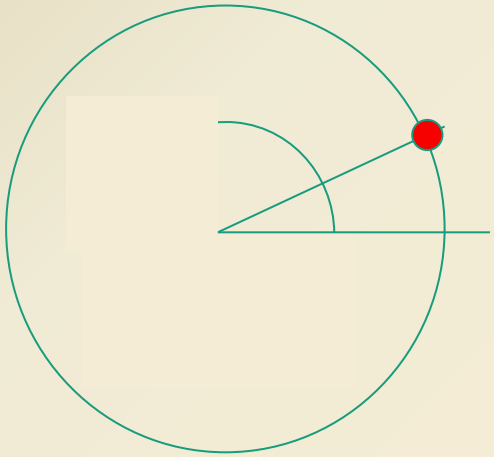
rsc … reactive sticking coefficient

Erosion trench on a magnetron target





Target, diameter approx. 400 mm



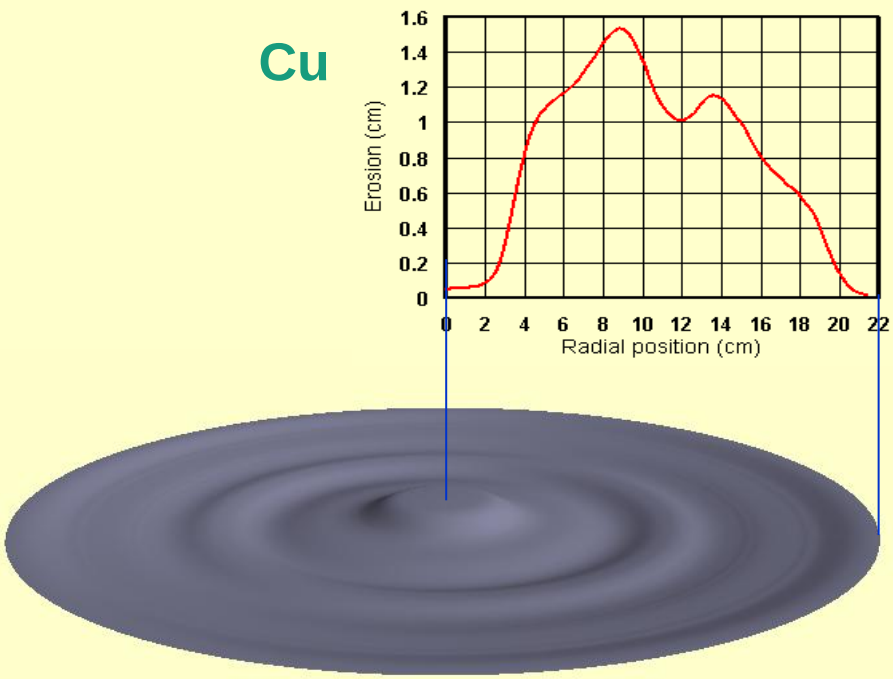
angle = 2 π R

Random number 0 ... R ... 1

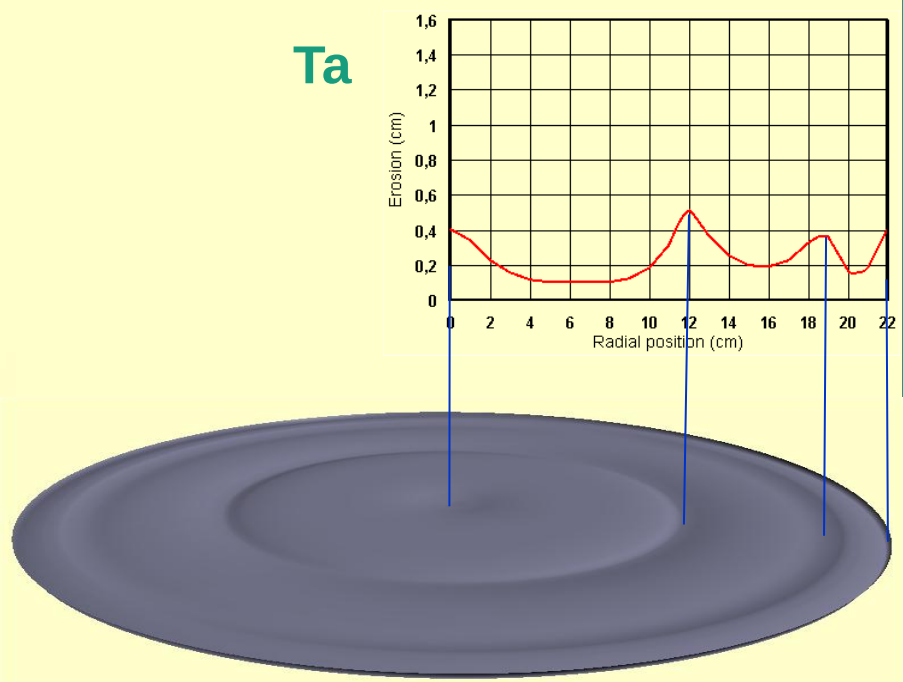
Modeling of target emission, erosion profile

chnology

Cu



Ta



Random Numbers, by Acceptance-Rejection Method

Random number, distributed with probability density f(x) = dW/dx by the acceptance-rejection method

Step 1. Normalization

$$f_n(x) = \frac{f(x)}{f_{max}}$$

Step 2. R1

choose R1, uniformly distributed random numbers in interval (xu, xo)

R1 = R * (xo – xu) + xu, $\qquad$ 0 < R < 1

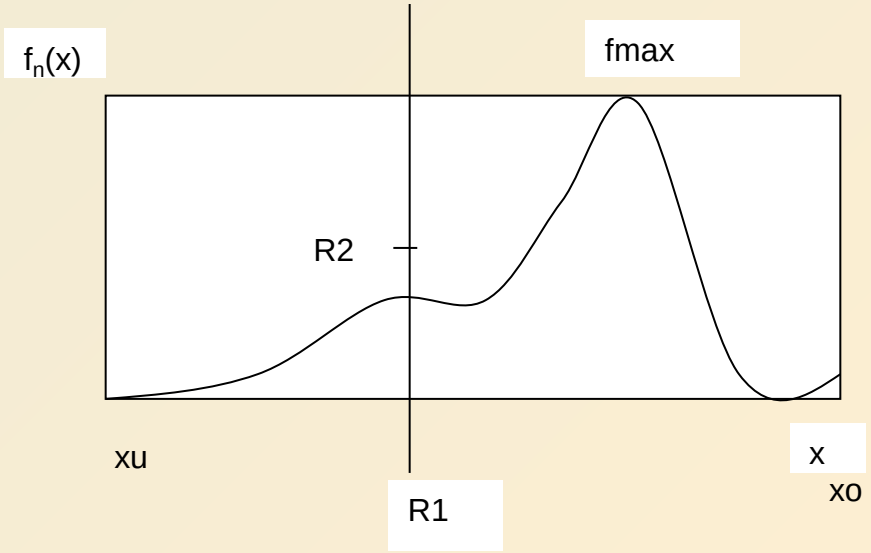
Step 3. choose R2 = R * fmax,

R1 is then randomly distributed if

$$R_2 < f_n(R_1)$$

(acceptance)

else rejection of R1, R2



Given: $f(x)$ as vector $f[i]$ at $x[i]$, i = 0 ... n-1

Step 1. Determination of the discrete probability mass function $F[j]$ at $x[i]$

$$f[j] = N \sum_{i=0}^{j} \frac{f(x[i+1]) + f(x[i])}{2} (x[i+1] - x[i])$$

Step 2. Normalization, e. g. trapezoidal rule

$$N = \frac{1}{\sum_{i=0}^{j-2} \frac{f(x[i+1]) + f(x[i])}{2} (x[i+1] - x[i])}$$

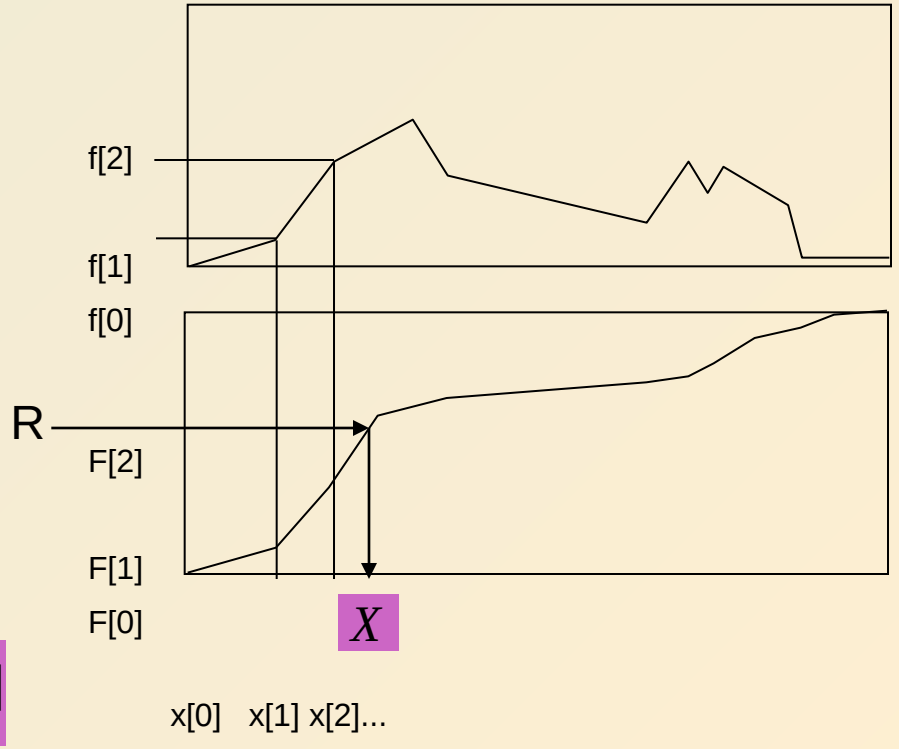
Step 3. Determination of R

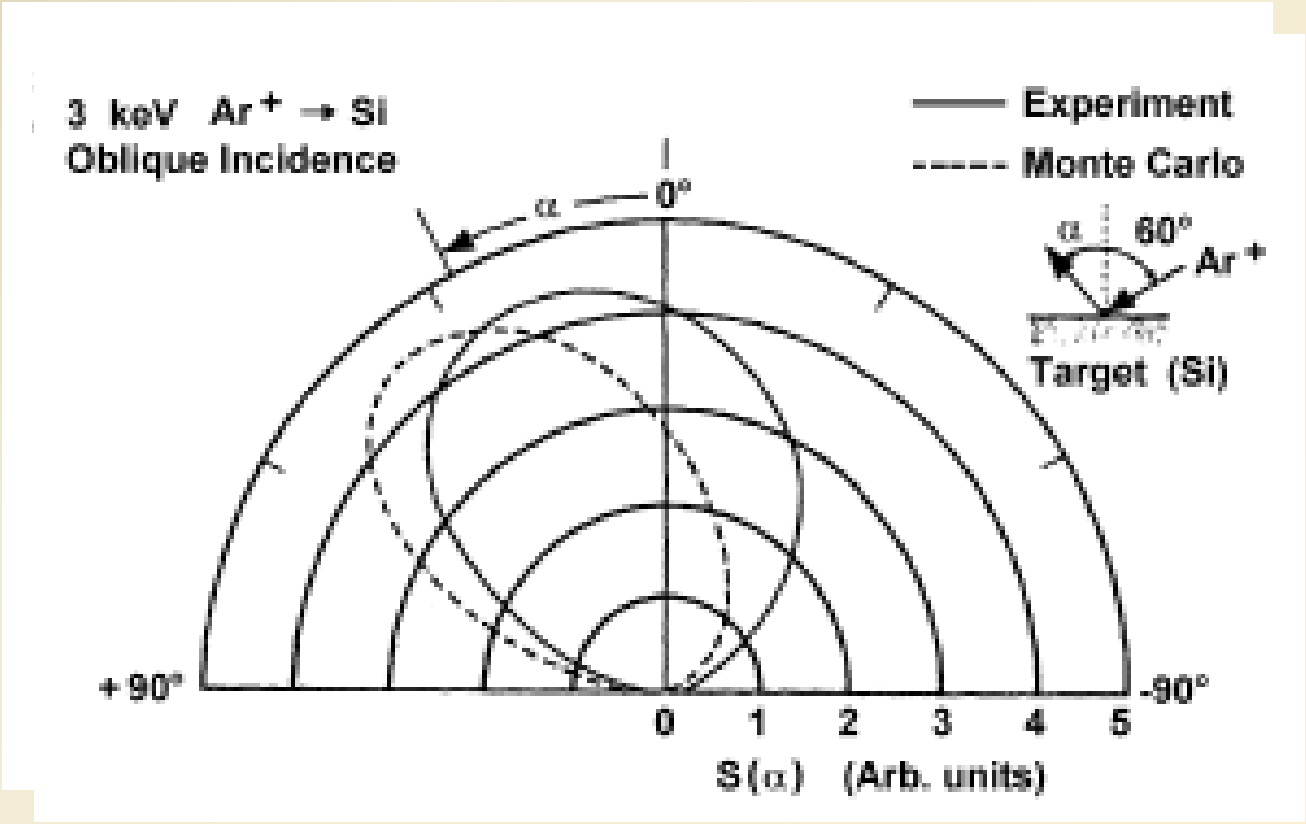
Determination of interval

$$F[i] < R < F[i+1]$$

Interpolation

$$X = \frac{x[i+1] - x[i]}{F[i+1] - F[i]} (R - F[i]) + x[i]$$





Angular distributions of sputtered Si atoms for 3 keV, Ar^+ ion bombardment at an incident angle of 60°

