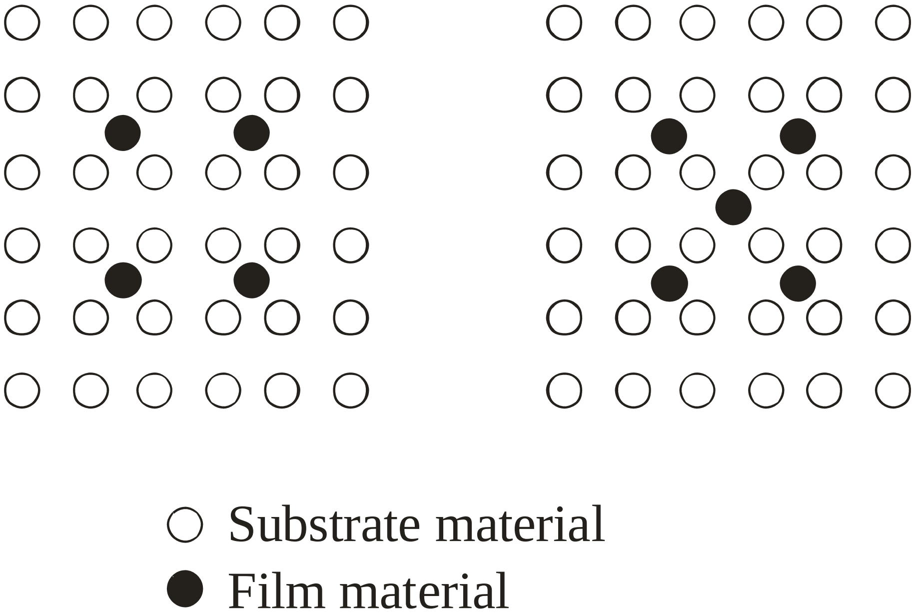
Repetition: Epitaxy

Epitaxy is the deposition of layers, which are monocrystalline in large regions

- **Homoepitaxy:**
  Substrate material = film material
- **Heteroepitaxy:**
  Substrate material ≠ film material

Repetition: Heteroepitaxy I

Epitactic relation:

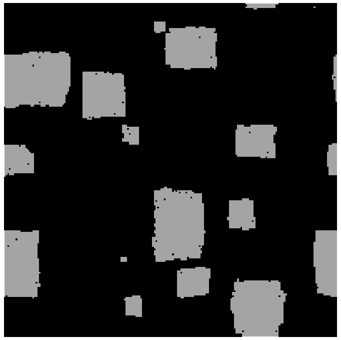


Van-der-Waals epitaxy:

The interaction between substrate material and film material is so weak, that film atoms can arrange themselves in a crystallographically favorable manner.

Repetition: Heteroepitaxy II

High temperature epitaxy:

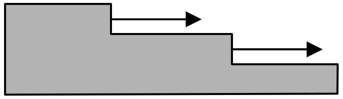


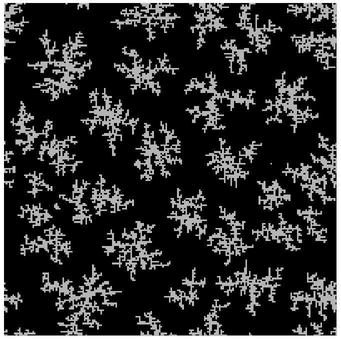
The crystallographically favorable arrangement of the atoms is reached by a high substrate temperature.

Low temperature epitaxy :

The crystallographically favorable arrangement of the atoms is reached by local defect structures

- Vicinal surfaces
- Dendritic Islands

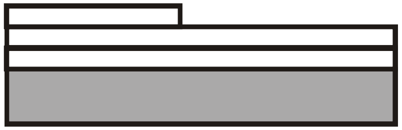




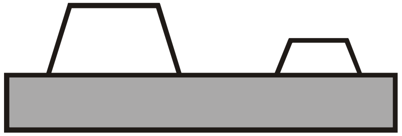
Repetition: Growth Modes

Growth modes:

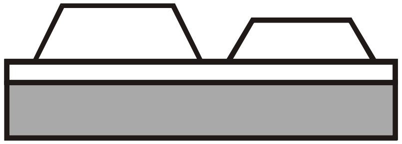
A: Substrate material
B: Film material



Frank-Van der Merwe:
layer by layer $W_{AB}>W_{BB}$



Volmer-Weber:
islands, $W_{AB}<W_{BB}$



Stranski-Krastanov:
layer/island, $W_{AB}>W_{BB}$
stress relief by 3d islands

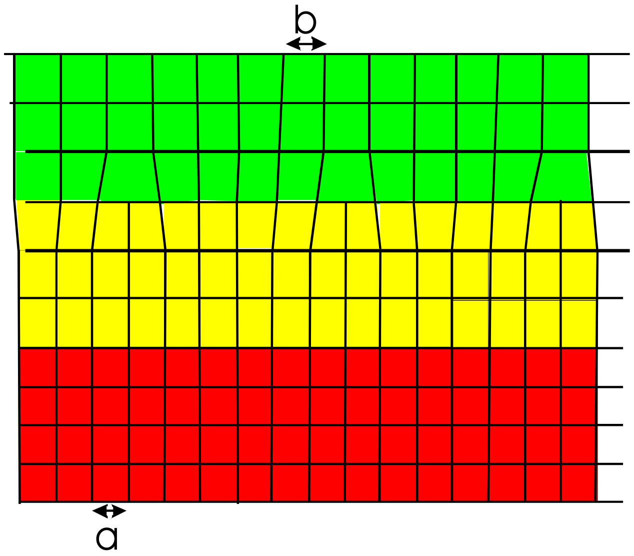
While the Frank-van der Merwe and Volmer-Weber Growth modes lead to mostly stress free films, in the Stranski-Krastanov-mode significant stresses are induced in the first growth phases.

Repetition: Stress/Film Growth

Detailed mechanism:

Lattice Mismatch Δ:

$$\Delta = \frac{a-b}{a} \cdot 100 [\%]$$

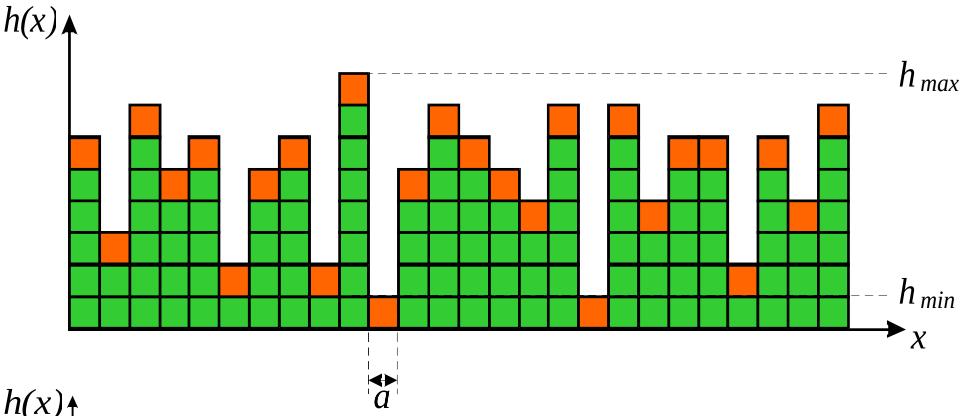


Film, lattice constant b

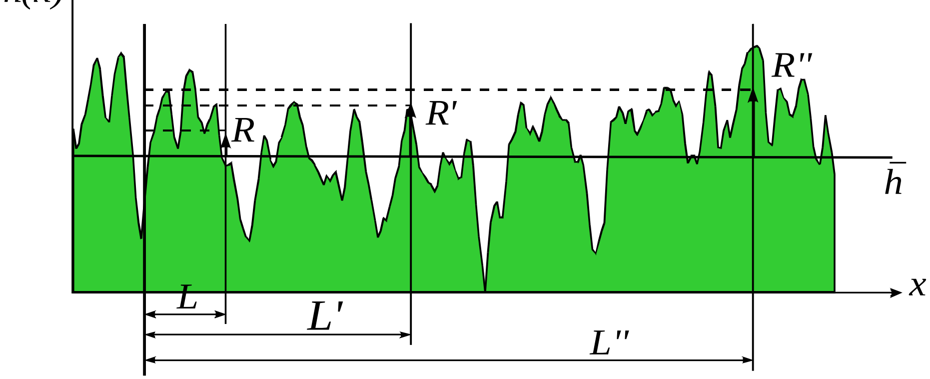
Pseudomorphic transition zone

Substrate, lattice constant a

Repetition: Roughness Types

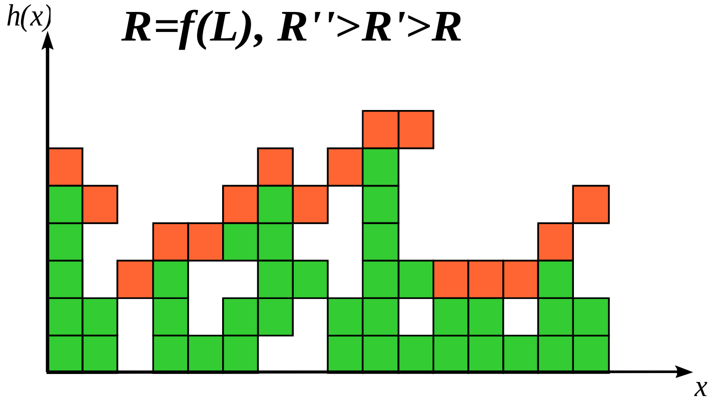


Stochastic roughness



Self similarity

$R = f(L),\ R'' > R' > R$

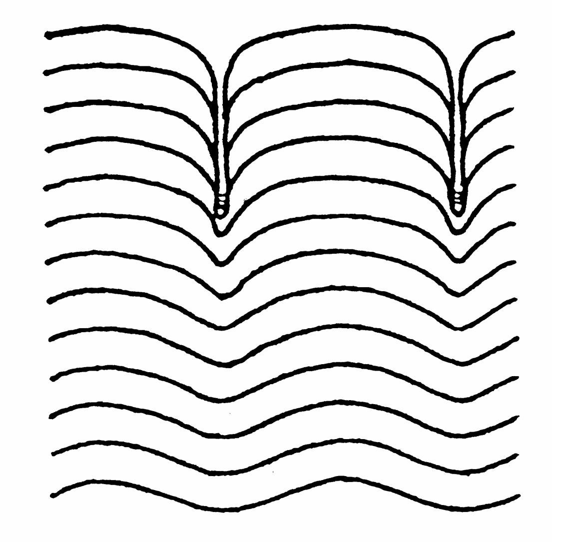


Ballistisc aggregate

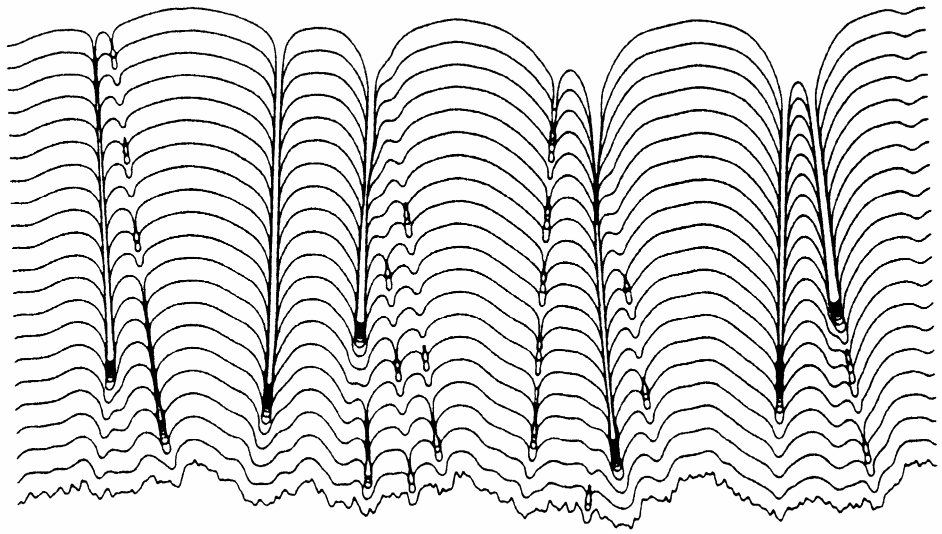
Repetition: Shadowing

Peaks grow faster than valleys

- + Formation of columnar structures (a)
- + Pore formation in combination with surface diffusion (b)



(a)



(b)

Repetition: Roughness Values

R_a-value: mean absolute deviation

$$R_a = \frac{1}{N}\sum_{i=1}^{N}\left|\bar{h} - h_i\right|$$

R_q- or RMS-value:
mean quadratic deviation

$$R_q = R_{RMS} = RMS = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\bar{h} - h_i\right)^2}$$

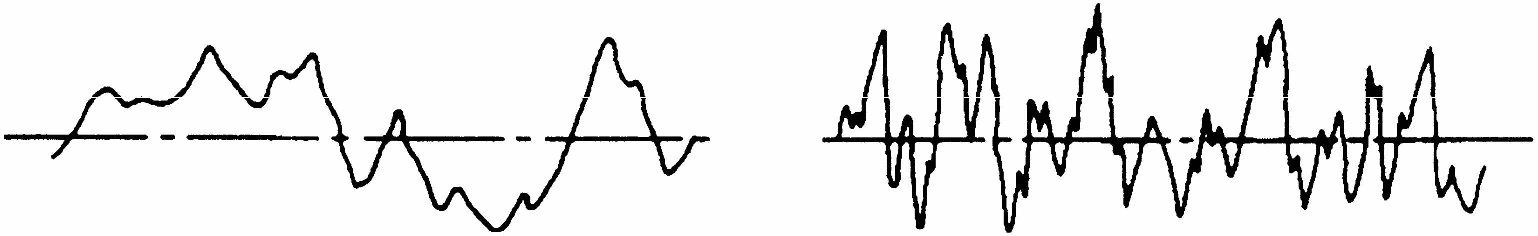
Repetition: Correlation Functions

Non normalized quantities	**Normalized quantities**
Autocovariance function $R(\tau) = \left\langle h(x) \cdot h(x+\tau) \right\rangle dx$	**Autocorrelation function** $\rho(\tau) = R(\tau) / R(0)$
Structure function $S(\tau) = \left\langle [h(x) - h(x+\tau)]^2 \right\rangle$ $S(\tau) = 2R_q^2[1 - \rho(\tau)]$	

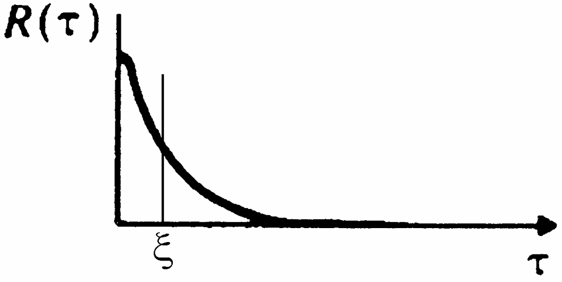
Note: All heigth values are measured from the mean heigth $\bar{h}$.

