Repetition: Sputter Yield

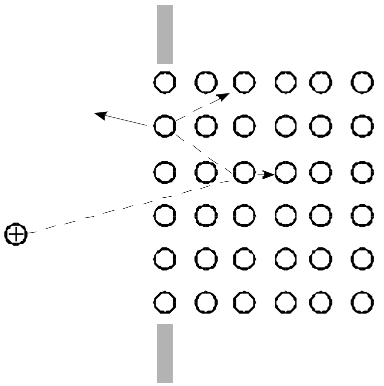
$$Y = \frac{\langle n \rangle}{n^{+}}$$

<n> = mean number of particles emitted per impingement
n^{+} = number of impinging ions

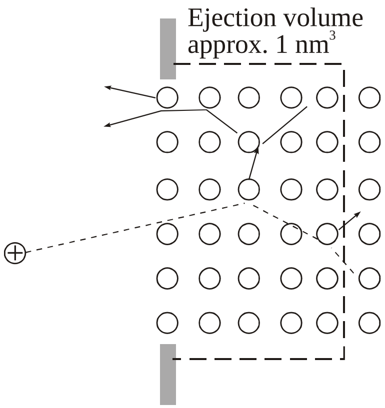
Y is dependent on several parameters of the ions and of the target material.

Repetition: Sputtering Regimes

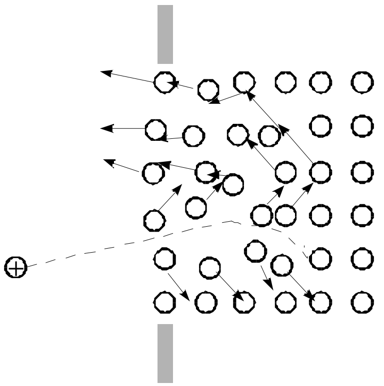
- **Single Knock On**



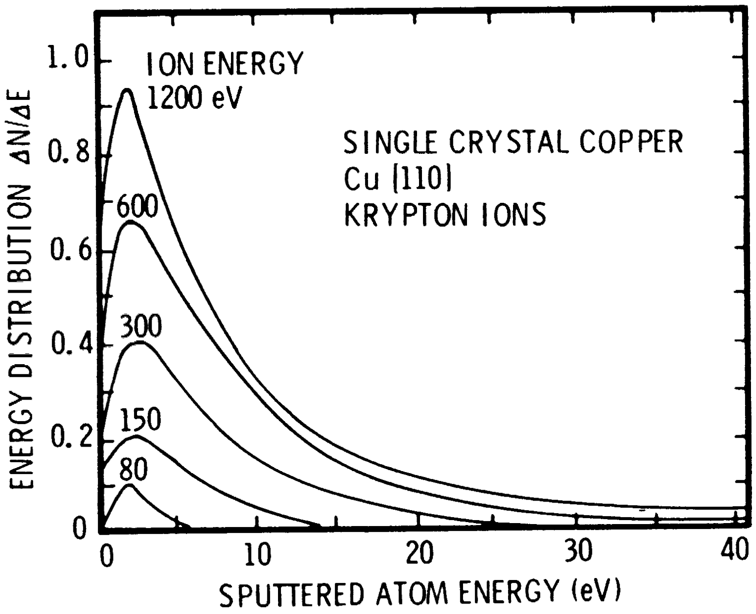
- **Linear Collision Cascade**

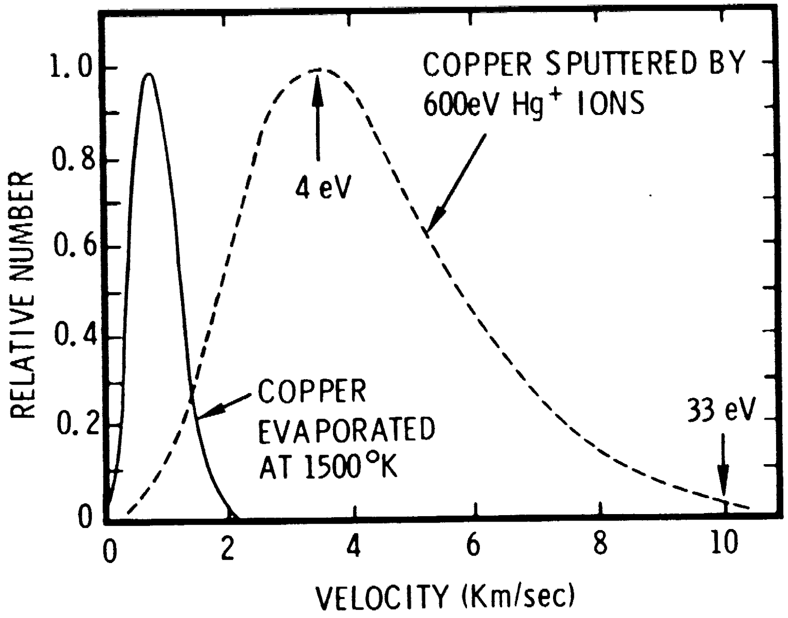


- **Thermal Spike**



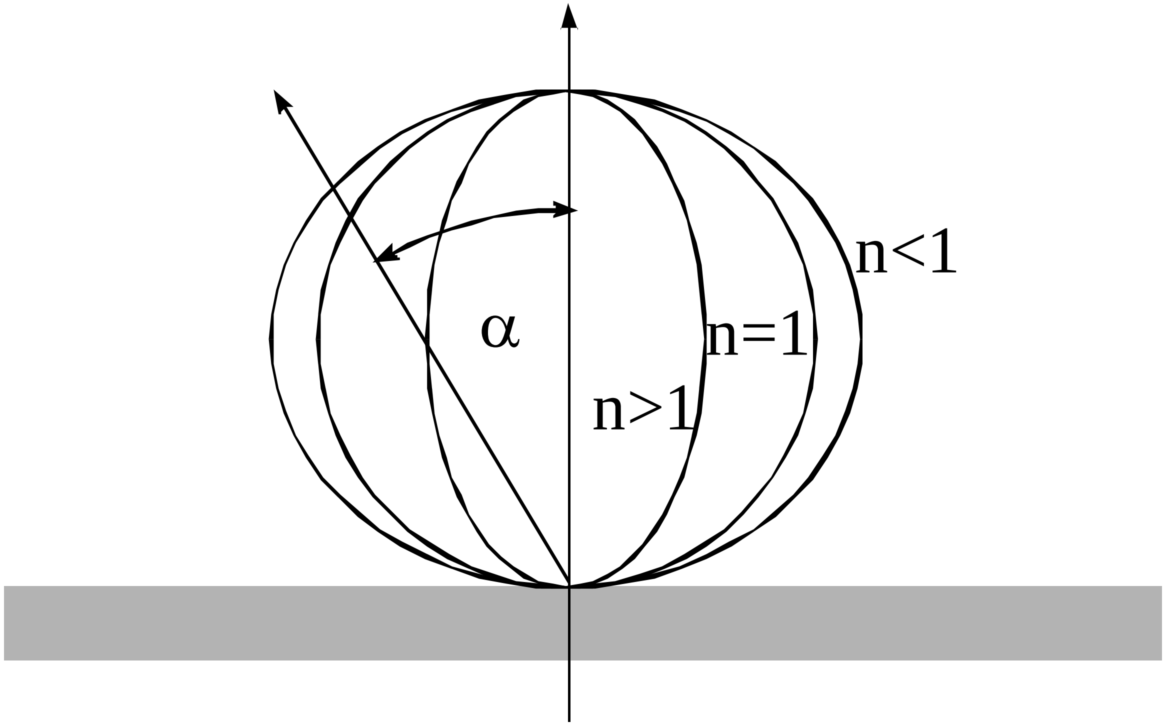
Repetition: Energy of Ejected Particles





The energy distribution of sputtered particles is significantly different from that of thermally evaporated ones.