Example: Particle Emission from Target with Cosine Distribution

Angular dependence of the probability density of emission $f(\varphi,\Theta)$

$$f(\varphi,\Theta) \propto \sin(\varphi)\cos(\varphi) \qquad \sin(\varphi)\cos(\varphi) = 1/2\sin(2x)$$

Step 1. Probability mass function

$$F(z) = N\int_0^z f(\varphi)d\varphi$$

Step 2. Normalization

$$F(z) = 1 = N\int_0^{\pi/2} f(\varphi)d\varphi \qquad N = \frac{1}{\int_0^{\pi/2}\sin(\varphi)\cos(\varphi)d\varphi}$$

Step 3. Integration

$$R = F(z) = N\int_0^z \sin(\varphi)\cos(\varphi)d\varphi$$

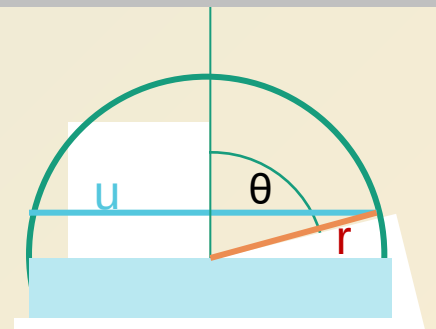
$$R = F(z) = \left[N\frac{1}{2}\sin^2(\varphi)\right]_0^z = N\frac{1}{2}\sin^2(z) = \frac{1}{\frac{1}{2}\sin^2(\pi/2)}\frac{1}{2}\sin^2(z)$$

Step 4. Inverse

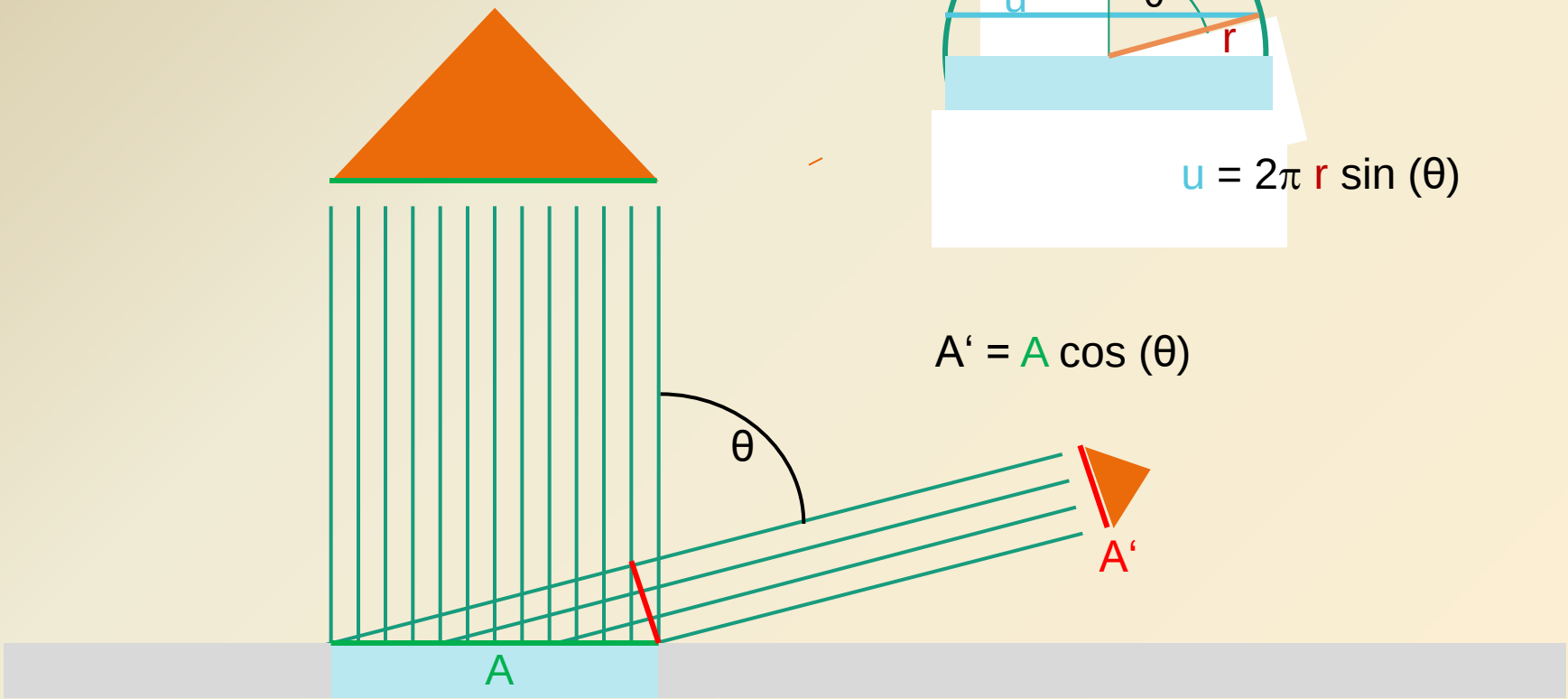
$$z = \arcsin\left(\sqrt{R}\right)$$

$$R = \sin^2(z)$$

Example: Particle Emission from Target with Cosine Distribution



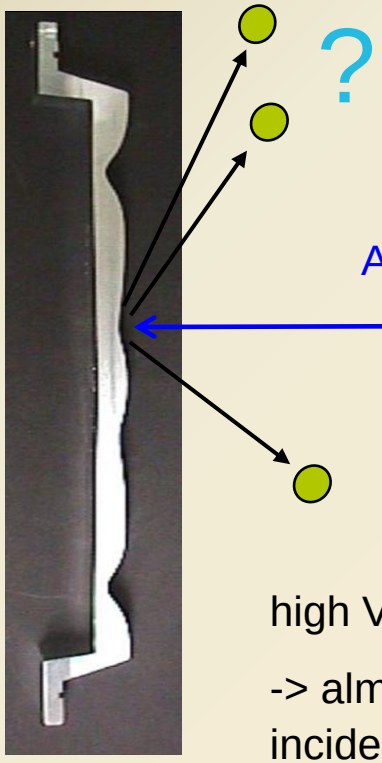
$u = 2\pi\, r \sin(\theta)$

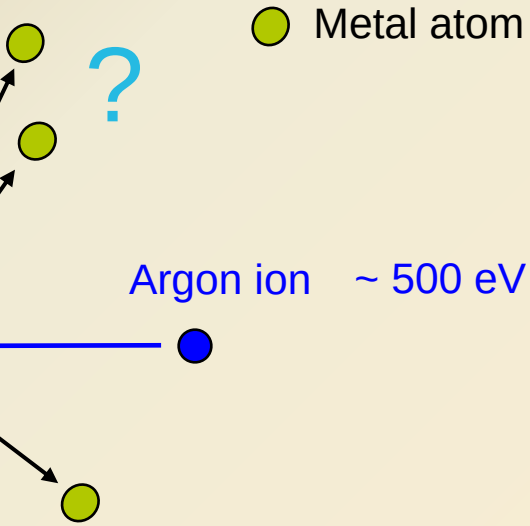


$A' = A \cos(\theta)$

$E \propto u\, A' \propto \sin(\theta) \cos(\theta)$

Goal: Calculation of angular and energy distributions of sputtered metal atoms

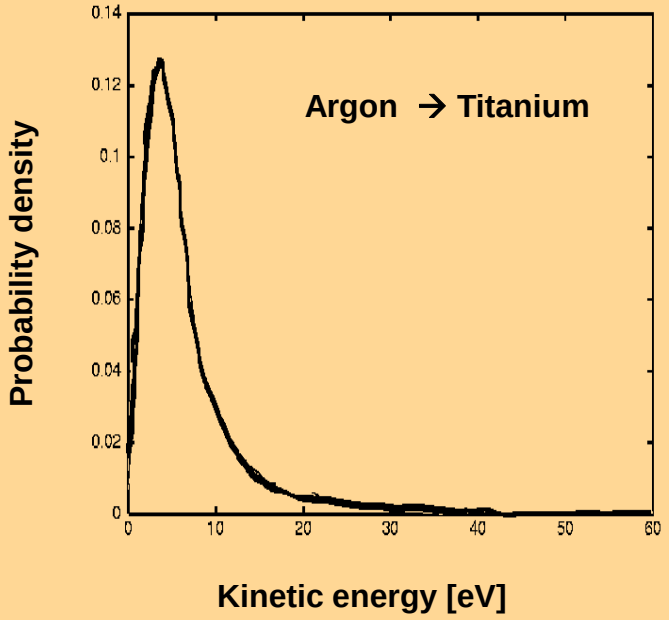




high V_{bias}

-> almost normal incidence of all projectiles

A typical energy distribution of sputtered particles:



95% sputtered atoms: E_{kin} < 25 eV

despite of the fact that projectile energy is about 500 V

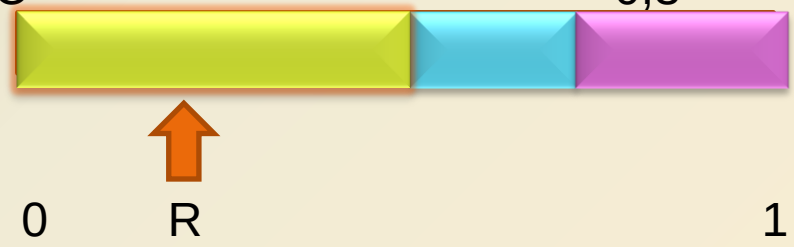
4. Collision

mole fraction

Species A 0,5

Species B 0,2

Species C 0,3



$$S = 0$$

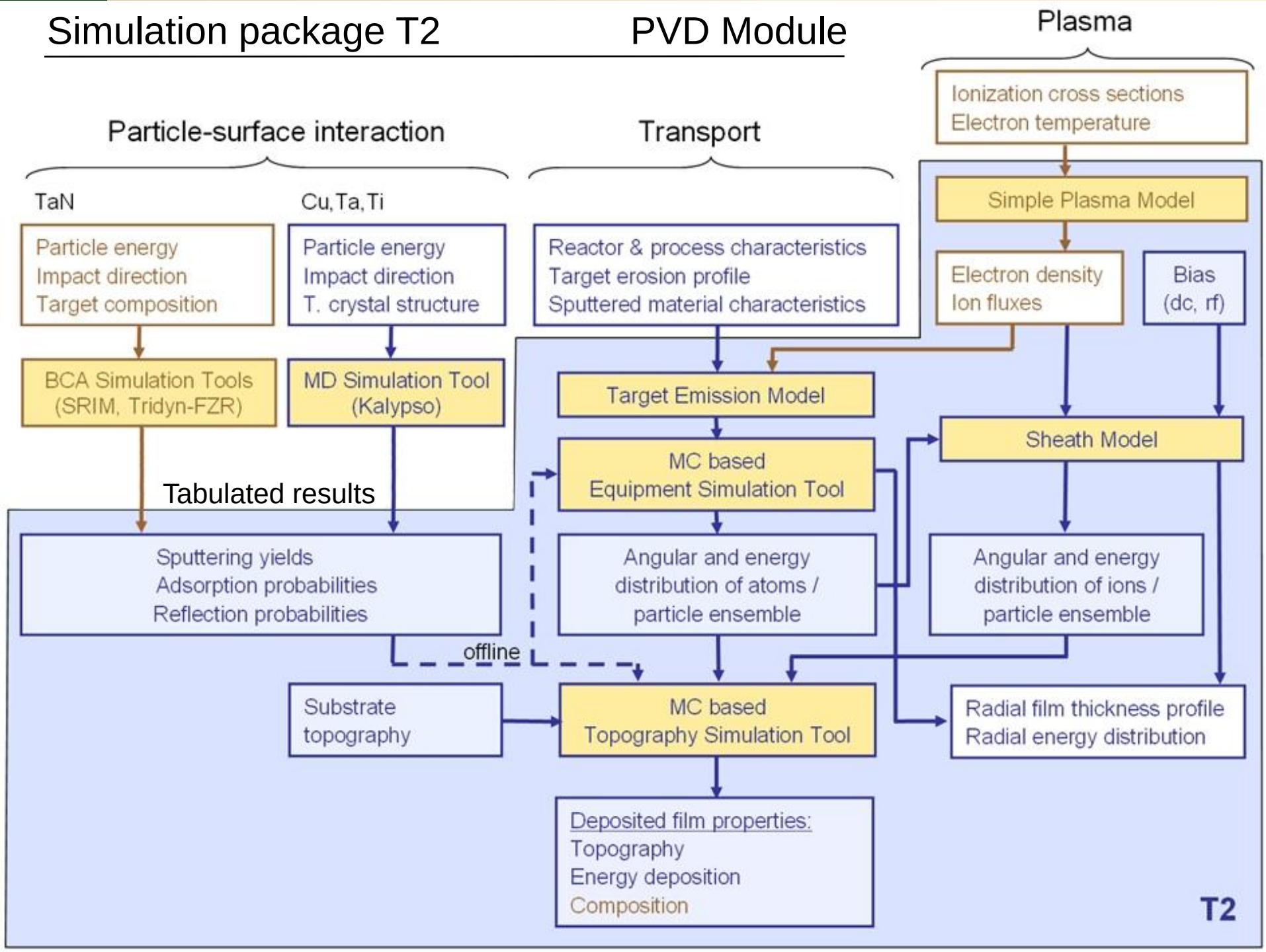
$$for(i = 0; i < numberOfSpecies; i++)\{$$

$$S = S + mole\_fraction_i$$

$$if\ (S > R) break; // i \text{ is index of collision partner}$$

$$\}$$

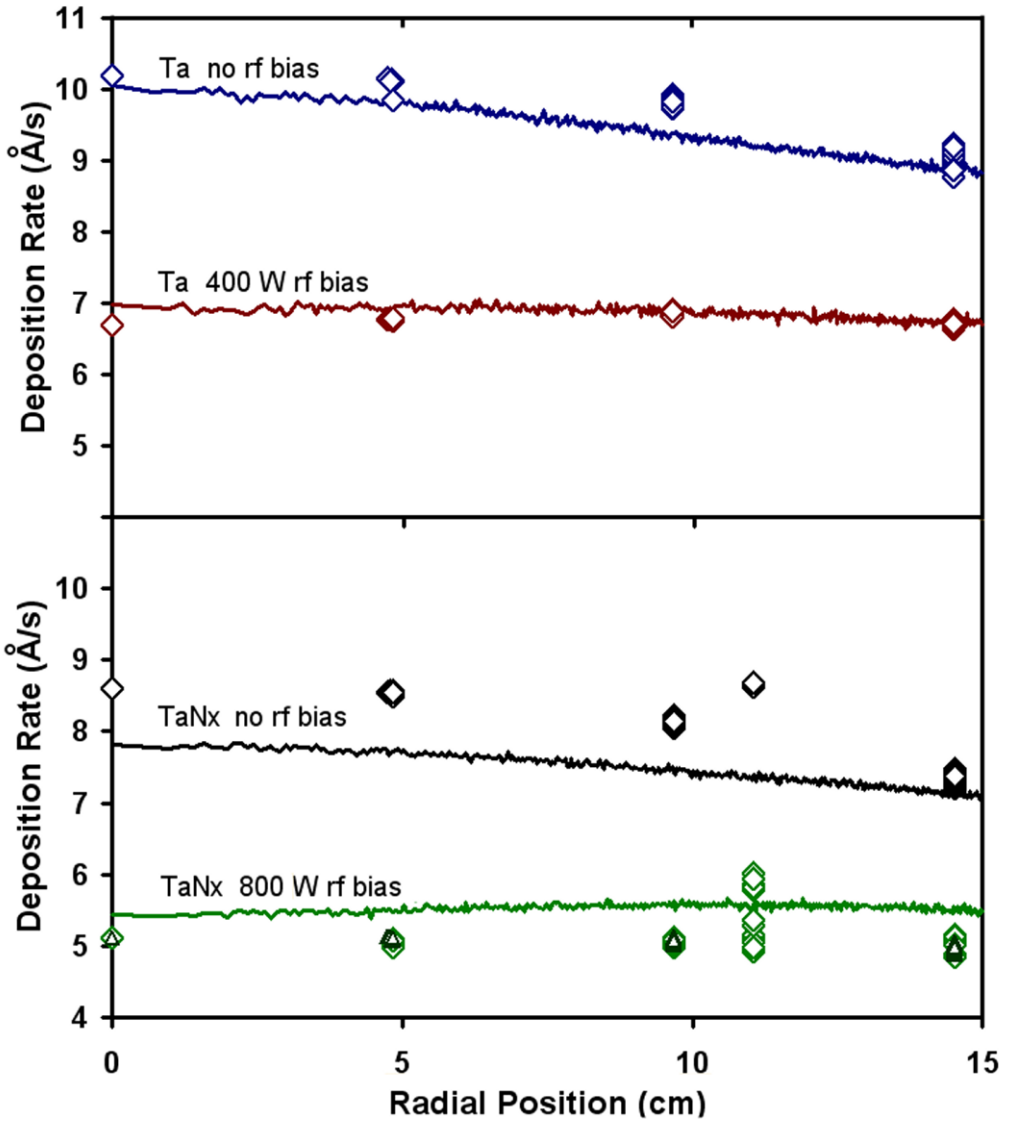
Simulation package T2 PVD Module



Results

Transport Simulation on different length scales

- **Reactor scale - Monte Carlo Transport Simulation**
- Feature - Monte Carlo Surface Kinematics Simulation
- Surface - Molecular Dynamics Approach



Radial dependence of simulated (lines) and measured (symbols) deposition rates for the deposition of Ta (upper frame) and TaN_x (lower frame) without and with rf bias applied to the wafer. Diamonds denote experimental deposition rates determined from thickness measurements by x-ray reflectometry and triangles designate deposition rates derived from measurements of the sheet resistance. The deposition rates at 11 cm are wafer-averaged values from different tools. The observed offset is presumably due to different target properties (age).

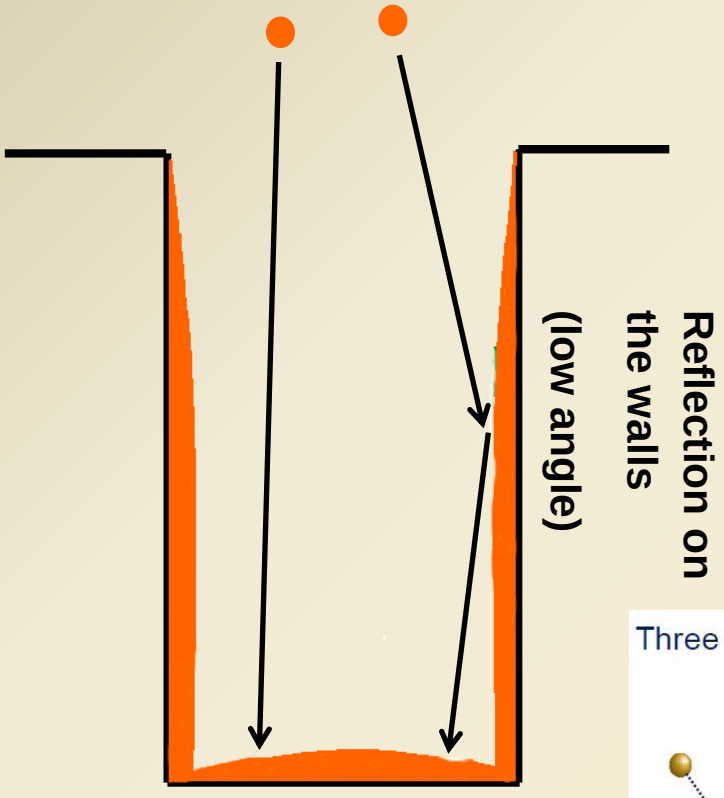
Calculation of

film growth

based on particle ensemble from reactor scale simulation

1. Start particle at wafer surface from collection
2. Modelling of particle flight near or in the feature (lattice based transport)
3. Modelling surface interaction (reflection, sputtering, sticking)
4. Repeat (10 000 000 and more)

IPVD situation



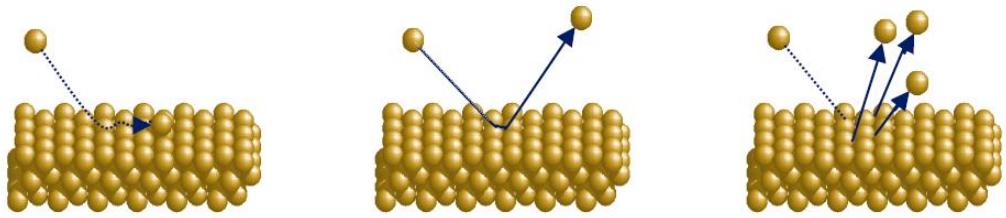
On the bottom mainly: Adsorption

Also some sputtering

With **Molecular Dynamics** we determine:

- probabilities of adsorption, reflection, and sputtering
- reflection or sputtering: the energy and angular distributions of reflected / sputtered atoms and the quantity of sputtered atoms

Three major types of surface reactions:



Start of a super-particle **X** of the collection taken from the reactor simulation or from an analytical distribution above the microskopic structur (angular and energy distribution)

↓

particle transport (particle size: X, real number)

↓

MD: surface reaction (depending on energy and angle of striking)

adsorbed = **X** * (1 – N)

reflected/sputtered/etched = **X** * N

N

↓

yes X > min?

no

N = 0	adsorption
0 > N > 1	partial adsorption (rsc = 1 - N)
N = 1	reflection
N > 1	sputtered, etched

rsc ... reactive sticking coefficient

Molecular (classical) dynamics

Quantum mechanics
(Schrödinger equation)

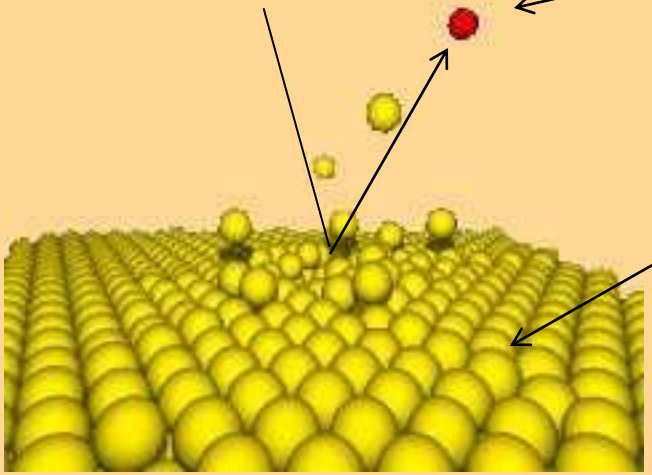
- no need for parameters
(solution from first principles)