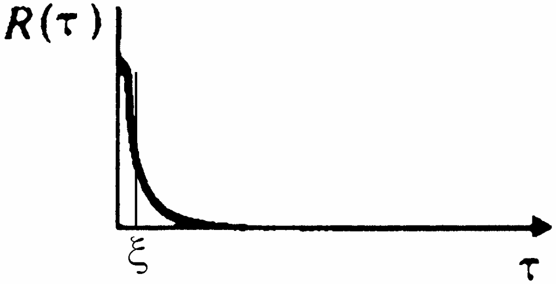
Repetition: Correlation Length ξ

Surface profile



Autocovariance function

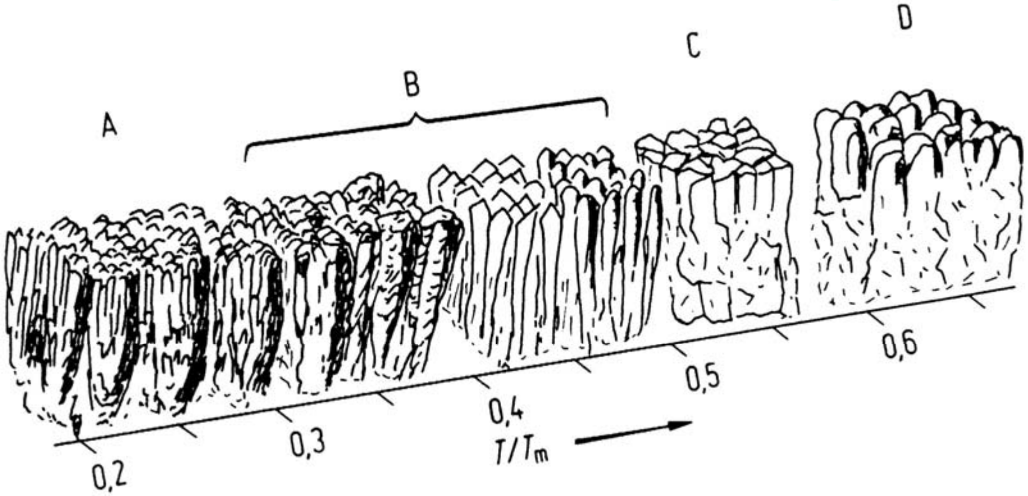




Within ξ the profile exhibits similar heigth values.

Periodicities are present, if R(τ) exhibits maxima at $\tau \neq 0$.

Film Structure and Film Properties



The film structure influences:

- + Density
- + Mechanical properties
- + Electric properties
- + Magnetic properties
- + Electronic properties

Application Profiles

Depending on the application a certain film structure can be advantageous or disadvantageous:

+ Tool ⇒ dense, fine grained

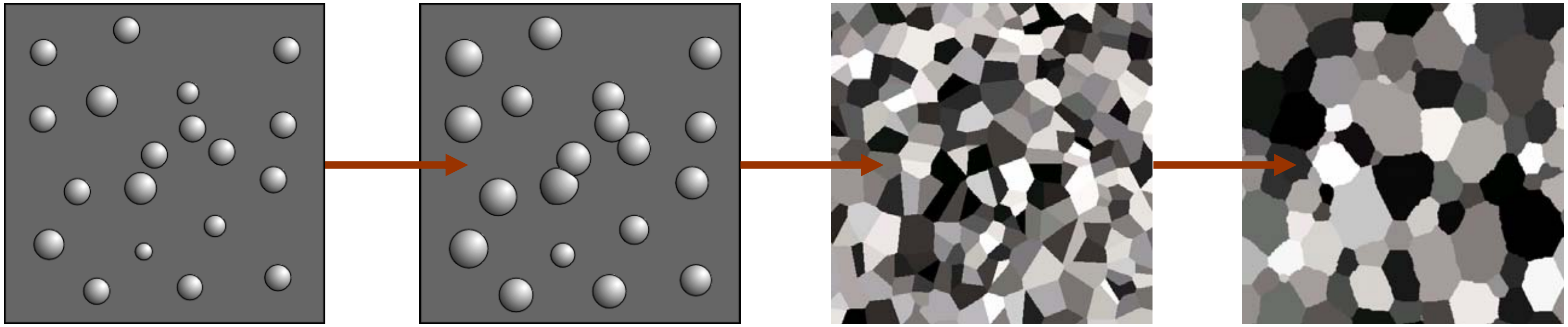
+ Biolog. material ⇒ porous, soft

+ Elektronics ⇒ dense, monocrystalline

+ Therm. barriers ⇒ porous, hard

Structure Zone Models

Growth phases of a coating



Nucleation on substrate

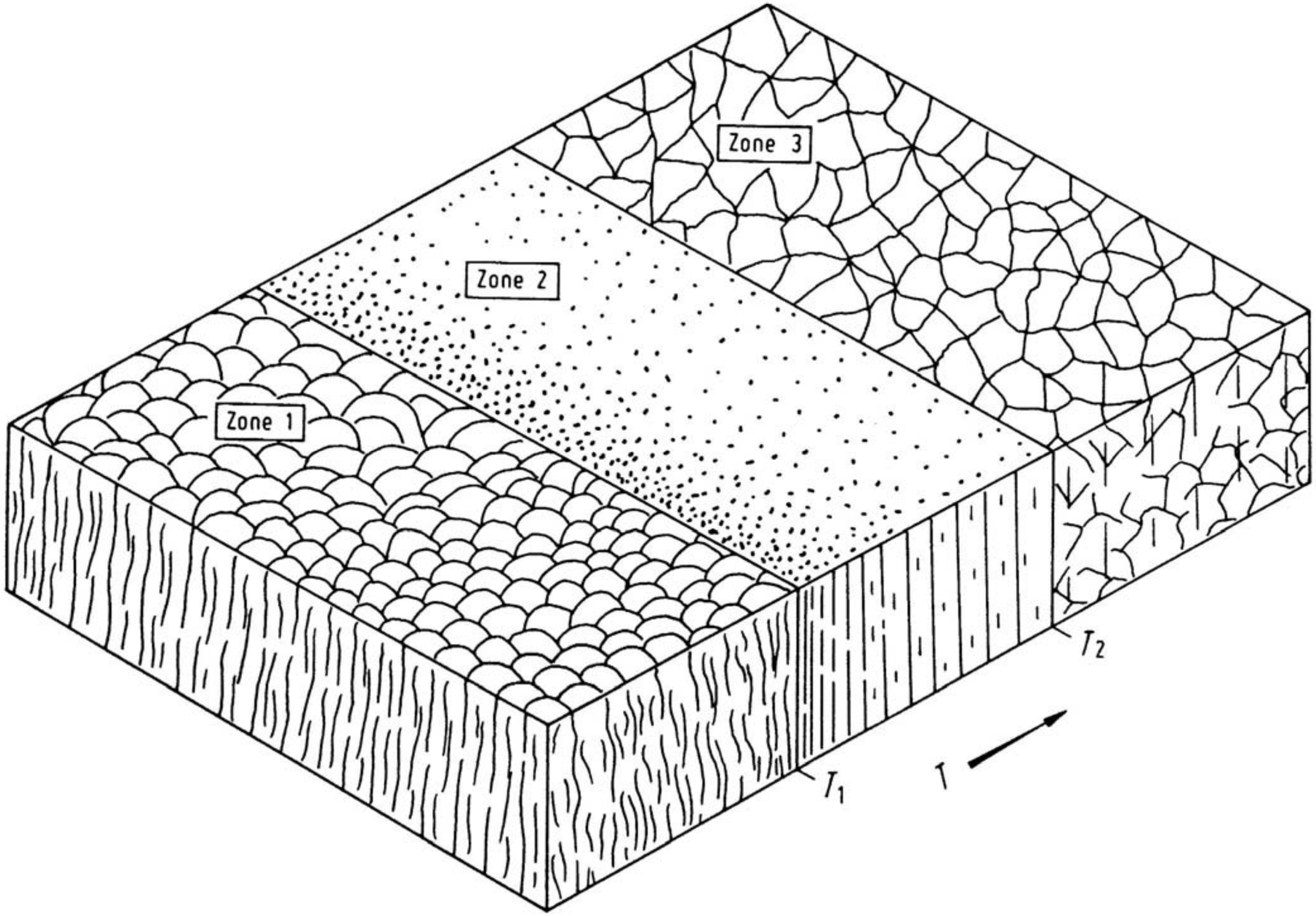
Partial coalescence and interface formation