Repetition: Angular Distribution at Emission

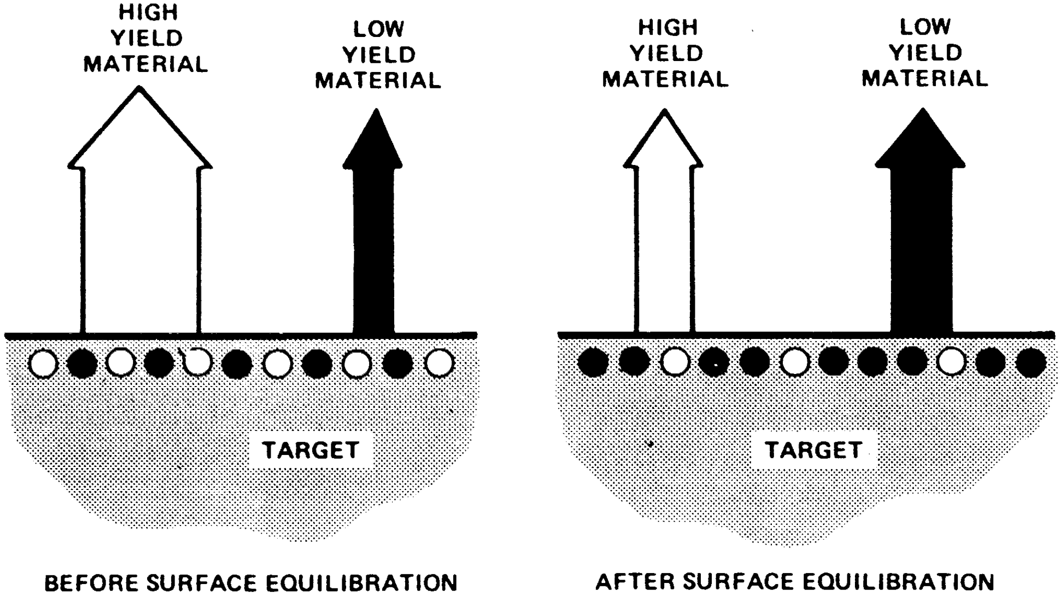


$$n(\alpha) \propto \cos^n \alpha$$

$n \leq 1$ E < 1 keV

$n > 1$ E > 1 keV

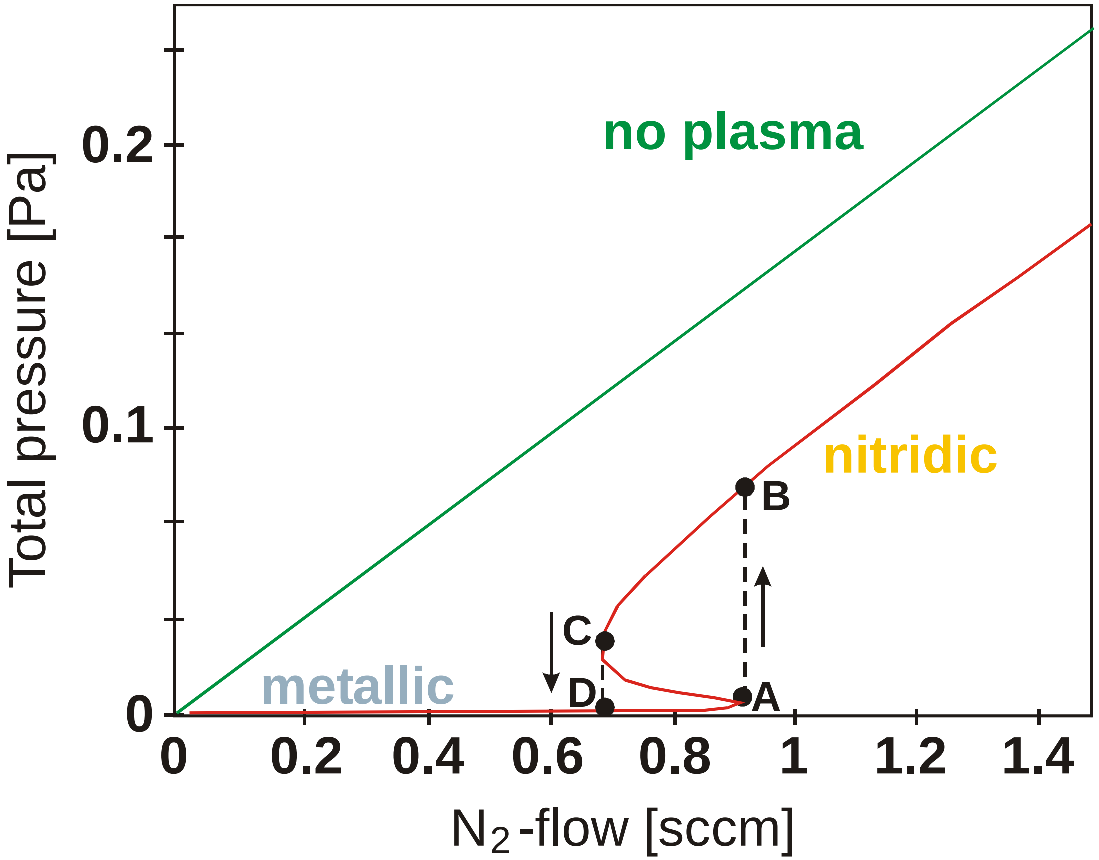
Repetition: Sputtering of Alloys



In the case of the homogenous distribution of the constituents the vapor composition is (after a transient regime) identical to the target composition.

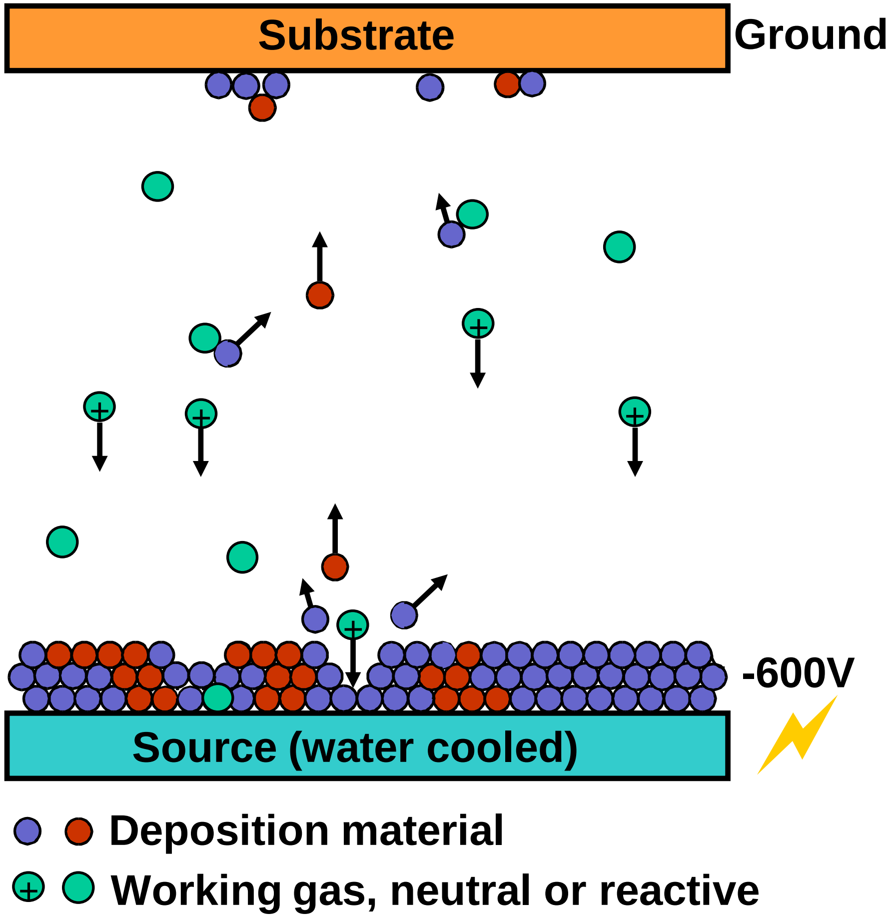
Repetition: Reaktive Processes (TiN)

Pressure in the chamber in dependence on the N_2- flow:



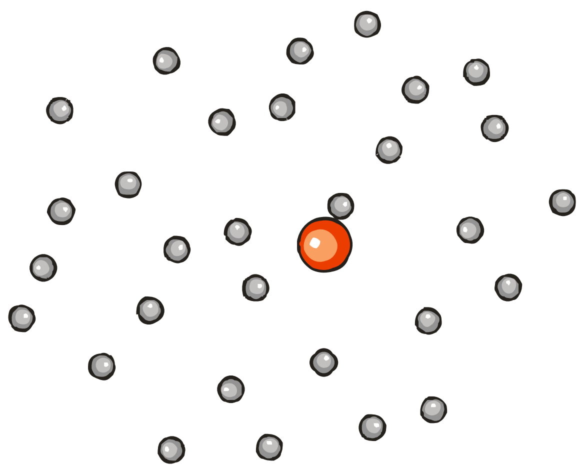
At first all N_2 is consumed; the unstable operating point A would be the optimum working condition

Gas Phase Transport



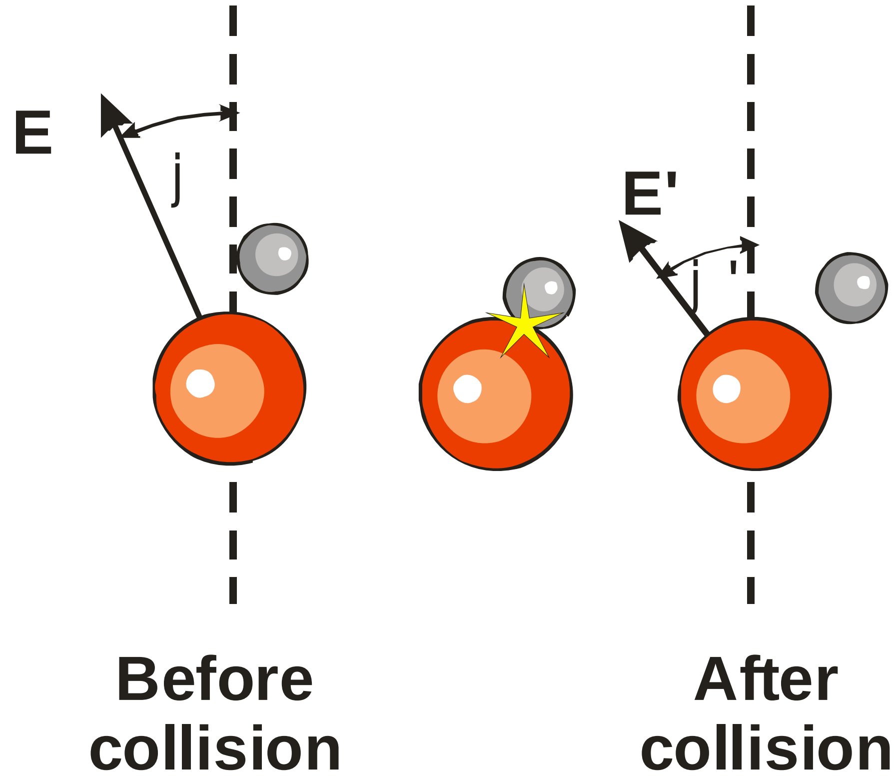
Modification of energy- and angular distribution of the coating material during the transport from source to substrate.

Film Particle Trespasses Gas Phase



$$E' = E - \Delta E$$

$$\varphi' = \varphi - \Delta\varphi$$



Per collision the particle suffers a mean energy loss ΔE and a mean change of the angle Δφ.

Mean Energy Loss I

Initial condition: particle 1 at rest, particle 2 moves.
Wanted: energy loss of particle 2.

$$\left\langle \frac{E'}{E} \right\rangle = 1 - \frac{1}{2} \cdot \frac{4 \cdot \mu}{(1+\mu)^2}, \quad \mu = \frac{m_1}{m_2}, \quad \langle \Delta E \rangle \approx E \cdot \left(1 - \left\langle \frac{E'}{E} \right\rangle \right)$$

E ... Energy particle 2 before collision
E' ... Energy particle 2 after collision

Light working gas: $\mu = 0.1 \Longrightarrow \langle E'/E \rangle = 0.83$

Equal masses: $\mu = 1 \Longrightarrow \langle E'/E \rangle = 0.5$

Heavy working gas: $\mu = 10 \Longrightarrow \langle E'/E \rangle = 0.83$

Mean Energy Loss II

Situation after 5 Collisions:

Light working gas: $\mu = 0.1 \Longrightarrow (\langle E'/E \rangle)^5 = 0.4$

Equal masses: $\mu = 1 \Longrightarrow (\langle E'/E \rangle)^5 = 0.03$

Heavy working gas: $\mu = 0.1 \Longrightarrow (\langle E'/E \rangle)^5 = 0.4$

For more realistic collision processes there are energy dependent collisional cross sections. The slower a particle is, the larger is it's cross section. Furthermore at a certain point the velocity distribution if the gas atoms has to be taken into account.

Mean Scattering Angle I

Mean scattering angle θ of particle 2:

$$\langle \cos\varphi \rangle = 1 - \frac{\mu^2}{3}, \quad \mu = \frac{m_1}{m_2} < 1$$

$$\langle \cos\varphi \rangle = \frac{2}{3 \cdot \mu}, \quad \mu = \frac{m_1}{m_2} > 1$$

Light working gas: $\mu = 0.1 \Rightarrow \langle \varphi \rangle = 4.6°$

Equal masses: $\mu = 1 \Rightarrow \langle \varphi \rangle = 48.2°$

Heavy working gas: $\mu = 10 \Rightarrow \langle \varphi \rangle = 86.2°$

Mean Scattering Angle II

Number f collisions n, to cover 360° (complete loss of directional information):

Light working gas:

$$\mu = 0.1 \Rightarrow \langle \varphi \rangle = 4.6°$$

$$n = 79$$

Equal masses:

$$\mu = 1 \Rightarrow \langle \varphi \rangle = 48.2°$$

$$n = 8$$

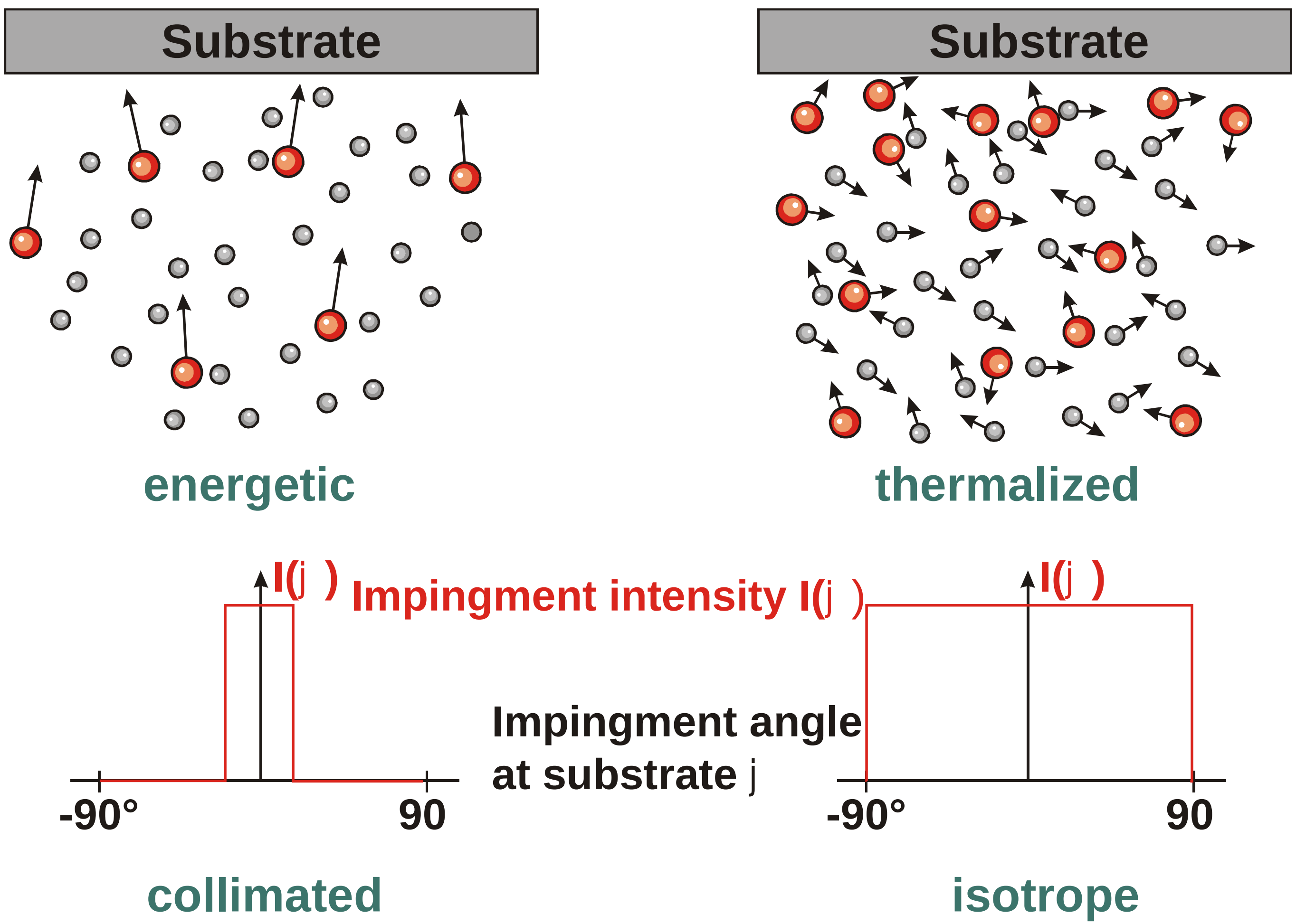
Heavy working gas:

$$\mu = 10 \Rightarrow \langle \varphi \rangle = 86.2°$$

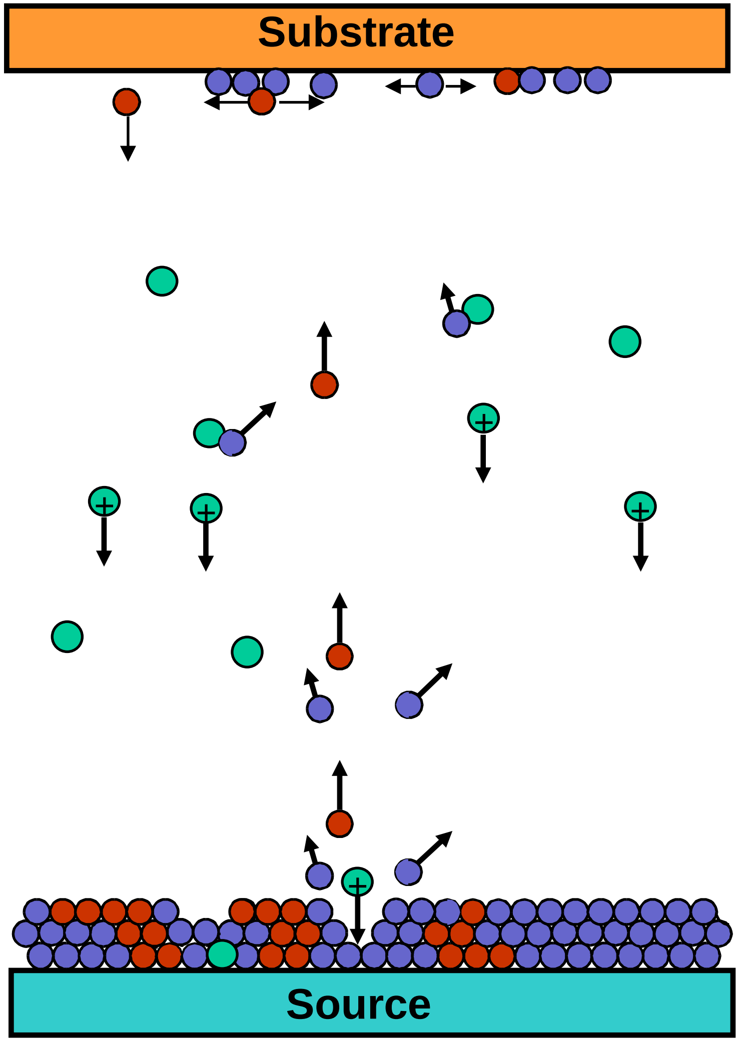
$$n = 5$$

Summary Gas Phase Scattering

As a result of collisions in the gas phase two limiting cases can be distinguished:



Elementary Steps of Film Deposition



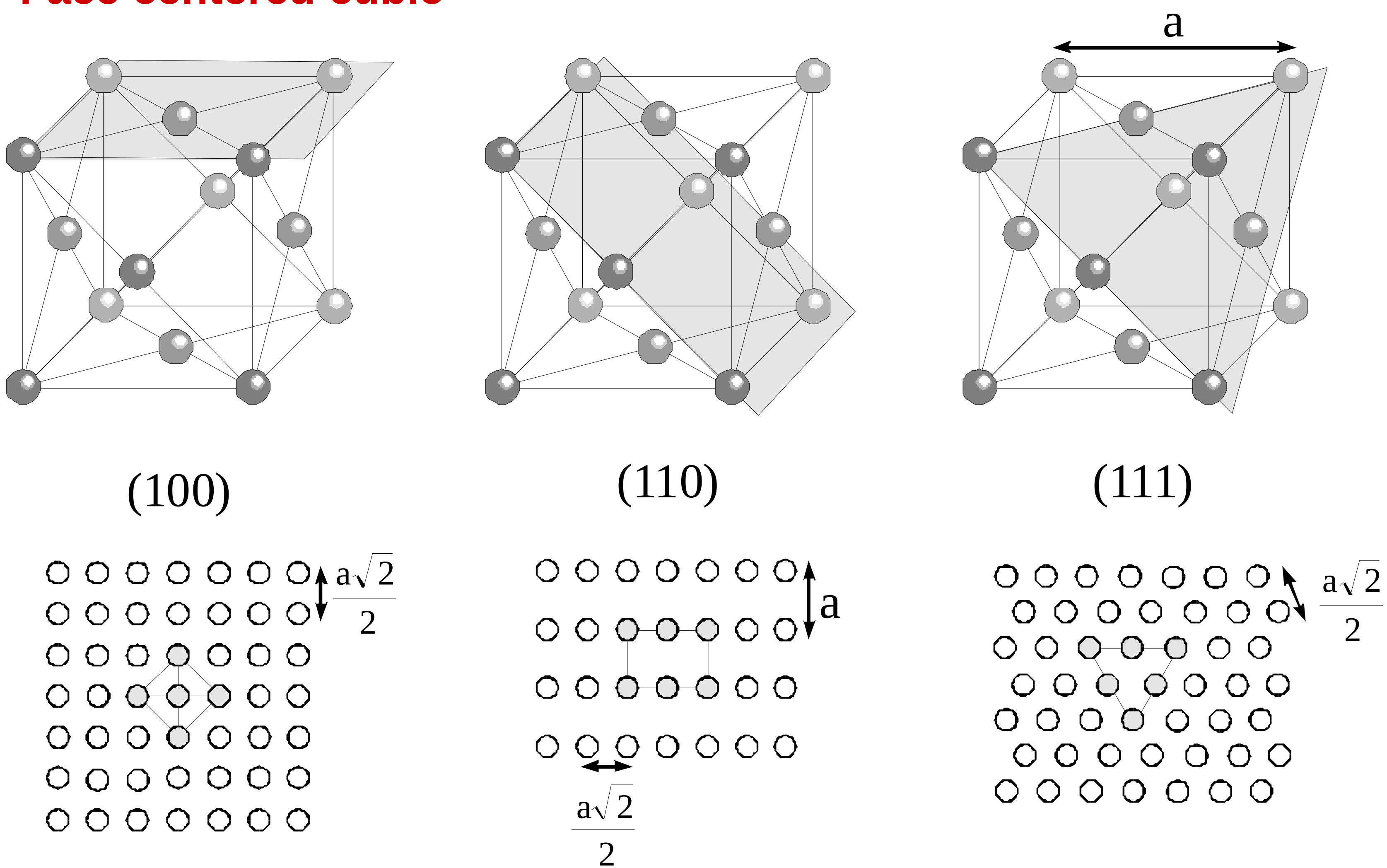
Impingment at substrate

Transport

Ejection from source

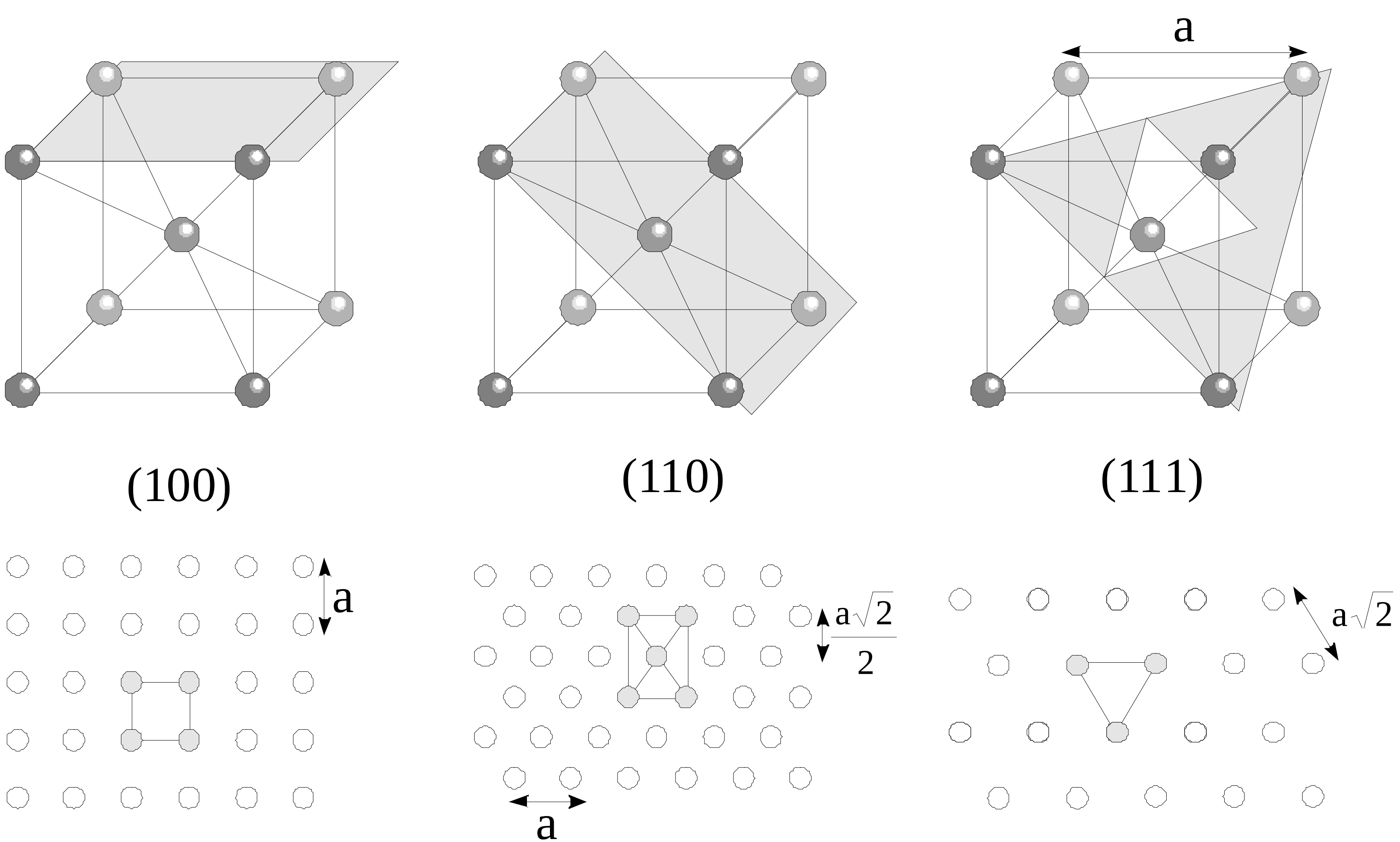
Surface Types I

Face centered cubic

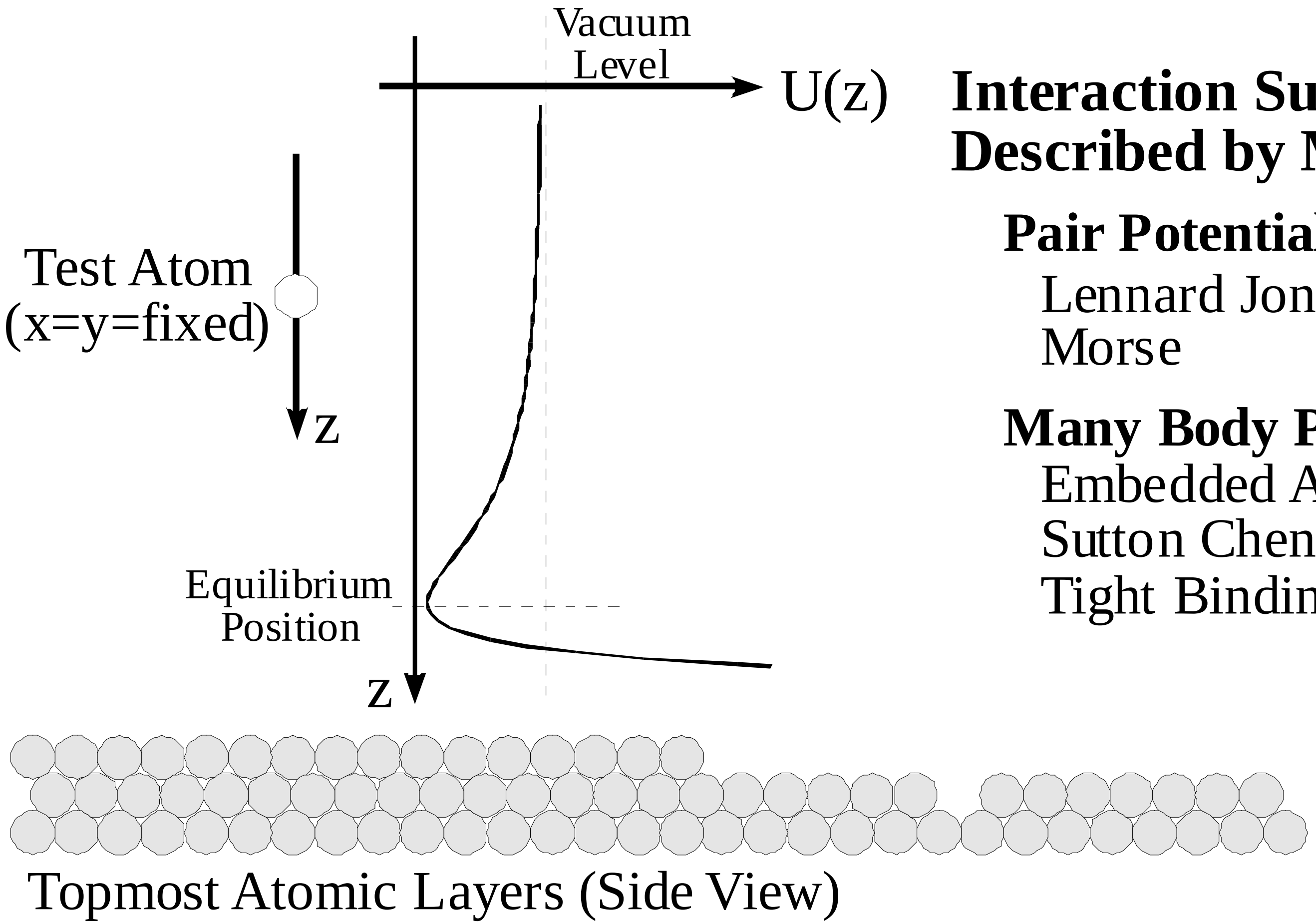


Surface Types II

Body centered cubic



Determination of Potential Energy Surfaces

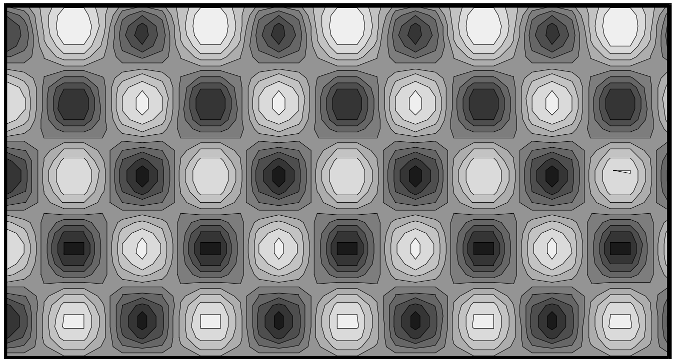


Interaction Surface/Test Atom Described by Model Potentials

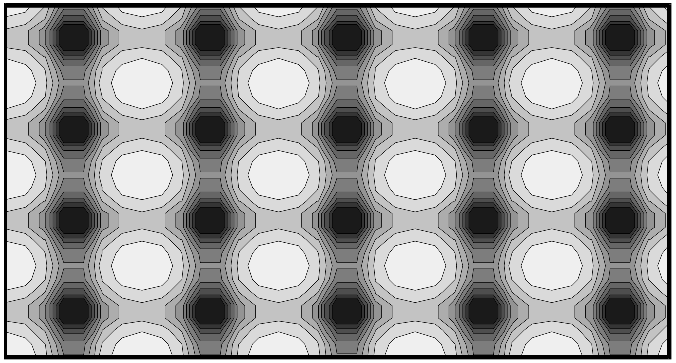
Pair Potentials:
- Lennard Jones
- Morse