→

Classical approximation
(Newton equations)

- a semiempirical classical
interaction model is needed

Simulation of sputtering and deposition:



Projectile: an Ar or metal ion
- sputtering: E_{kin} ~ 200 eV - keV
- deposition: 0 – 150 eV

Target: a metal crystal
- the size depends on $\mathbf{E_{kin}}$ of projectile
- for $\mathbf{E_{kin}}$ ~ 500 eV: ~ 10 000 atoms,

The interaction model

Metal - metal:

$r \in (0, \approx 0.5\, r_{NN})$:

Short range repulsive (pairwise) interaction

screened Coulomb potential (ZBL)

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} \frac{Z_\alpha\, Z_\beta\, e^2}{4\pi\varepsilon_o\, r_{ij}} \sum_{k=1}^{4} c_k^{\alpha\beta}\, e^{-b_k^{\alpha\beta}\, r_{ij} / a^{\alpha\beta}}$$

$Z_{\alpha,\beta}$ - atomic no. $\quad c_k^{\alpha\beta}, b_k^{\alpha\beta}, a^{\alpha\beta}$ - params

---

$r \in (\approx 0.9 r_{NN}, r_{cut-off})$:

Attractive (many-body) interaction (TB-SMA)

$E(123) \neq E(12) + E(13) + E(23)$

$$E = \sum_i \left[\sum_{j>i} A\, e^{-p\, x_{ij}} - \sqrt{\sum_{j \neq i} \xi^2\, e^{-q\, x_{ij}}} \right]$$

$$x_{ij} = \frac{r_{ij}}{r_o} - 1$$

A, ξ, p, q, r_o - parameters dependent on α and β

$r \in (\approx 0.5 r_{NN}, \approx 0.9 r_{NN})$:

A (pairwise) effective spline potential

a connection between the repulsive potential and an effective attractive potential derived from the bulk environment

Noble gas - metal: ***Short range repulsive potential only*** (ZBL)

MD code Kalypso

The integration loop: Verlet algorithm

For each particle in the system:

$$\mathbf{r}_{n+1} = \mathbf{r}_n + \mathbf{v}_n \Delta t + 0.5\mathbf{F}_n \Delta t^2 / m$$

$$\mathbf{v}_{n+1} = \mathbf{v}_n + 0.5(\mathbf{F}_{n+1} + \mathbf{F}_n)\Delta t / m$$

m ... mass of the particle

$\mathbf{r}_n, \mathbf{v}_n$ ... position/velocity at time $n\Delta t$

$\mathbf{F}_n$ ... force at time $n\Delta t$

= negative gradient of the interaction potential

Δt ... time step (~ 10^{-15} s)

- depends on E_{kin} and mass the projectile
- can be set to vary during the simulation (as the E_{kin} of particles is decreasing)

Program features

• default crystal structures and faces:

FCC (100, 110, 111)
BCC (100, 110) and so on

• processing the crystal

possibility to generate an arbitrary crystal face

• impact zone (points)
relation to the primitive surface cell

• lattice vibrations (hot target)

• models for inelastic energy losses

• thermostating

• configurable output

M.A. Karolewski

- **Kalypso: a software package for molecular dynamics simulation of atomic collisions at surfaces**
- A suite of graphically-oriented computer programs for molecular dynamics simulations of projectile collisions with metallic targets
- free-boundary or periodic targets
- many-body potentials
- a variety of inelastic loss models, able to carry out simulations of fluence-dependent processes

https://sites.google.com/site/kalypsosimulation/Home/**downloads**

DEMO

Results

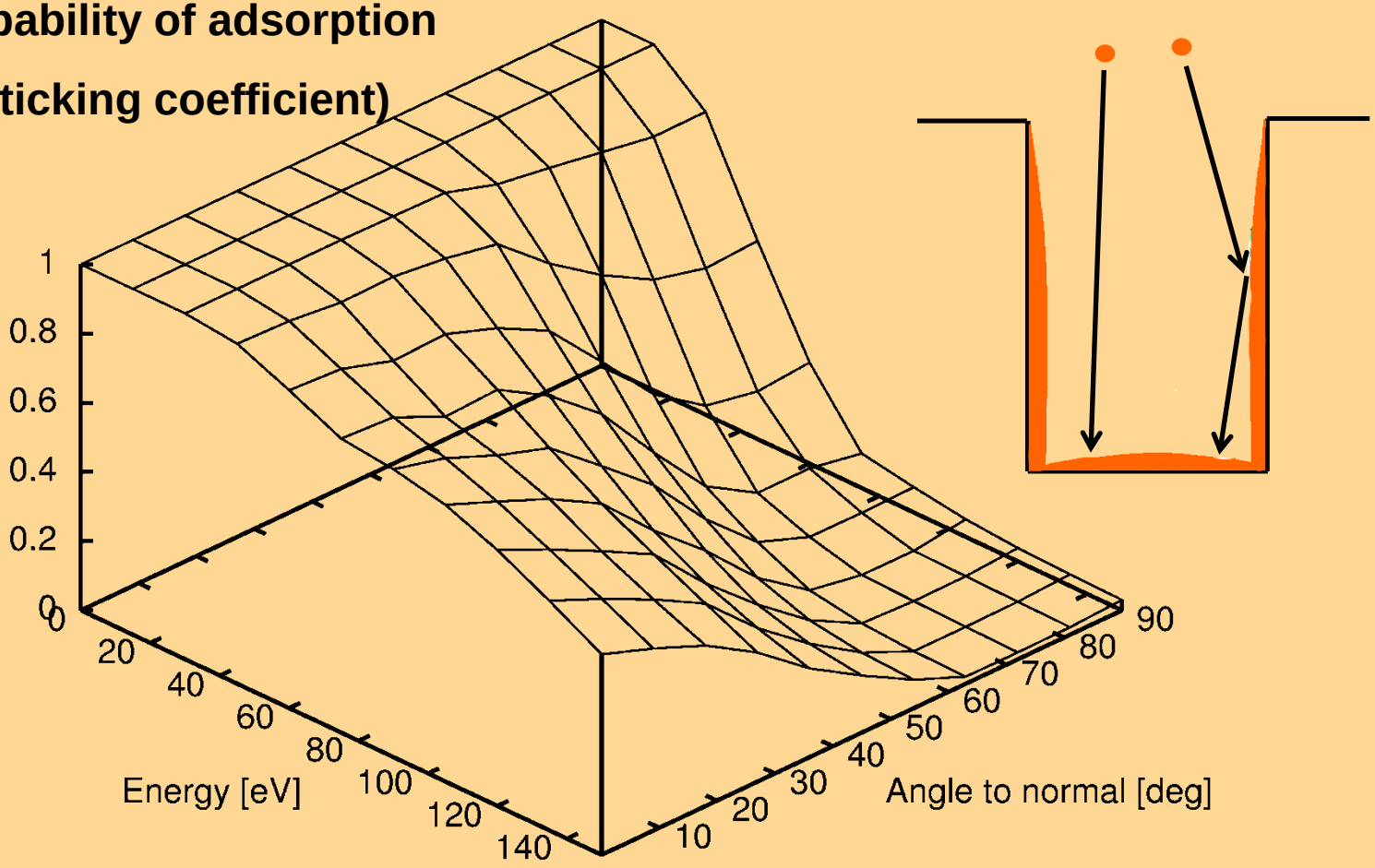
Transport Simulation on different length scales

- Reactor scale - Monte Carlo Transport Simulation
- Feature - Monte Carlo Surface Kinematics Simulation
- **Surface - Molecular Dynamics Approach**

IPVD Deposition: Ti^+ (0-150eV) ⟶ bcc Ti(100)

Probability of adsorption

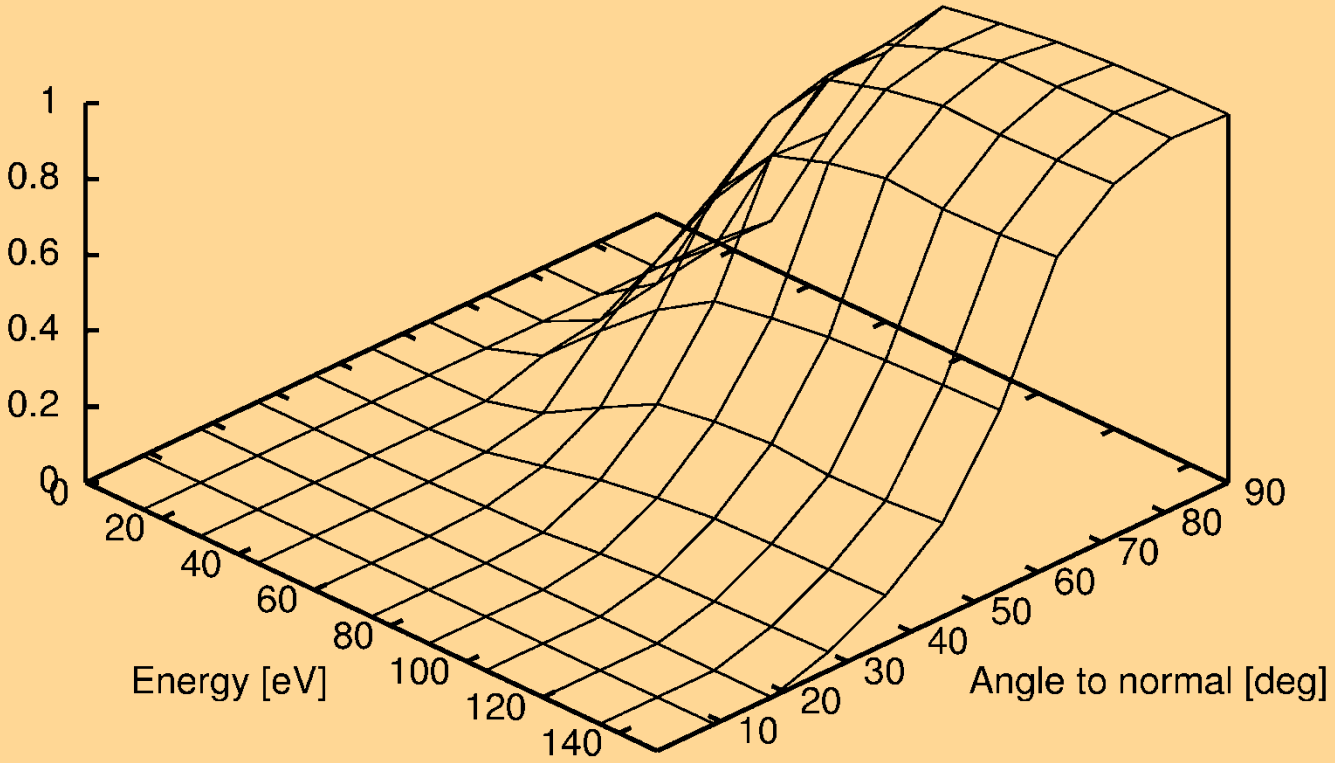
(sticking coefficient)



MD calculation by A. Kersch

IPVD Deposition: Ti^+ (0-150eV) ⟶ bcc Ti(100)