Total coalescence and polycrystal formation

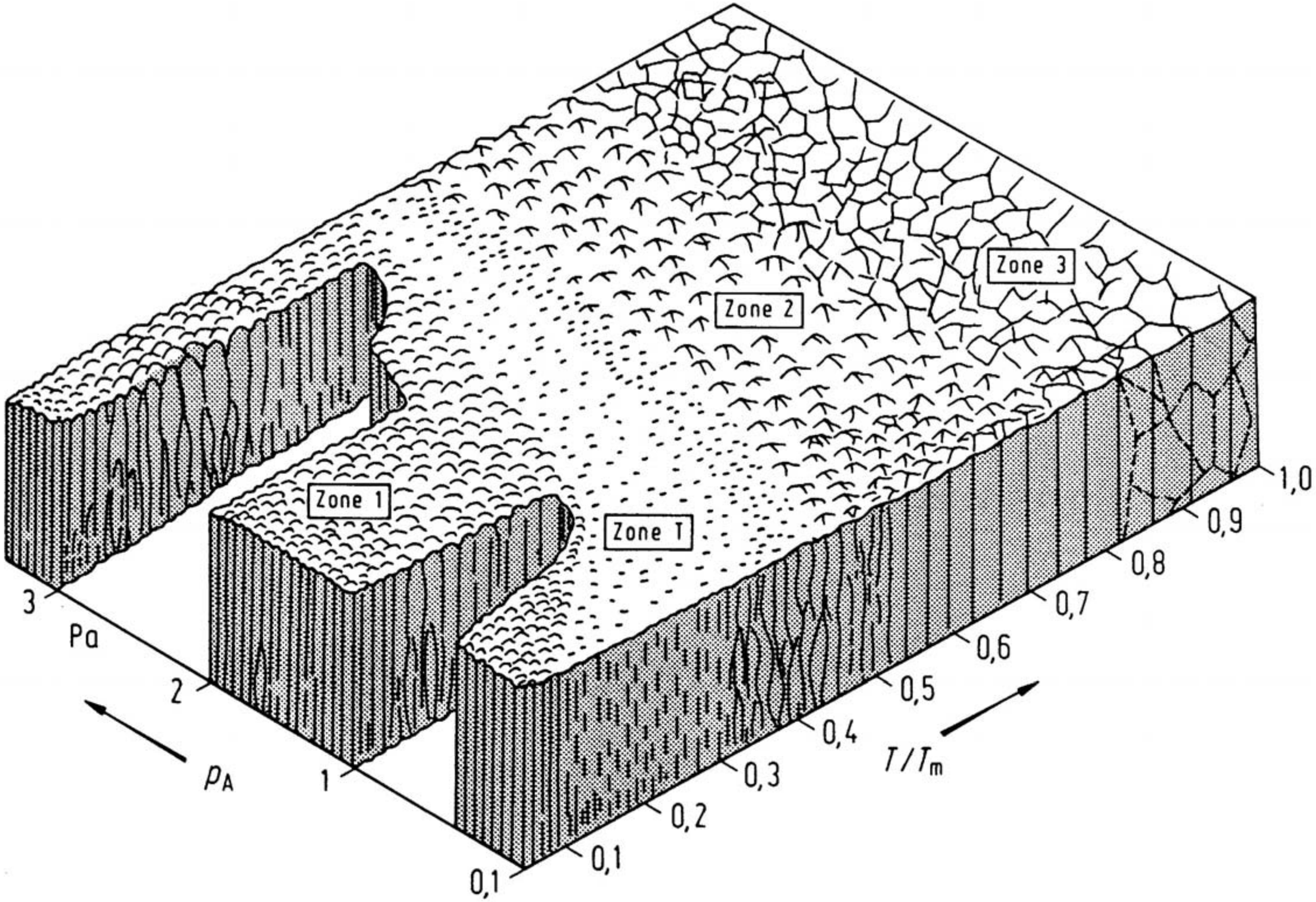
Growth of polycrystal grains

Structure zone models yield a qualitative image of film growth, morphology and crystallography in dependence on the coating parameters.