Many Body Potentials:
- Embedded Atom
- Sutton Chen
- Tight Binding

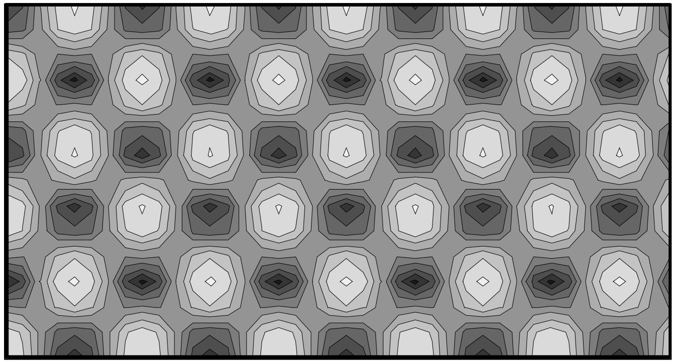
Elementary Potential Energy Surfaces



(100)



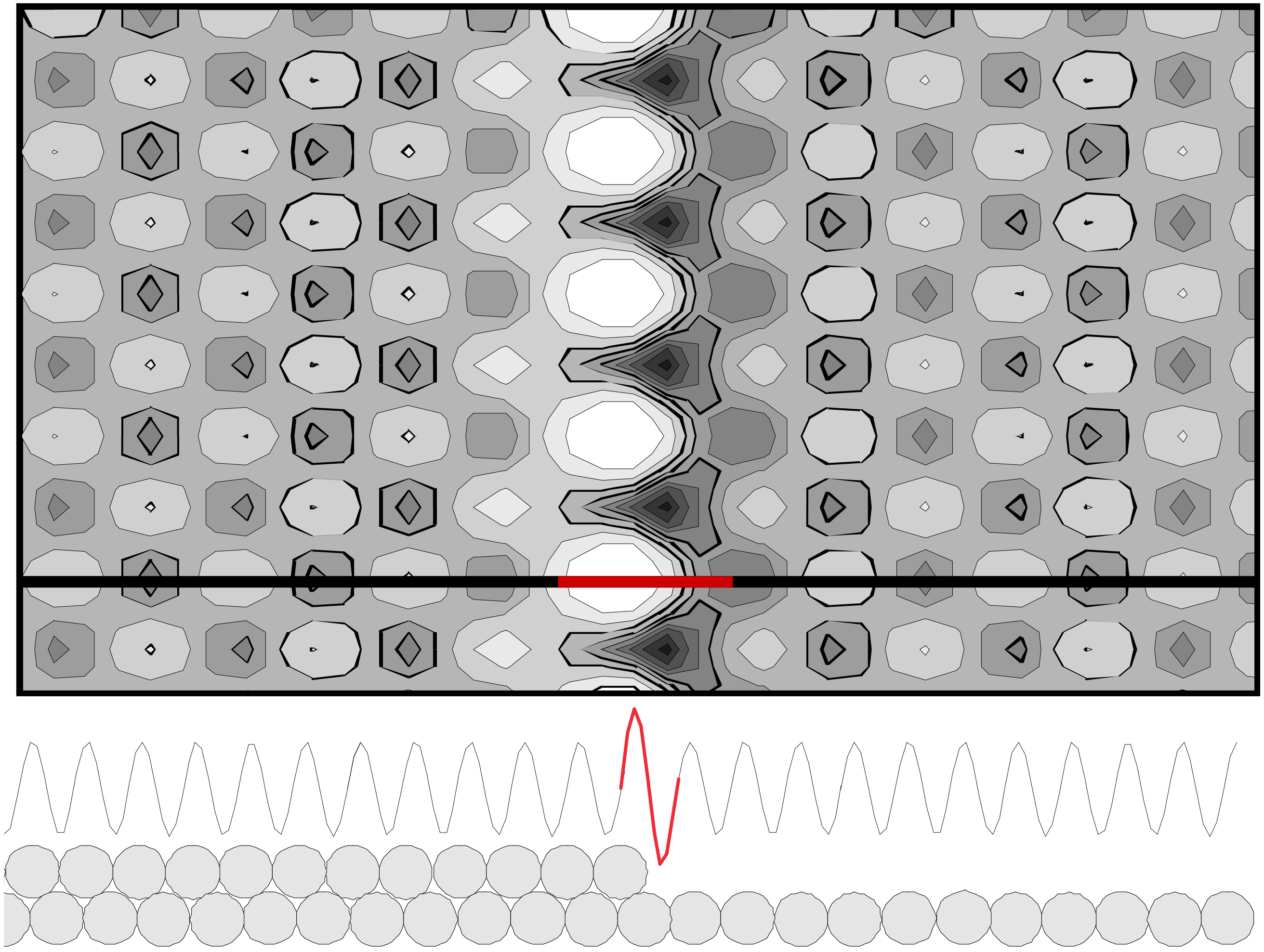
(110)



(111)