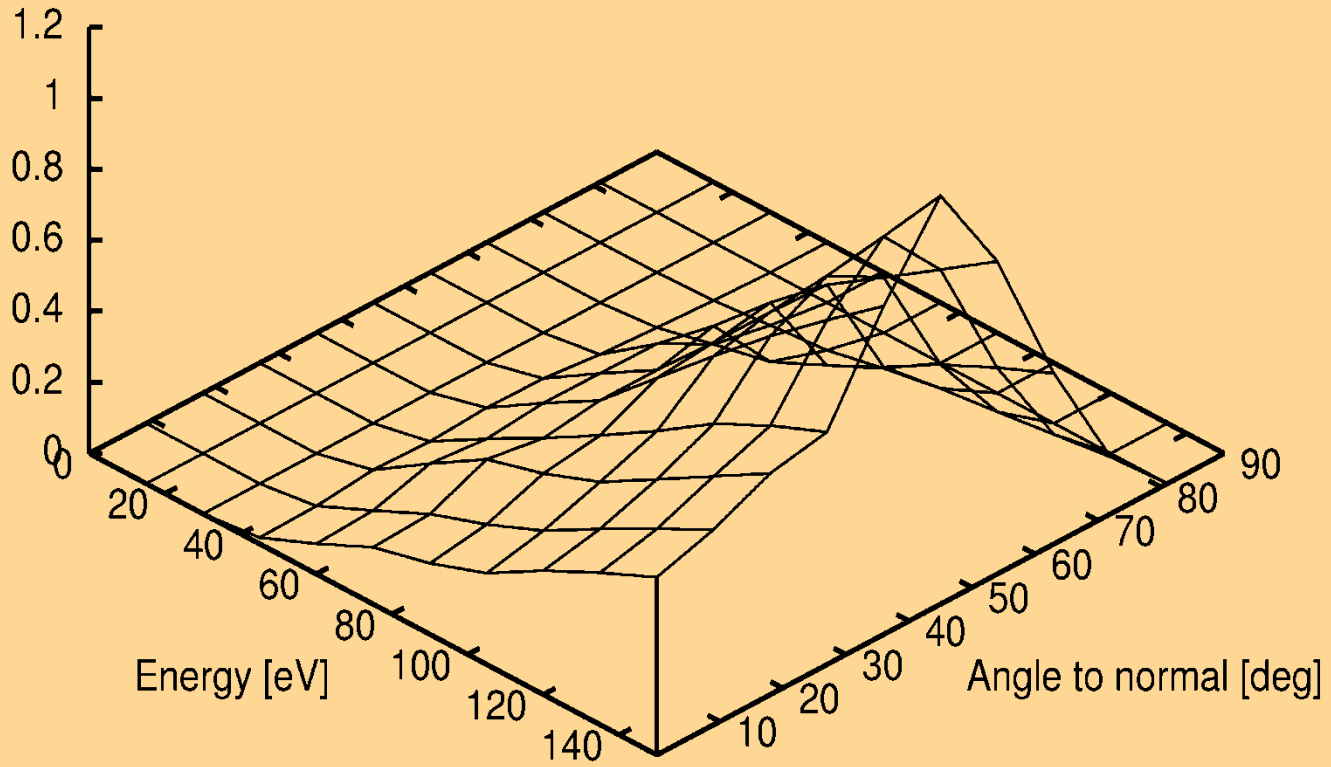
Probability of reflection



MD calculation by A. Kersch

IPVD Deposition: Ti^+ (0-150eV) ⟶ bcc Ti(100)

Sputtering yield



MD calculation by A. Kersch

6. Calculation of surface interaction

rsc = 1… save particle (position, direction, energy)

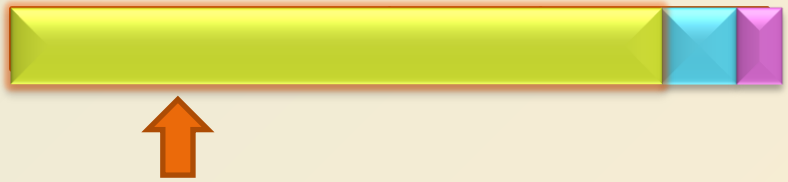
or MD based calculation of adsorption/sputtering/reflexion probability

surface interaction

Adsorption 0,85 (rsc … reactive sticking coefficient

Reflexion 0,1

Sputtering 0,05



$$f_{ads} + f_{reflex} + f_{sputt} = 1$$

$$if\left(f_{ads} > R\right): \text{Adsorption}$$

$$if\left(f_{reflex} > R\right): \text{Reflexion}$$

else Sputtering

feature scale simulation

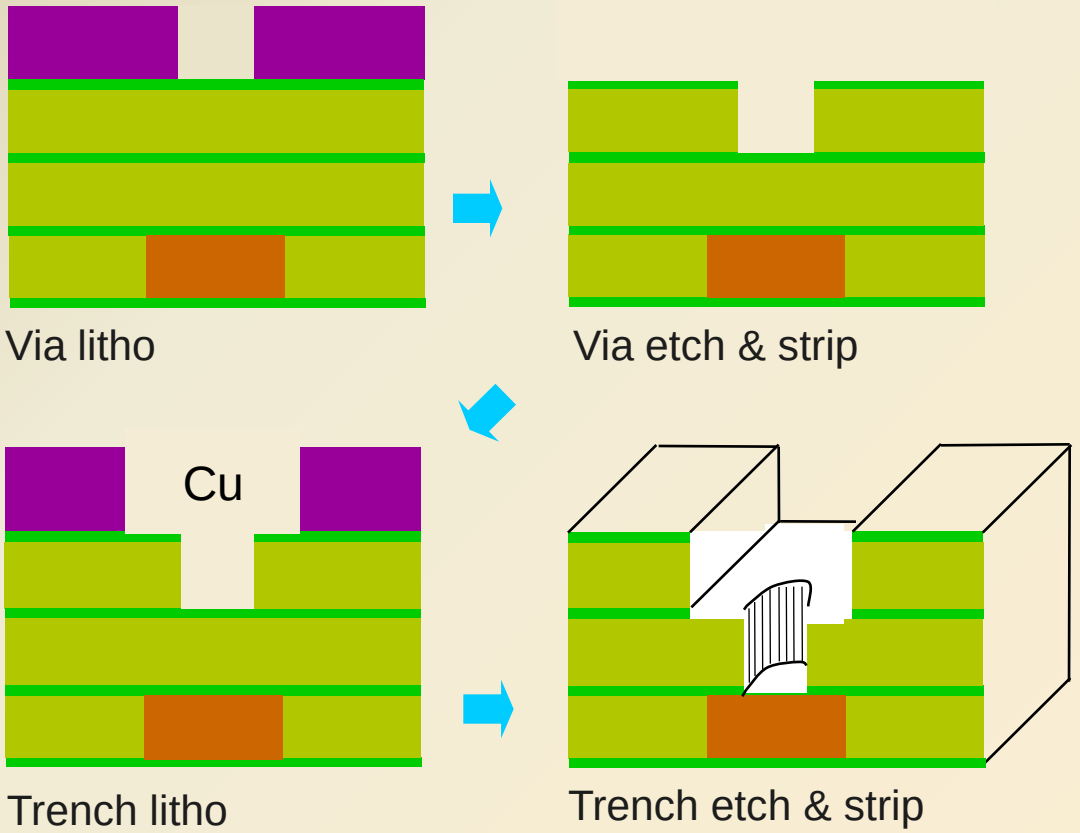
Sputtering rate, emission angle, energy of sputtered particles

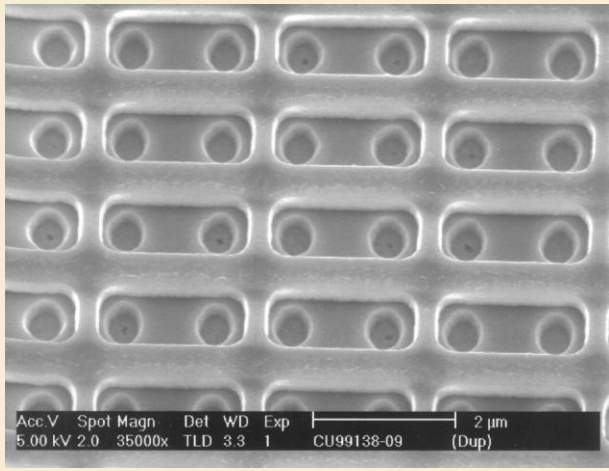
Results

Transport Simulation on different length scales

- Reactor scale - Monte Carlo Transport Simulation
- **Feature - Monte Carlo Surface Kinematics Simulation**
- Surface - Molecular Dynamics Approach

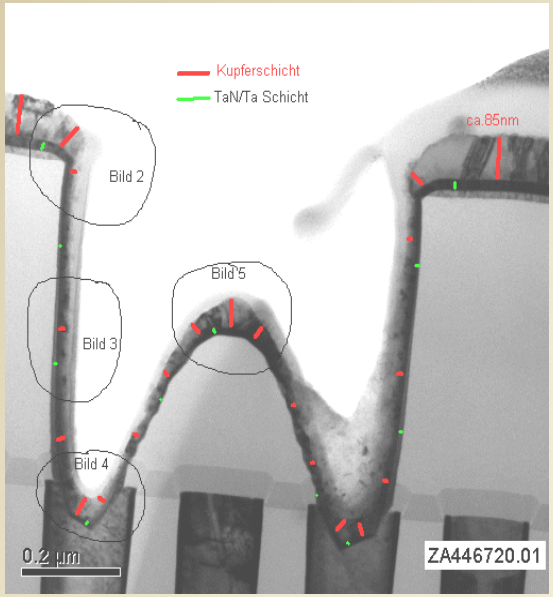
It uses two dielectric etch processes, one via etch and one trench etch
Metal layers are deposited into via holes and trenches

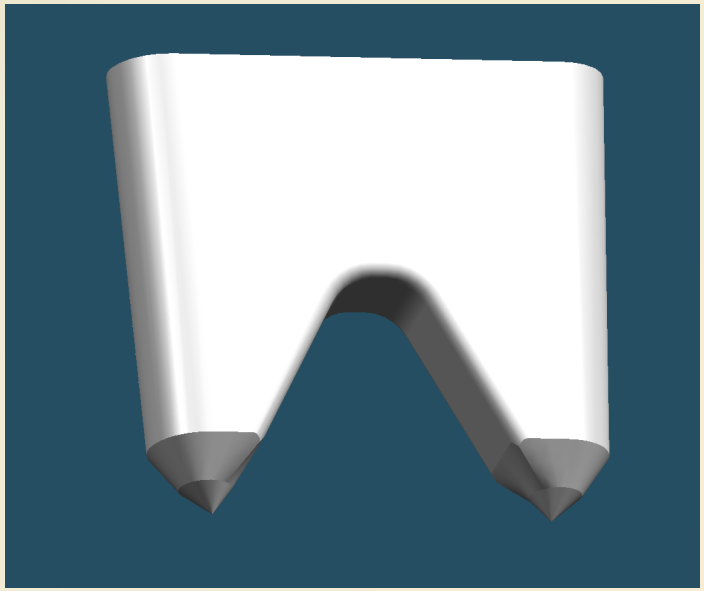




source: IMEC 2003

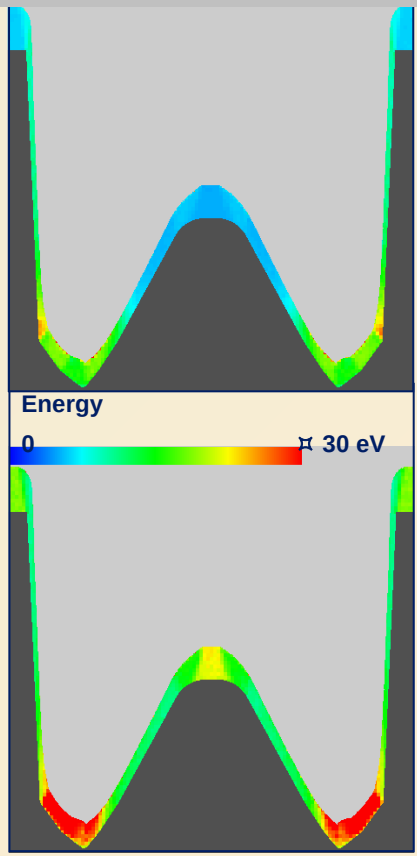
Cu seed layer deposition in a minimum size dual damascene test structure

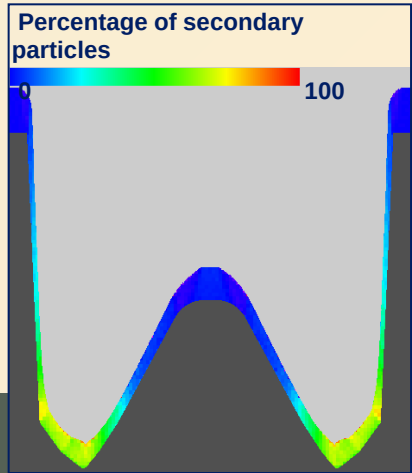




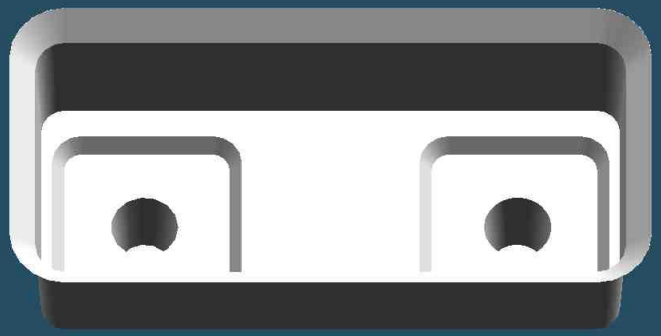
PVD:

Simulation of seed layer deposition



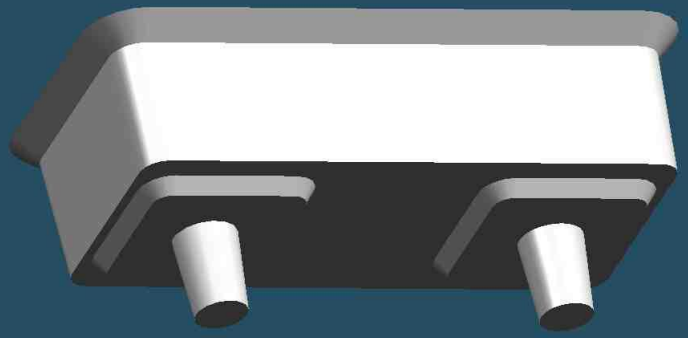


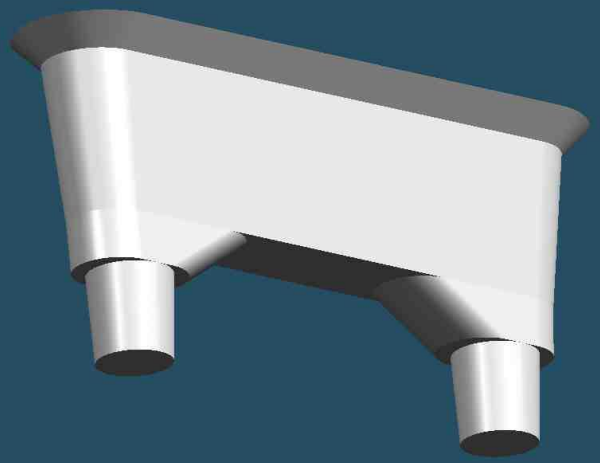
PVD Feature Scale Simulation, Structure Input: Via-Interconnect-Via



V1 covered landed center

V1 isolated center



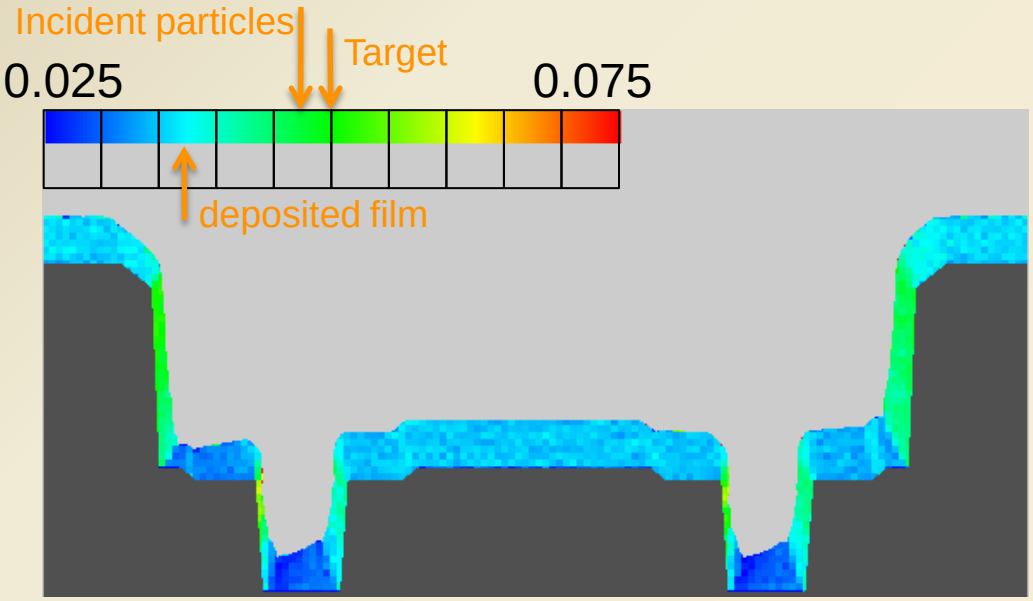


PVD Feature Scale Simulation, Results, Self Forming Barriers

Composition

$$\frac{Mg}{Cu + Mg}$$

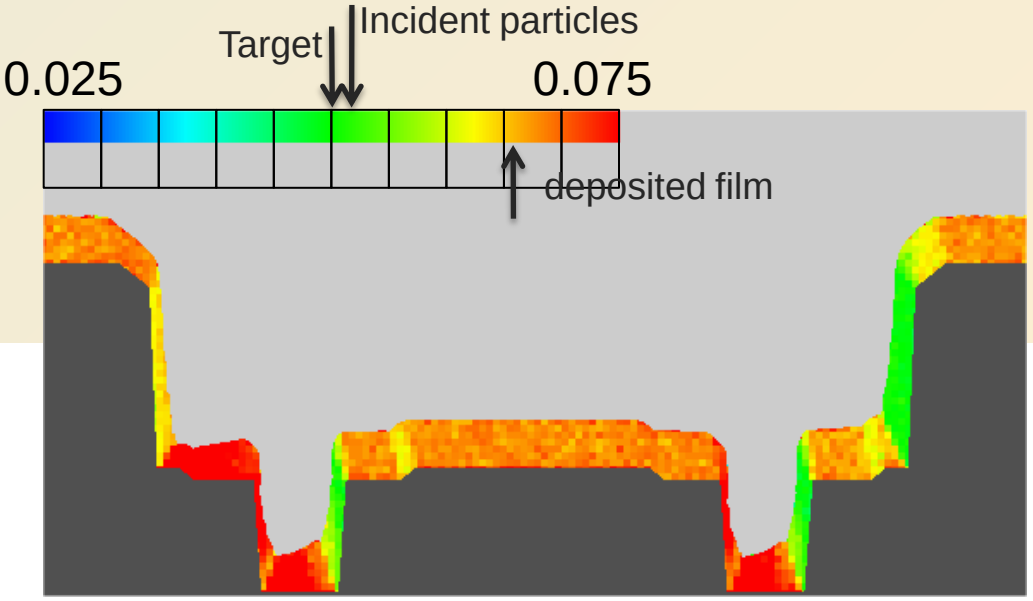
Target	0.0500
Incident parts	0.0468
Film (average)	0.0371