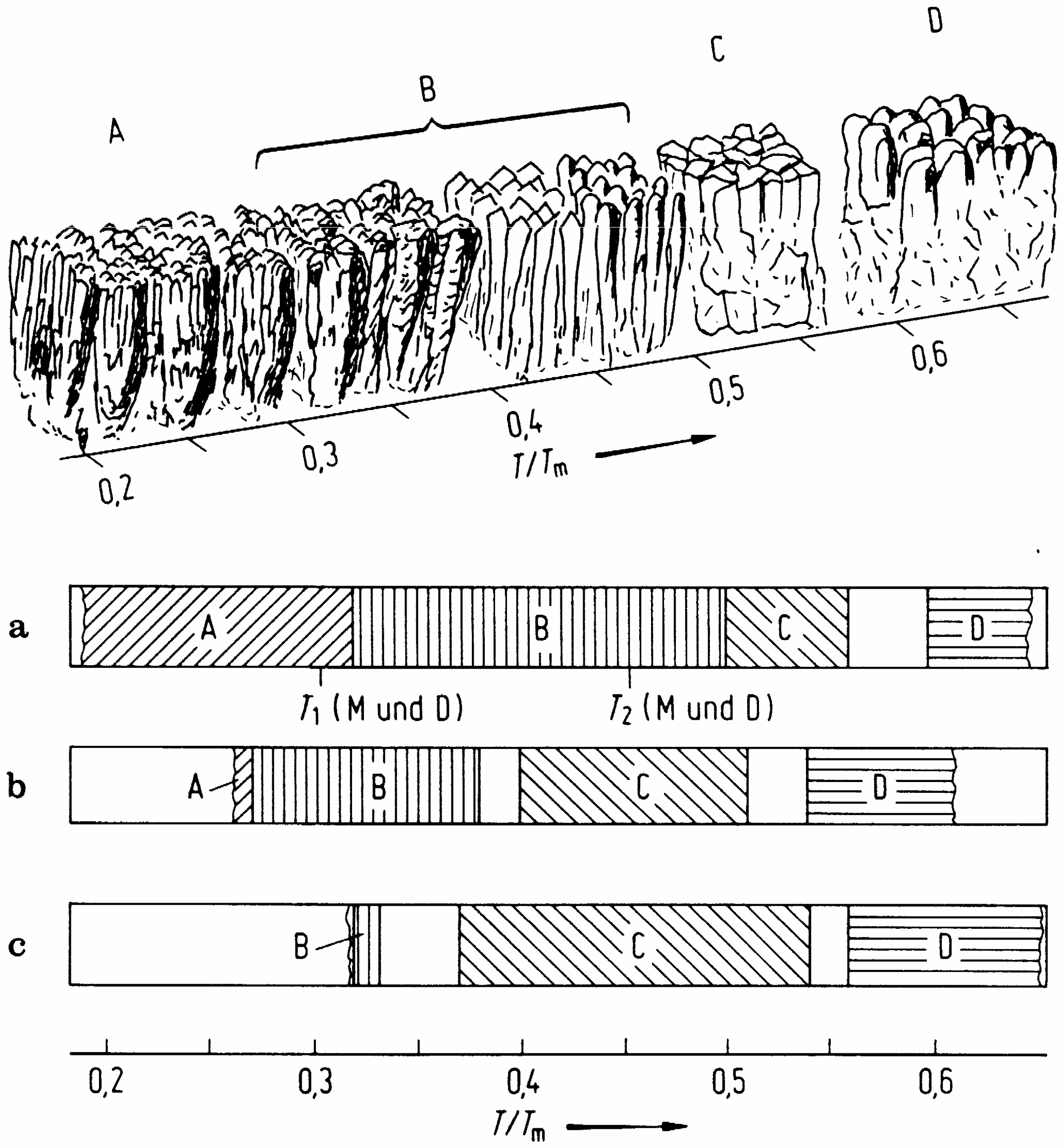
Movchan-Demchishin: Evaporation



Thornton: Sputtering



Ion Plating


A
B
C
D
0,2
0,3
0,4
0,5
0,6
T/Tm
a
A
B
C
D
T1 (M und D)
T2 (M und D)
b
A
B
C
D
c
B
C
D
0,2
0,3
0,4
0,5
0,6
T/Tm

Zones and Growth Mechanisms

Zone	Mechanism	Char. feature
1: $T/T_M < 0{,}2$	Shadowing	Fibers, pores
T: $T/T_M < 0{,}4$	Particle energy	Nano grains
2: $T/T_M < 0{,}8$	Surface diffusion	Columnar crystlites
3: $T/T_M > 0{,}8$	Volume diffusion	3d - Grains

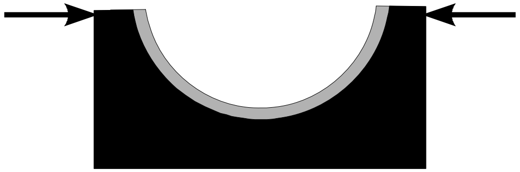
Stresses

Kinds of stresses:

$$\boxed{\sigma = \sigma_{\mathrm{MECH}} + \sigma_{\mathrm{T}} + \sigma_{\mathrm{I}}}$$

Mechanical stress:

σ_{MECH}



Generated by clamping of the substrate and subsequent unclamping

Thermal stress:

$$\sigma_{\mathrm{T}} = E_{\mathrm{S}}(\alpha_{\mathrm{S}} - \alpha_{\mathrm{U}})(T_{\mathrm{B}} - T_{\mathrm{M}})$$

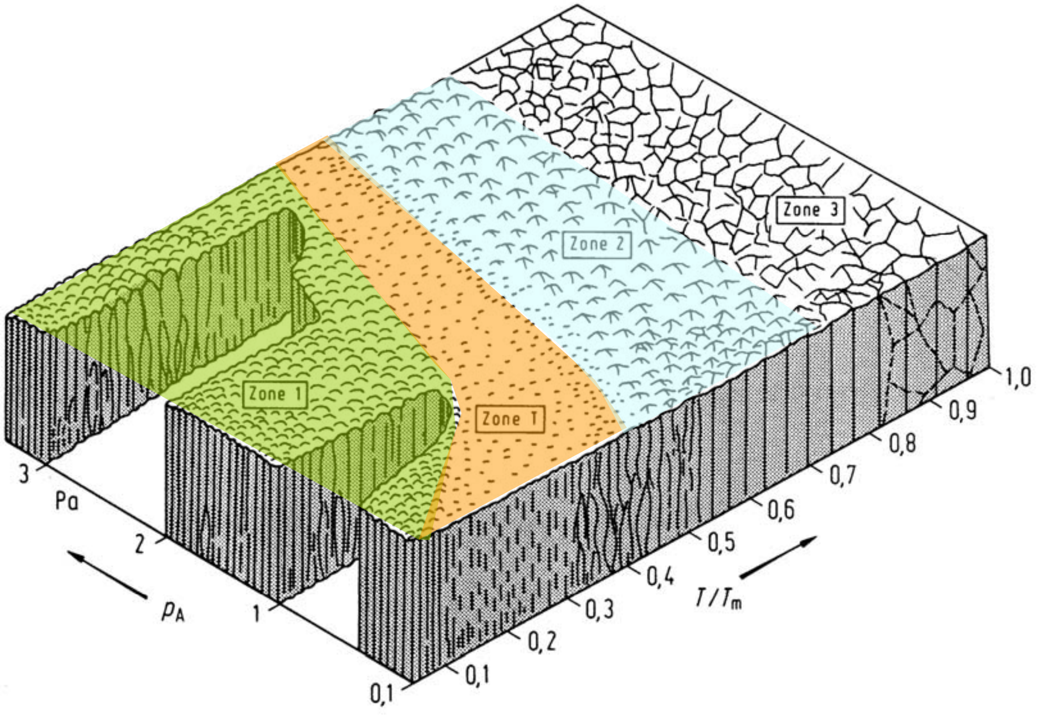
E_S ... Elastic modulus film
α_S ... CTE film
α_U ... CTE substrate
T_B ... Deposition temperature
T_M ... Measurement temperature

Generated by the different coefficients of Thermal Expansion (CTE) of substrate and coating

Stresses and Film Structure

Intrinsic stress:

σ_I **Intrinsic stresses are a direct consequence of the film structure and of the deposition conditions.**