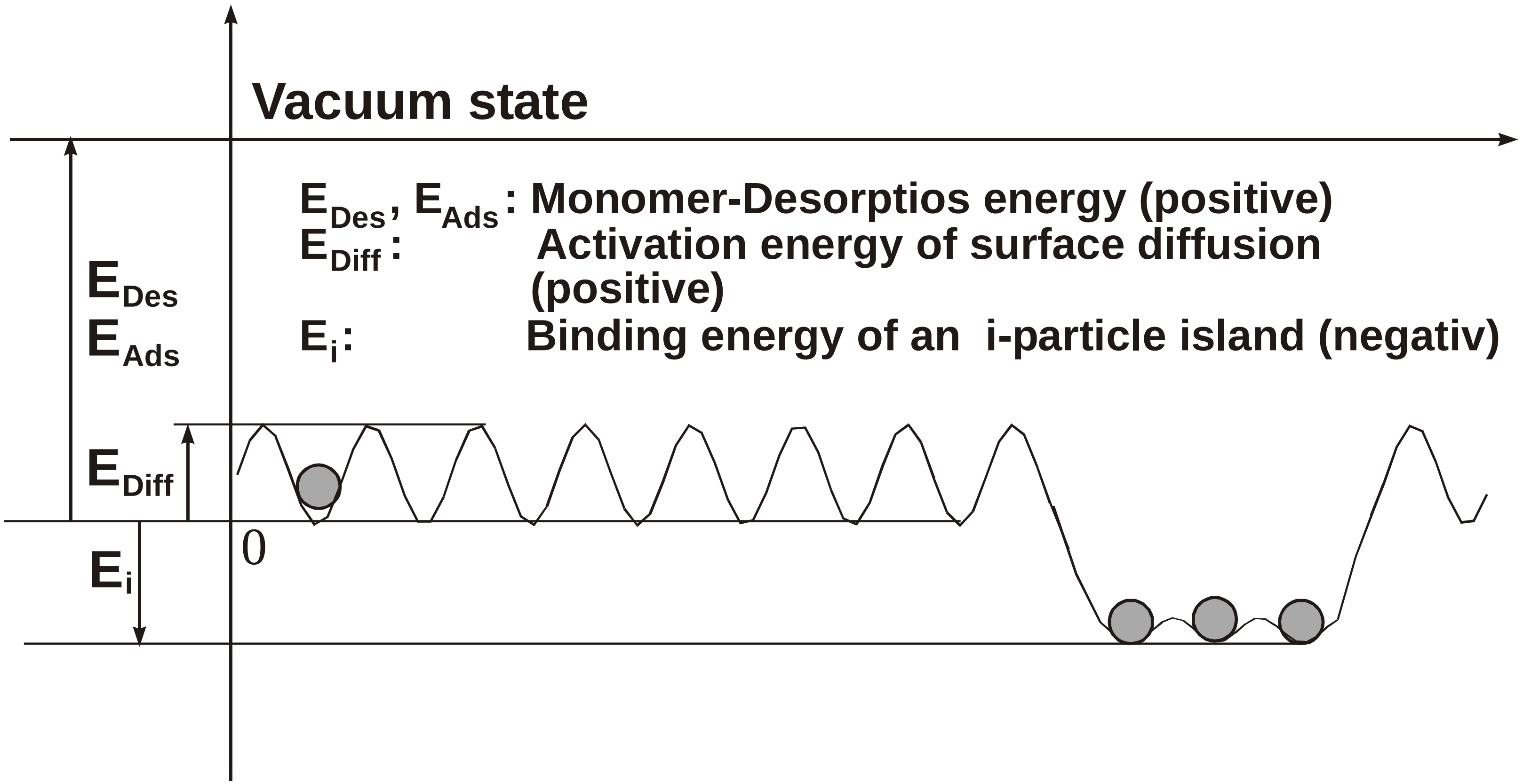
More Complex Surface Geometries

Stepped surface – Ehrlich Schwöbel barrier



Binding Energies

Important binding energies

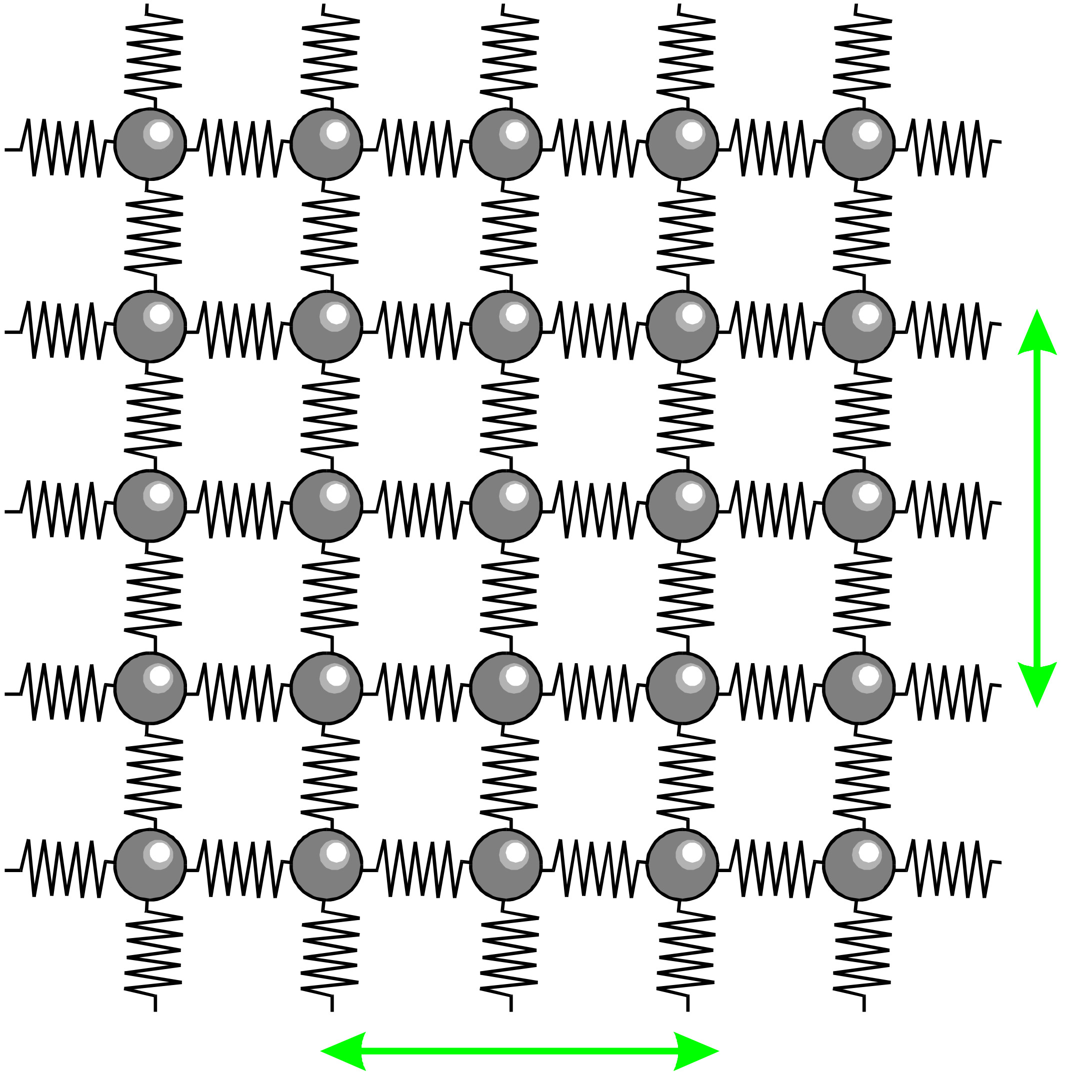


E_{Des}, E_{Ads} : Monomer-Desorptios energy (positive)

E_{Diff} : Activation energy of surface diffusion (positive)

E_i: Binding energy of an i-particle island (negativ)

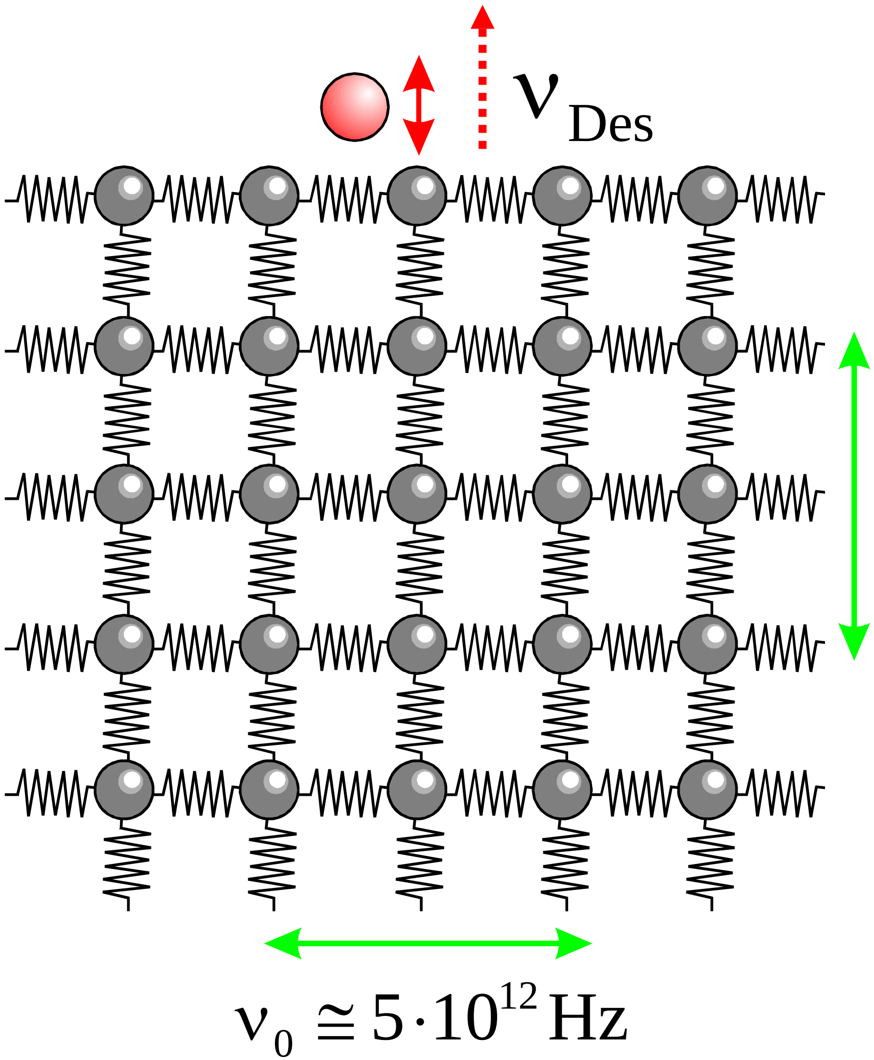
Elementary Processes: Phonon Oscillations