Cu95Mg05

$$\frac{Al}{Cu + Al}$$

Target	0.0500
Incident parts.	0.0519
Film (average)	0.0657

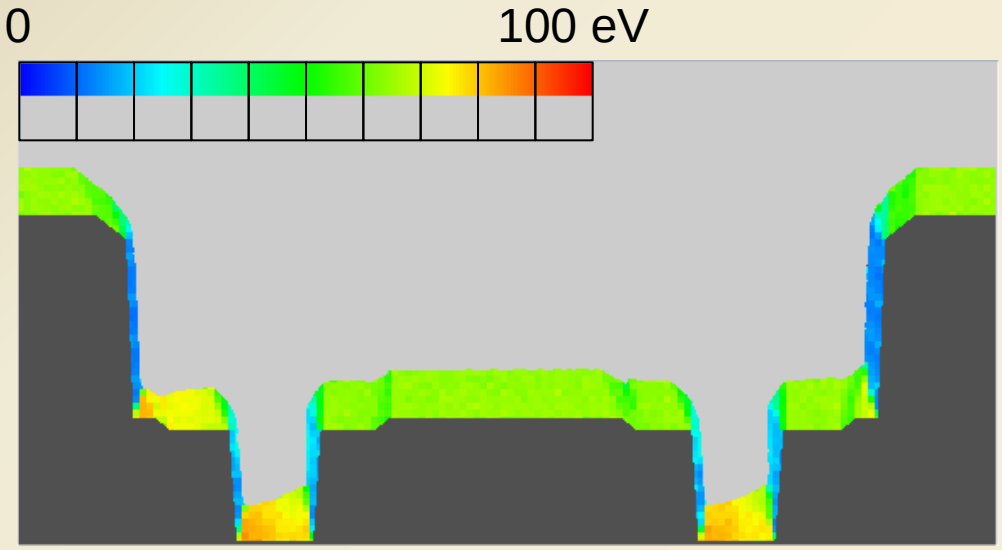


Cu95Al05

PVD Feature Scale Simulation, Wafer edge

Energy

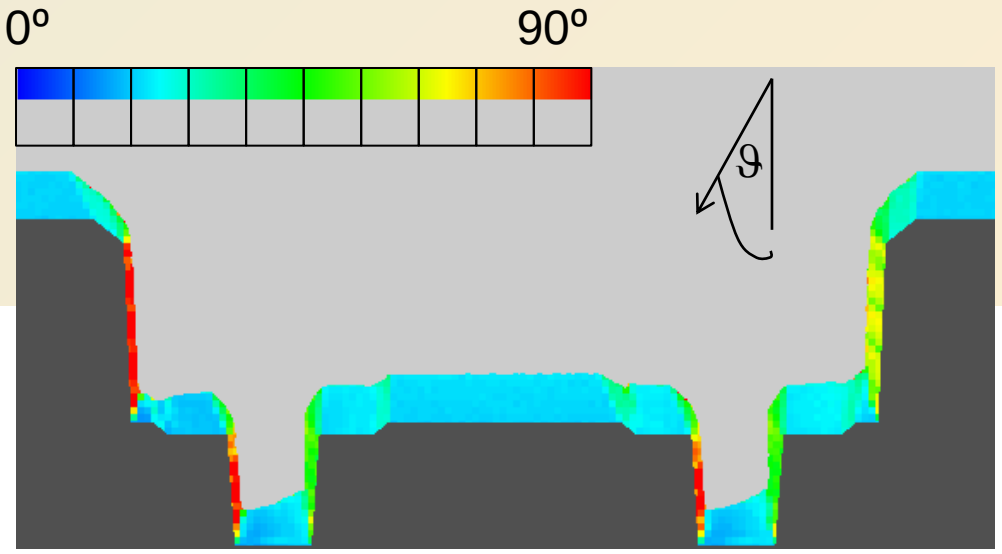
of incident particles



Cu95Mn05

Polar angle

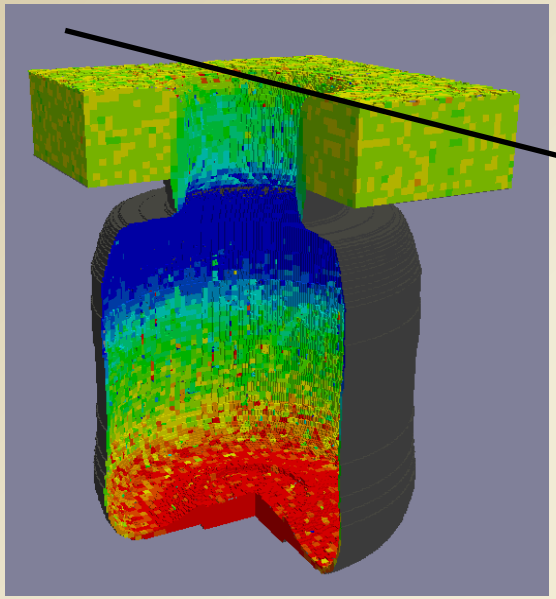
of incident particles

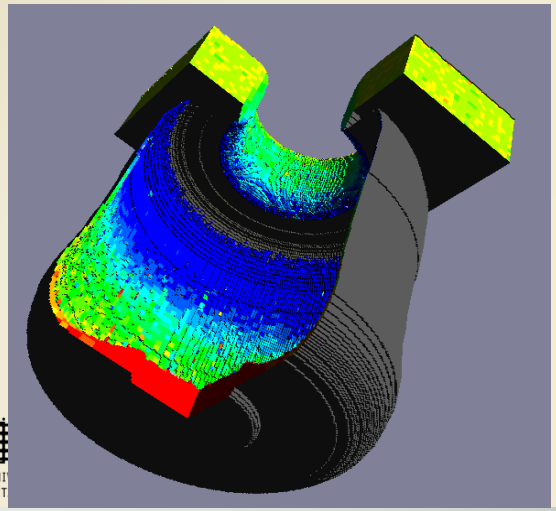


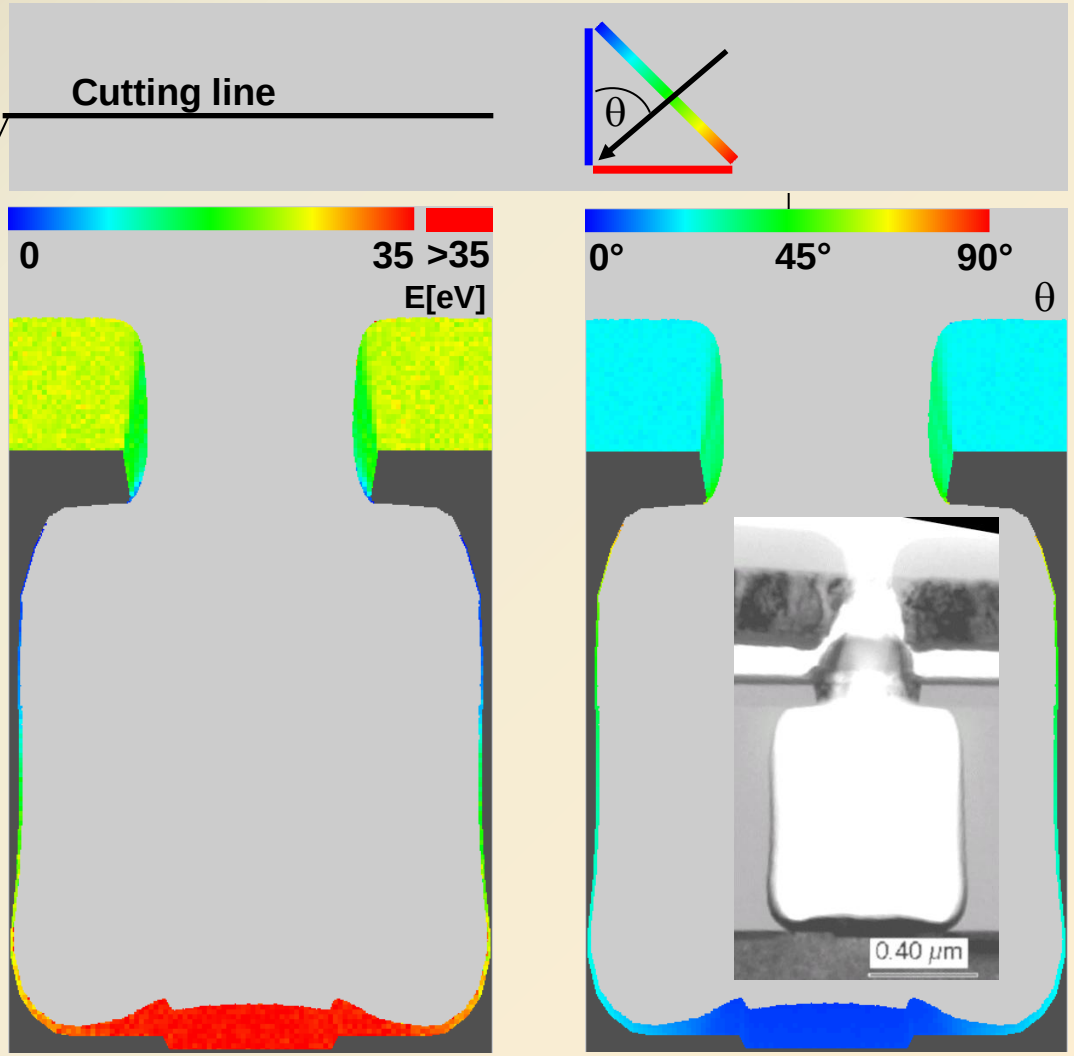
Cu95Mn05

Direction towards the wafer center

Ti deposition (Advanced HiFill process) in a bottle-shaped test structure







Energy deposition in eV/atom

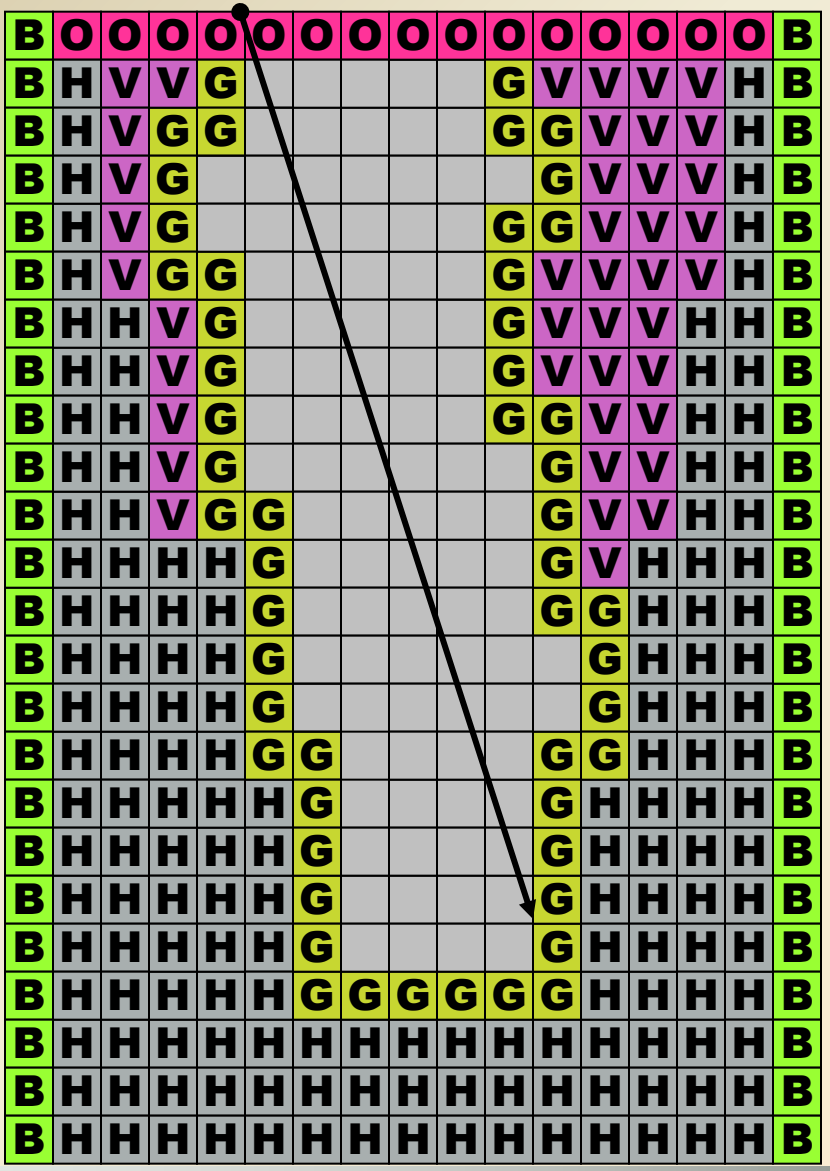
Influence on texture, density, surface diffusion

Average polar angle of incident Ti atoms

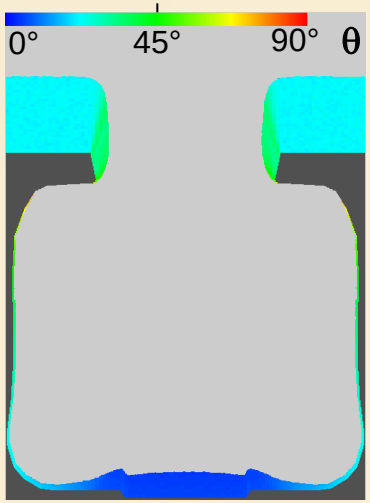
Influence on grain growth

Flow chart – Lattice Based Monte Carlo Topography Simulation in „T2“

Particle starts here

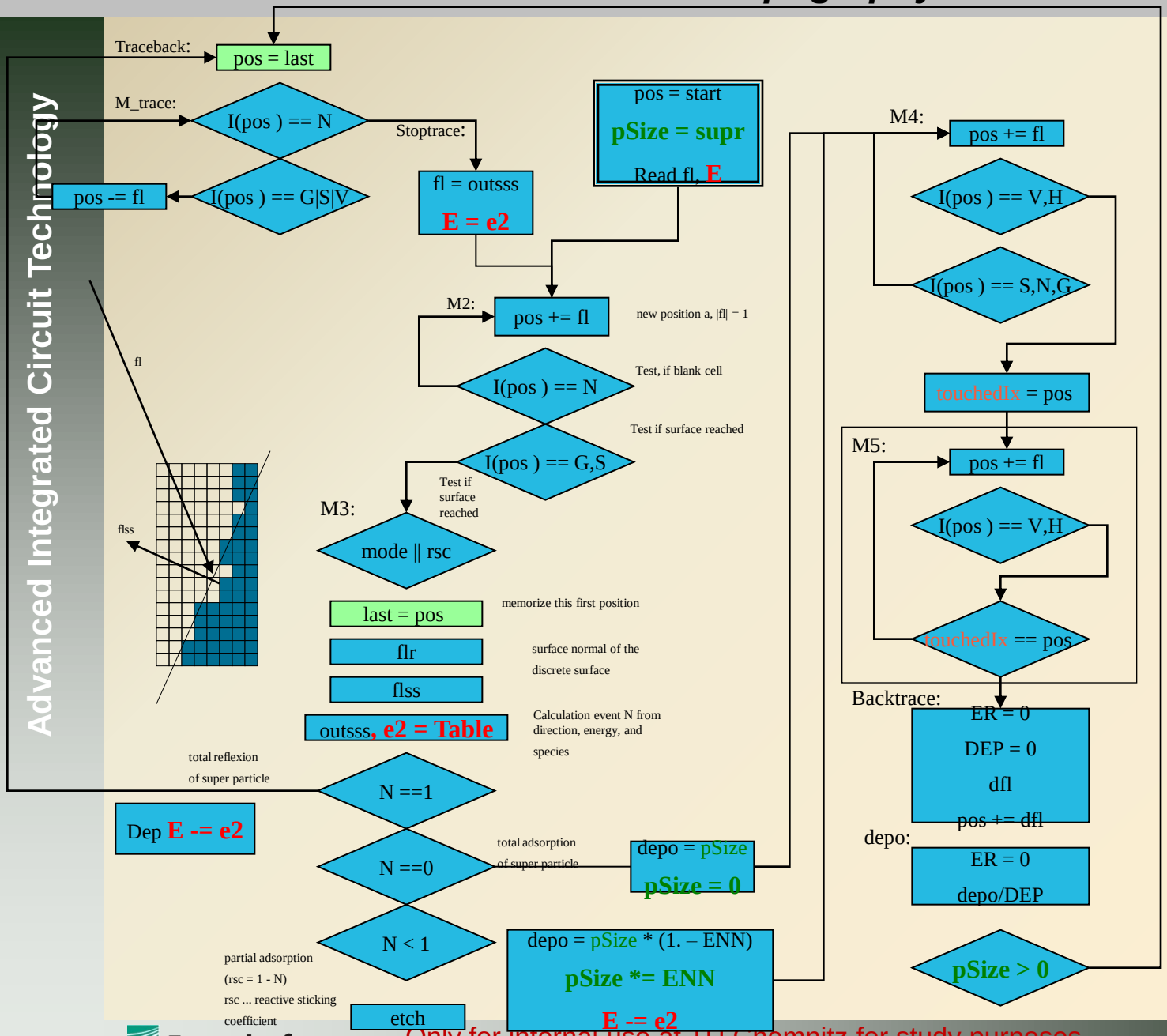


- **H** Material cell, structure definition
- **V** Material cell, grown
- **B** Boundary cell
- Blank cell
- **O** Boundary cell
- **G** Growing cell