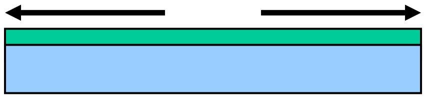


🟩 **Tensile stress**

🟧 **Compressive stress**

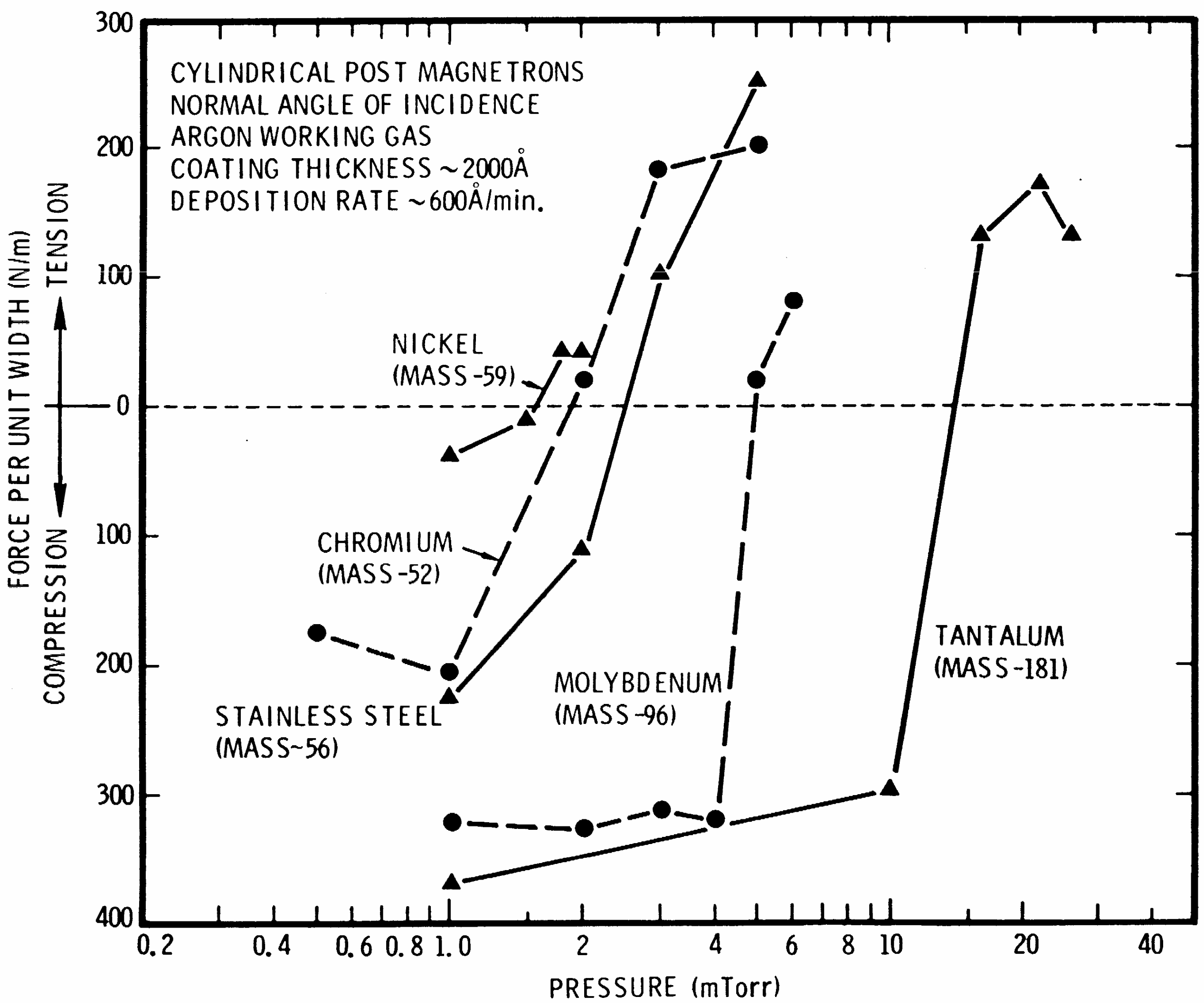
🟦 **Variable**

Compressive stress



Tensile stress

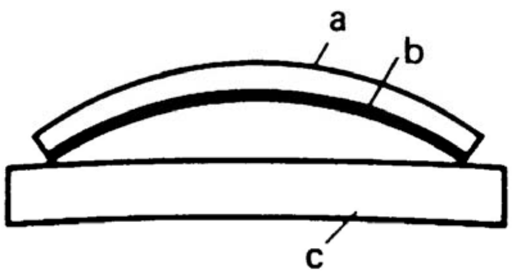
Intrinsic Stresses: Sputtering



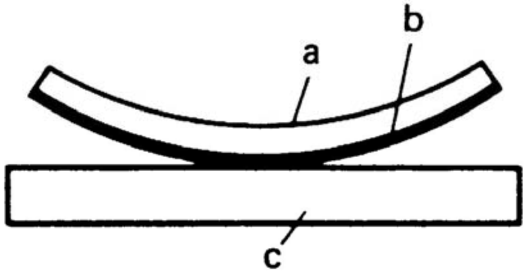
Stress Measurement: Fundamentals

Curved substrate:

Tensile stress



Compressive stress



a) Substrate
b) Film
c) Reference platelet

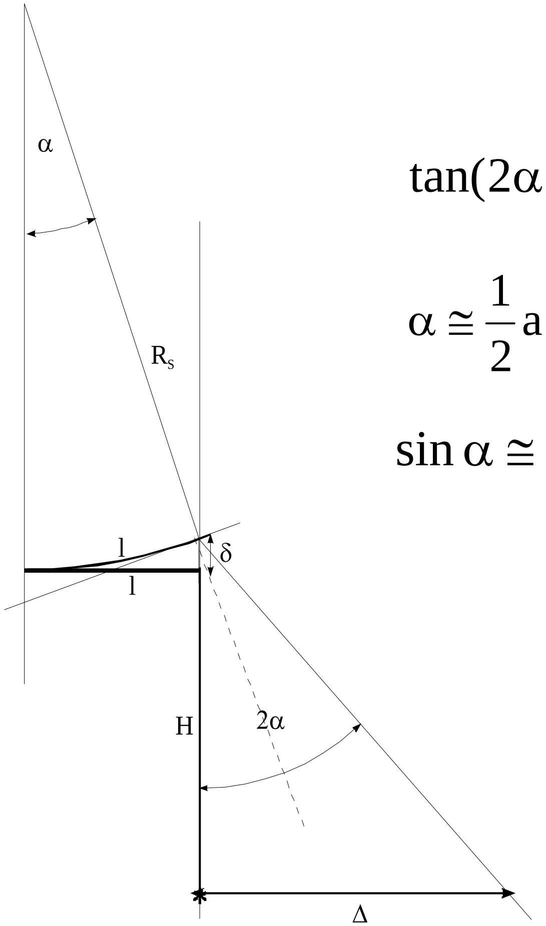
Total stress σ of a thin film:

$$\sigma = \frac{E_s d_s^2}{6(1-\nu_s)d_F}\left(\frac{1}{R_{s1}} - \frac{1}{R_{s2}}\right)$$

E_S ... Elastic modulus substrate
ν_S ... Poisson-number substrate
d_S ... Thickness of substrate
d_F ... Film thickness
R_{S1}, R_{S2} ... Radius of curvature before and after coating, respectively

Stress Measurement: Cantilever

Geometry:

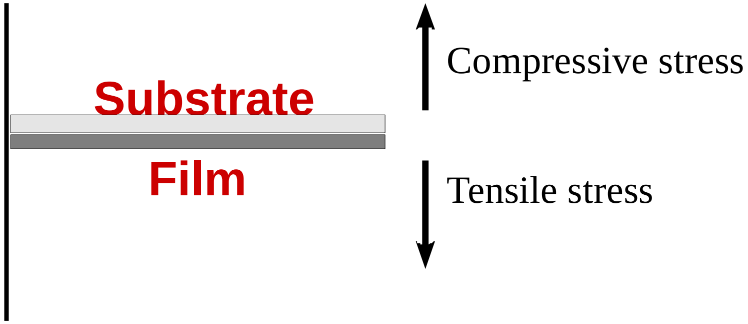


$$\tan(2\alpha) \cong \frac{\Delta}{H}$$

$$\alpha \cong \frac{1}{2}\,\mathrm{a\,tan}\left(\frac{\Delta}{H}\right)$$

$$\sin\alpha \cong \alpha = \frac{l}{R_S}$$

Principle:



Compressive stress

Substrate

Film

Tensile stress

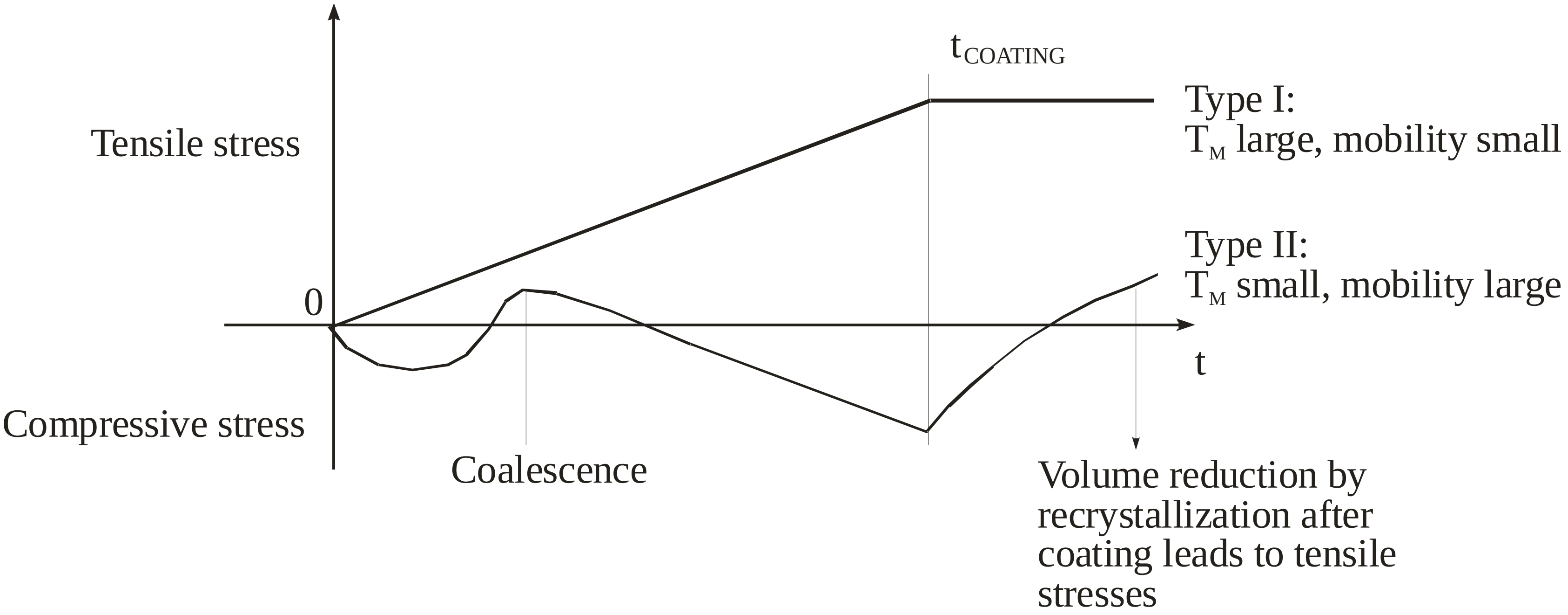
$$\boxed{R_S \cong 2\frac{l}{\mathrm{a\,tan}\left(\frac{\Delta}{H}\right)} \cong \frac{2lH}{\Delta}}$$

Neglections and prerequisites:

a) lateral displacement of the cantilever
b) vertical displacement of the cantilever (δ)
c) low ratios Δ/H

Stresses and Film Growth I

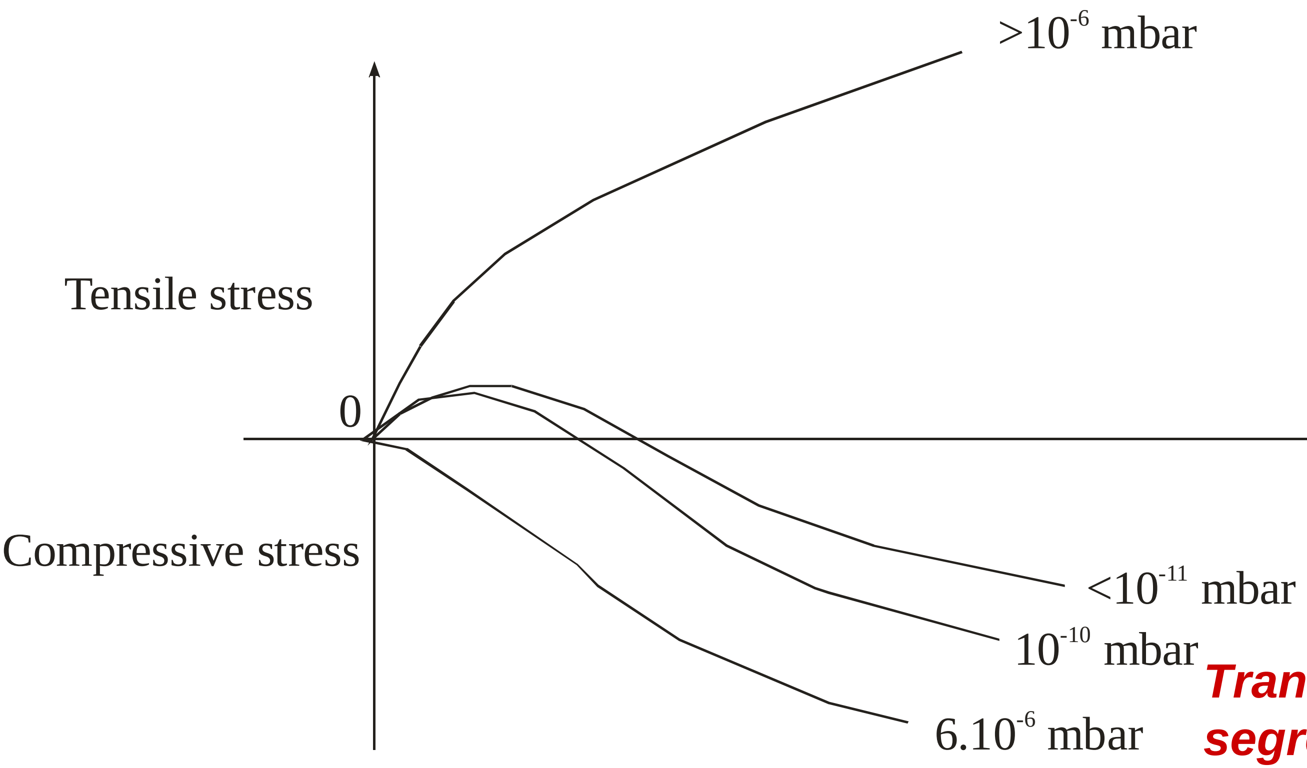
In-Situ-measurements by the cantilever method:



Influence of the film thickness on σ_I

Stresses and Film Growth II

In-Situ-measurements by the cantilever method : Evaporation of Al



Type I

Type II

Transition: segregation

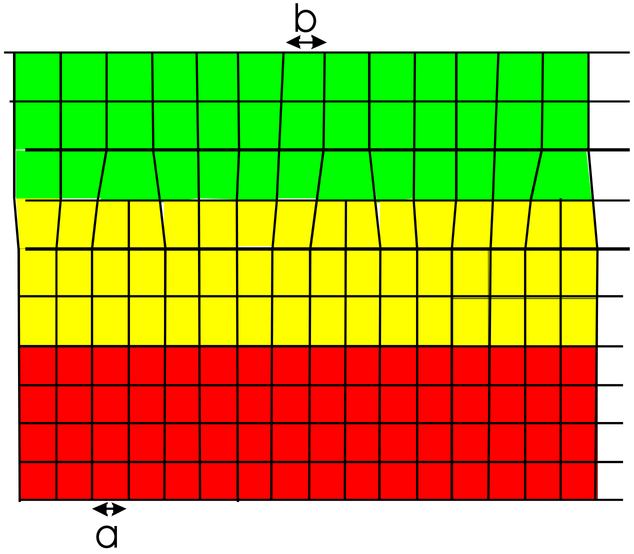
Influence of impurities in the residual gas During the evaporation process on σ_I