Phonon frequency:

$$\nu_0 \cong 5 \cdot 10^{12}\,\mathrm{Hz}$$

Elementary Processes: Desorption

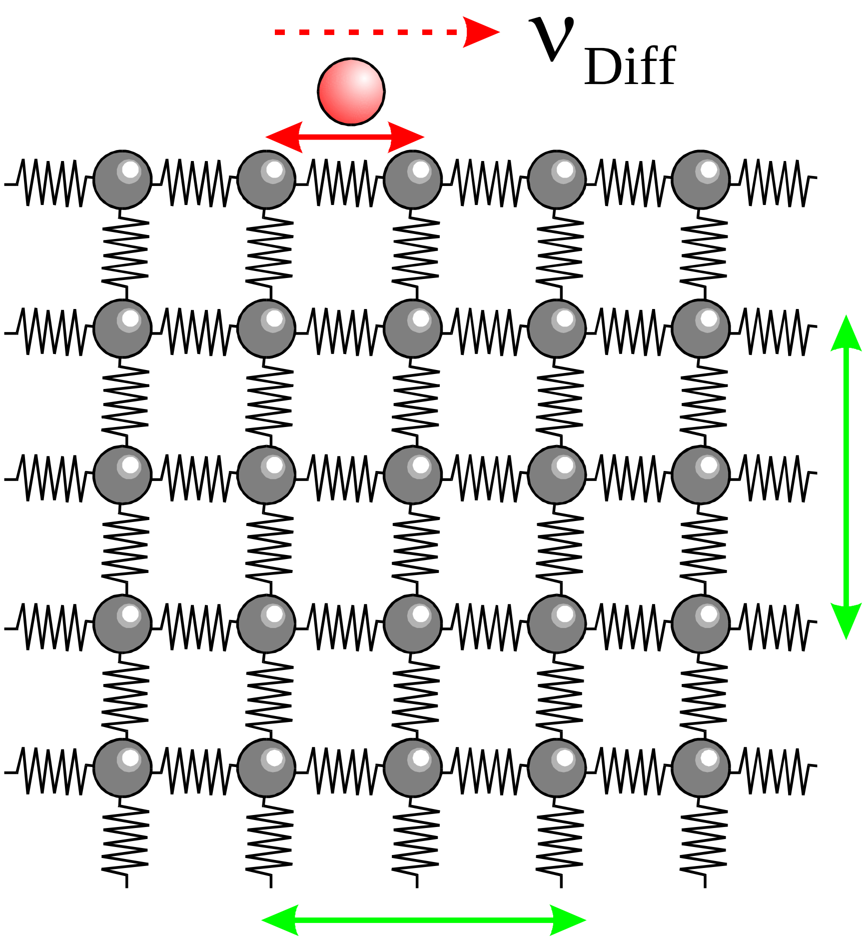


Desoprtion frequency:

$$\nu_{Des} = \nu_0 \cdot e^{-\frac{E_{Des}}{k_B T_S}}$$

$$E_{Des} \cong 1 - 3\,\mathrm{eV}$$

Elementary Processes: Surface Diffusion



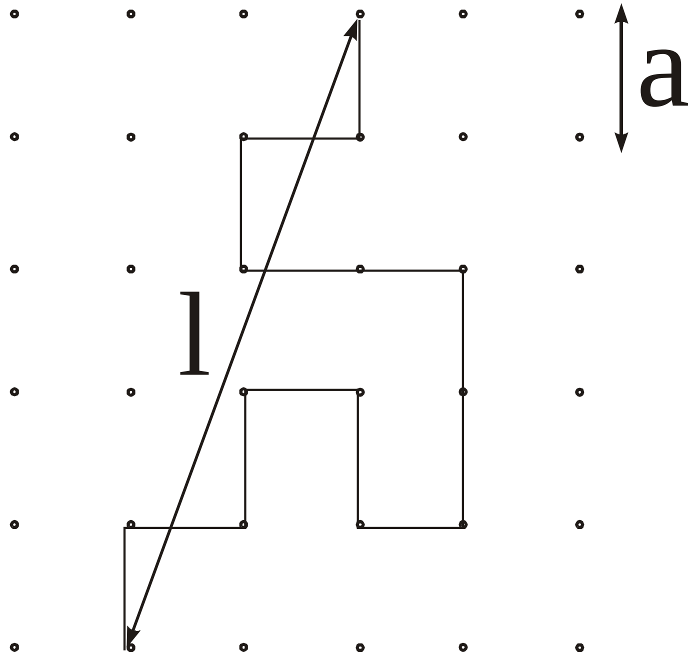
$$\nu_0 \cong 5 \cdot 10^{12}\,\mathrm{Hz}$$

Diffusion frequency:

$$\nu_{Diff} = \nu_0 \cdot e^{-\frac{E_{Diff}}{k_B T_S}}$$

$$E_{Diff} \cong 0.1 - 0.8\,\mathrm{eV}$$

Surface Diffusion: Random Walk



a...lattice constant

l...effective distance travelled by particle

Pythagoras:

$$l^2 = \left(\sum_{i=1}^{n_x} x_i\right)^2 + \left(\sum_{i=1}^{n_y} y_i\right)^2 \qquad x_i, y_i = \pm a$$

$$l^2 = \left(\sum_{i=1}^{n_x} x_i \sum_{j=1}^{n_x} x_j\right) + \left(\sum_{i=1}^{n_x} y_i \sum_{j=1}^{n_x} y_j\right)$$

$$\langle l^2 \rangle = \left\langle \left(\sum x_i \sum x_j\right) \right\rangle + \left\langle \left(\sum y_i \sum y_j\right) \right\rangle =$$

$$= \left\langle \sum_{i=1}^{n_x} x_i^2 \right\rangle + \left\langle \sum_{i=1}^{n_y} y_i^2 \right\rangle = (n_x + n_y) \cdot a^2 = N \cdot a^2$$

$$\langle l^2 \rangle = N \cdot a^2$$

Surface Diffusion: Diffusion Coefficient

$$\langle l^2 \rangle = N \cdot a^2$$

$$D = \nu_0 \cdot a^2 \cdot e^{-\frac{E_{Diff}}{k_B T_S}} \; [m^2 s^{-1}]$$

$$\nu_{Diff} = \nu_0 \cdot e^{-\frac{E_{Diff}}{k_B T_S}}$$

Einstein-relation:

$$N[s^{-1}] = \nu_{Diff}$$

$$\langle l \rangle \cong \sqrt{D\tau}[m]$$

τ = Diffusion time

Time Scales I

Lattice vibrations:

$$\nu_0 \cong 5 \cdot 10^{12}\,\mathrm{Hz}$$

T_S = 300 K

k_B = 1,38.10^{-23}J/K

Surface diffusion:

$$\nu_{Diff} = \nu_0 \cdot e^{-\frac{E_{Diff}}{k_B T_S}}$$

E_{Diff} = 0,2 eV=3,2.10^{-20} J

ν_{Diff} = 2,2.10^{9} Hz

$\tau_{Diff} = \nu_{Diff}^{-1}$ = 0.5 ns

Desorption:

$$\nu_{Des} = \nu_0 \cdot e^{-\frac{E_{Des}}{k_B T_S}}$$

E_{Des} = 2 eV=3,2.10^{-19} J

ν_{Des} = 1,2.10^{-21} Hz(!)

$\tau_{Des} = \nu_{Des}^{-1}$ = 10^{13} a

Time Scales II

$\tau_{Diff}/\tau_{Phonon}$ $=10^4$

τ_{Des}/τ_{Diff} $=10^{30}$ (!!)

Important phenomena happen on extremely different time scales!

Condensation Regimes

- **Complete condensation:**
  Each impinging particle remains on the surface because of the extremely low desorption frequency.
  Prerequisite: T_S <

- **Incomplete condensation:**
  Particles can desorb, an adsorption/desorption-equilibrium is created ein (see later).
  Prerequisite: T_S >