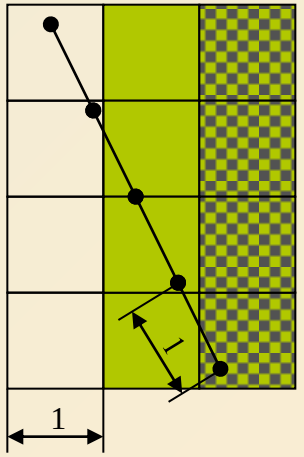


Average polar angle of incident atoms

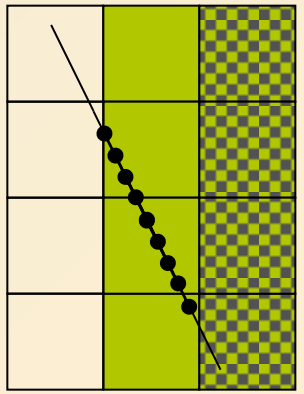
Flow chart – Lattice Based Monte Carlo Topography Simulation in „T2“



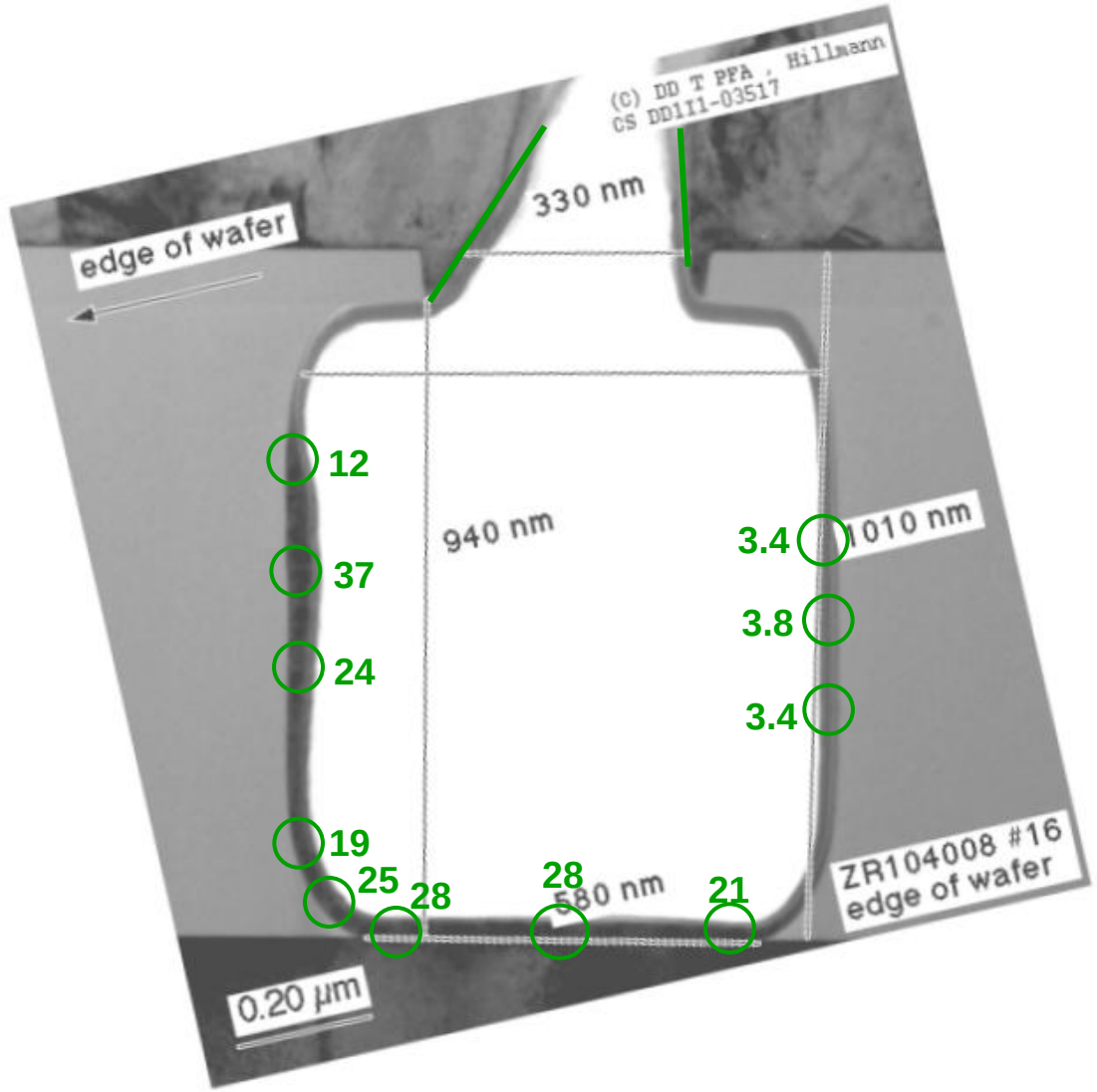
Transport:

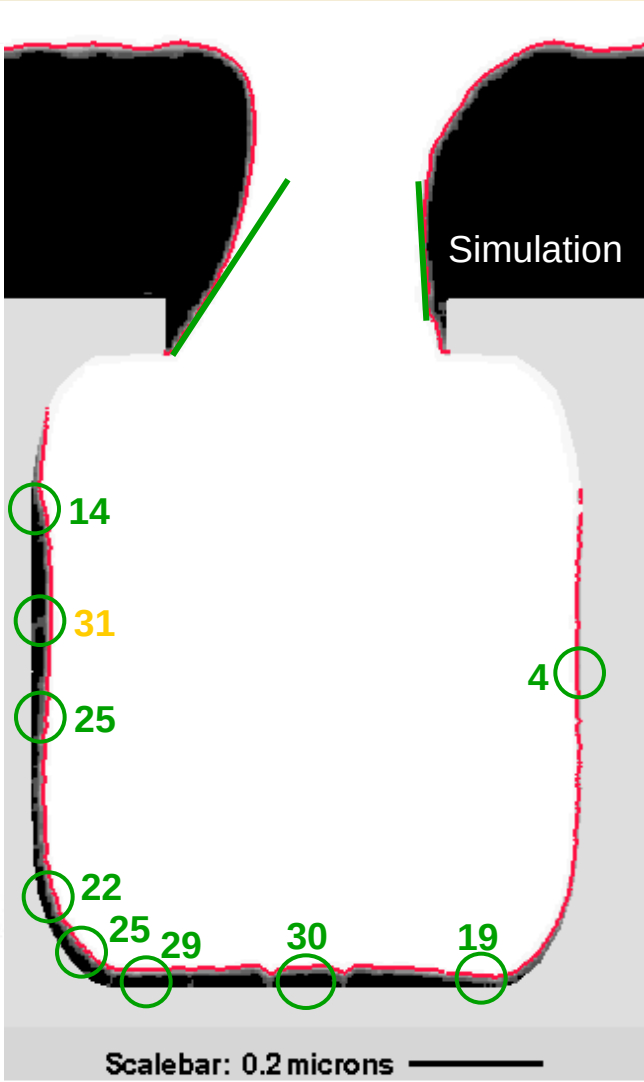


Backtracing:

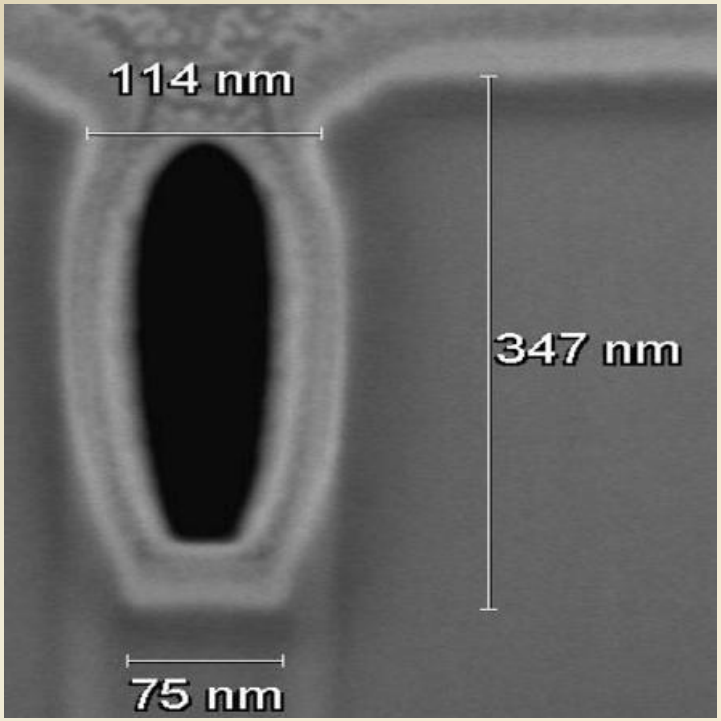


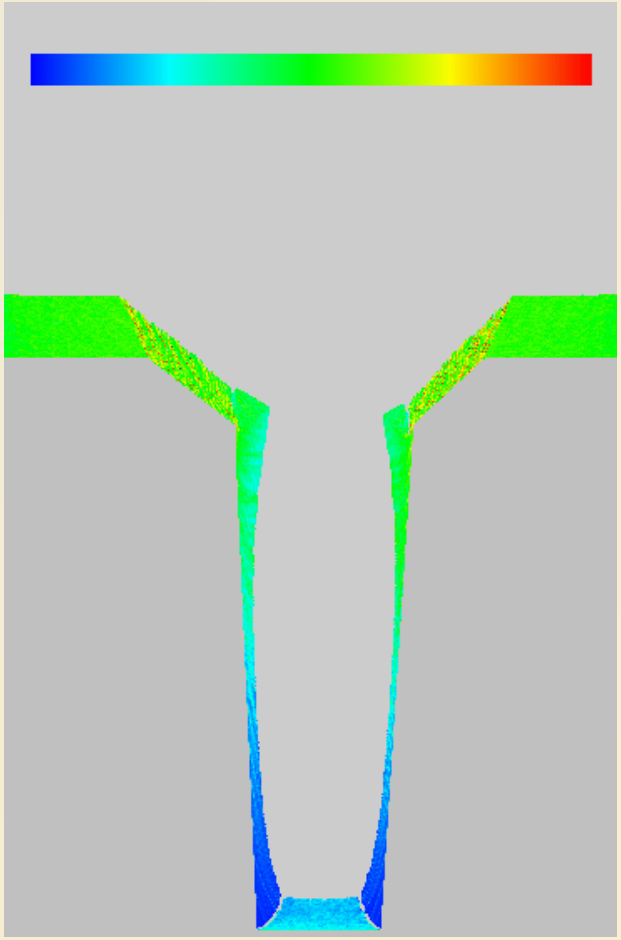
Titanium, wafer edge, rsc = 1





TaN-PVD: Feature scale





$$\frac{N}{Ta+N}$$

Summary

- Modeling of thin film deposition helps to understand better chemical/physical background of deposition processes
- Simulation to improve deposition rates, uniformity, fill behavior of vias and trenches by optimization of process conditions and reactor configuration
- Calculation of layer properties difficult to measure (energy deposition, layer composition (TixNx), minimum film thickness in deep trenches/vias)
- Time savings
- Cost reduction
  (example: vertical CVD batch reactor: up to 200 200mm wafers!)

Types of Computer Simulation

Advanced Integrated Circuit Technology

+

=

Static Simulation

Time is no consideration, snap-shot

Monte-Carlo Simulation

Is based on random numbers and/or stochastic theory

Dynamic Simulation

Time is most important
Sequences and processes are the focus

Continuous Simulation

Time flows in regular steps
Every time step causes a of state of system change
Models mostly systems of differential equations
Continuous simulation ist deterministic
Physical processes (e.g. vibration characteristics, analog circuits, fluid flow), chemical processes, weather and climate

Discrete Simulation

In time step events are evoked which determine the next system state

Application in production and logistics, Supply-Chains etc.

Hybride Simulation

Models representable with standard elements (e. g. random numbers, waiting lists, probability distributions)

Forecast of expected probabilities for different system states

Prognosis (traffic, airports, tollbooths, mail, etc.)