Lattice Mismatch and Self Organization I

Detailed mechanism:

Lattice Mismatch Δ:

$$\boxed{\Delta = \frac{a-b}{a} \cdot 100[\%]}$$



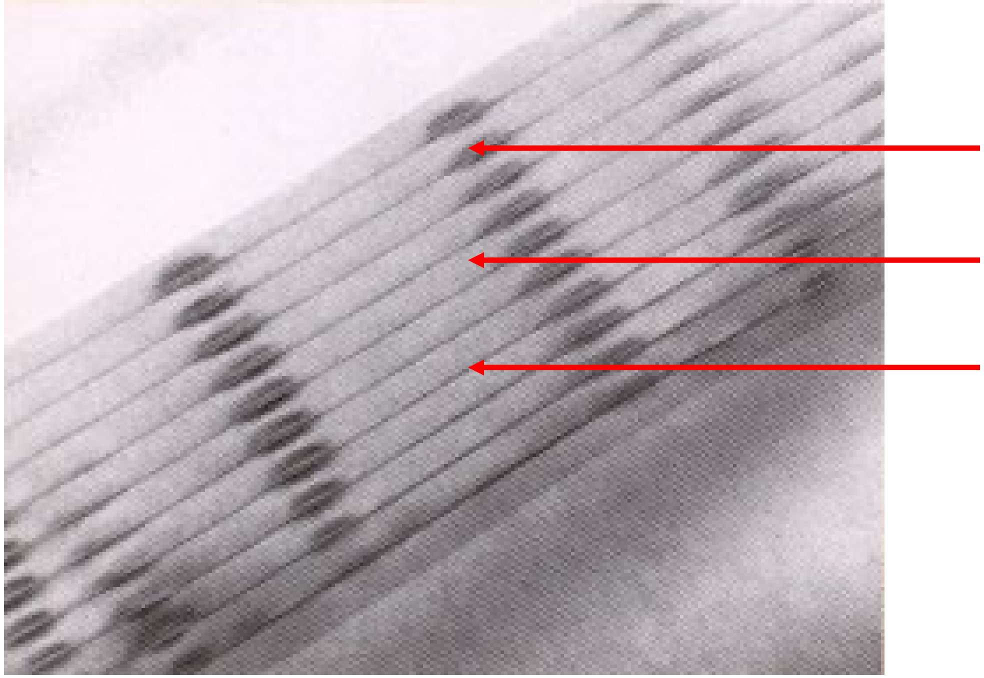
Film, lattice constant b

Pseudomorphic transition zone

Substrate, lattice constant a

Lattice Mismatch and Self Organization II

Example: self organization of island positions in InAs/GaAs Multilayers:



Quantum dot

Interlayer

Stranski-Krastanov wetting layer

The lattice strain in the interlayer generates a preferred nucleation position directly above an island.

Stress Measurement by X-Rays

Principle:

Measurement of the global strain of the elementary cell generated by:

- **+ Interstitial atoms**
- **+ Impurities**

Advantages:

- **+ Non-destructive**
- **+ In Situ possible**

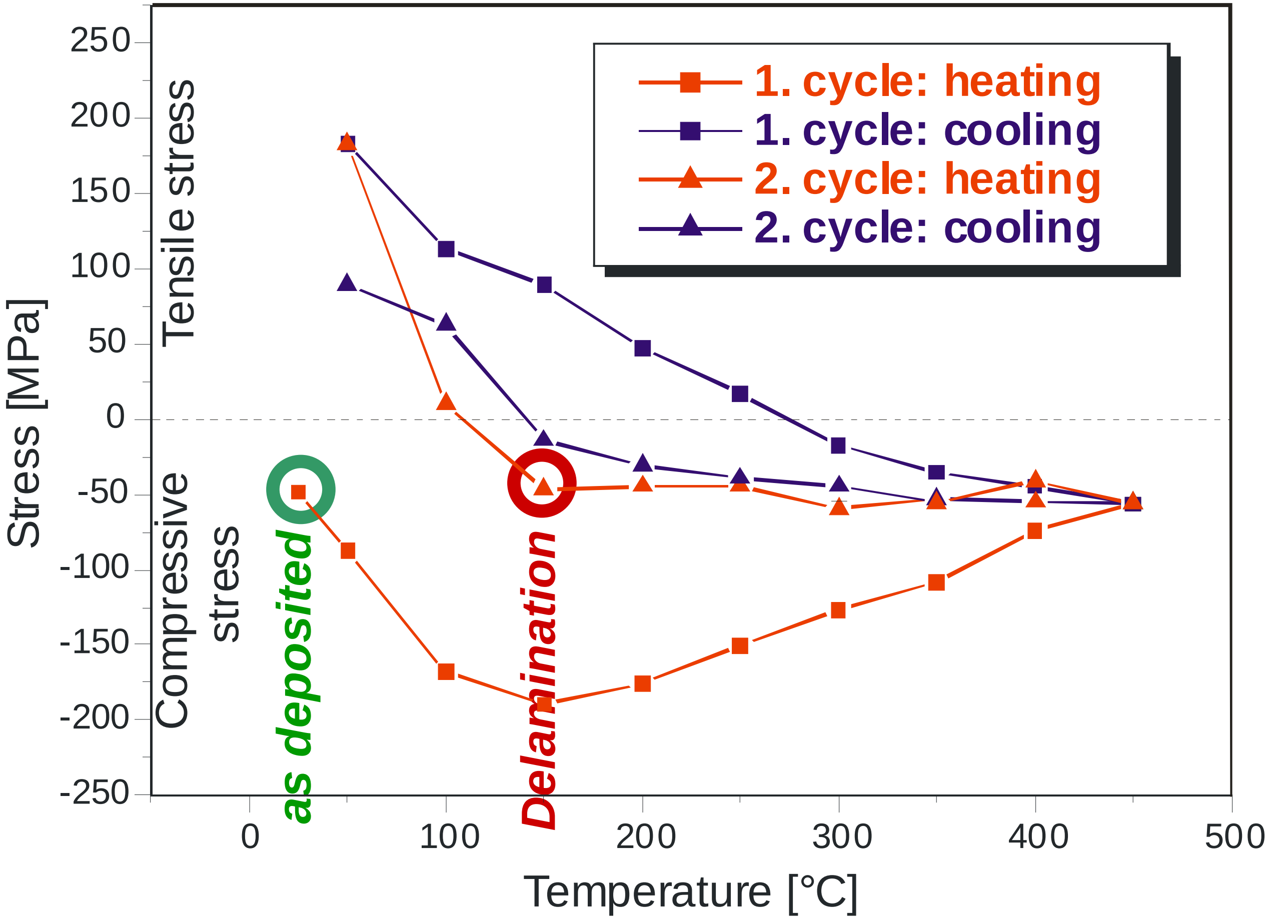
Disadvantages:

Several other influences:

- **+ Lattice defects**
- **+ Dislocations**
- **+ Impurities**
- **+ Foreign phases**

Example: Temperature Variation

Roentgenographic stress determination at variable temperature:



Carbon substrate coated with 4 µm Cu

α_{Cu} = 16 ppm/K

α_{C} = 2 ppm/K