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École polytechnique fédérale de Lausanne

Institute of Materials - Institute of Bioengineering
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SuNMiL
Supramolecular NanoMaterials and Interfaces Laboratory

Heterophase Interfaces and Thin Films
Lesson 12

MSE 304

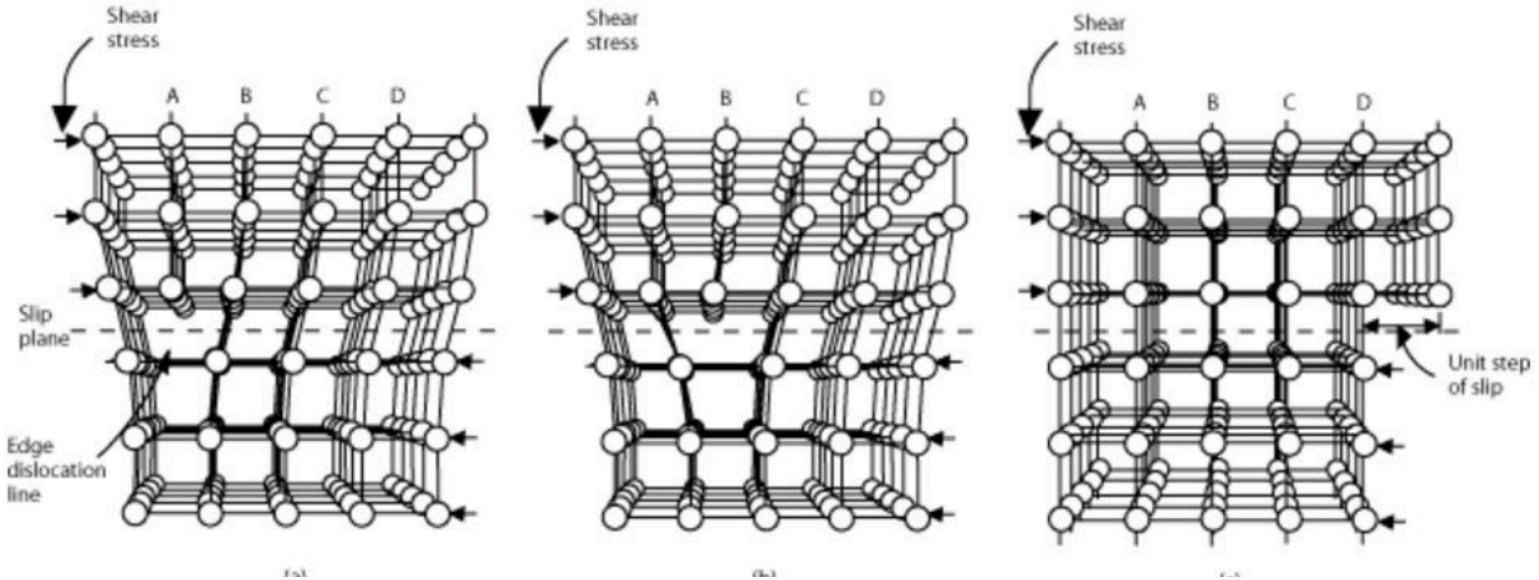
Francesco Stellacci

桑缪 썬밀 सानमिल ΣouNMιΛ سنمل CaHMПЛ

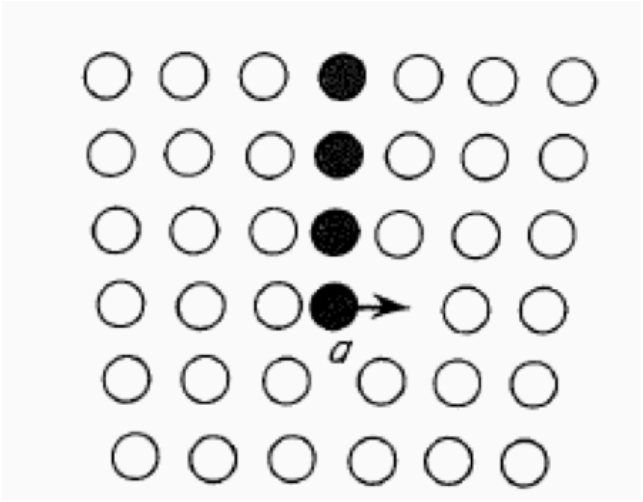
Key Topics in the Previous Class

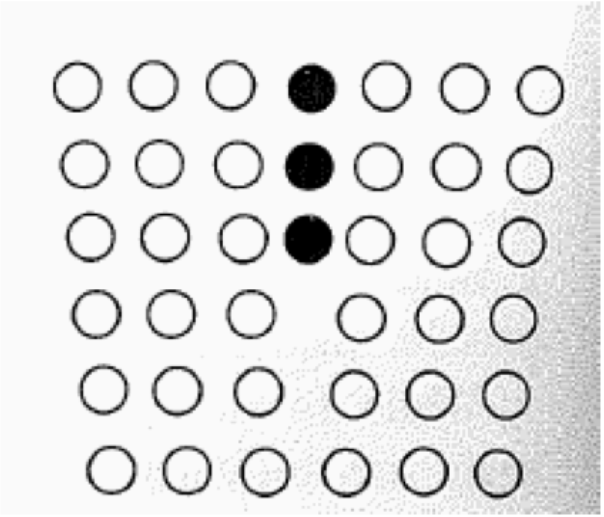
Slip Planes in a Crystal Structure

Glide Motion of Dislocations



Climb Motion for Dislocations





Glide and Climb Motion for Dislocations

Glide vs. Climb

Glide/slip: *conservative movement within the slip plane*

Climb: *non-conservative movement away from the slip plane*

let's consider a dislocation AB that moves to A'B' in the direction $\vec{t}$

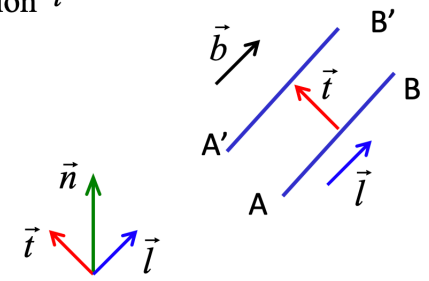
$\vec{n} = \vec{l} \times \vec{t}$ - surface normal

$\vec{b} \cdot \vec{n} = 0$ - conservative motion, glide

$\vec{b} \cdot \vec{n} > 0$ - addition of material

$\vec{b} \cdot \vec{n} < 0$ - removal of material

} climb



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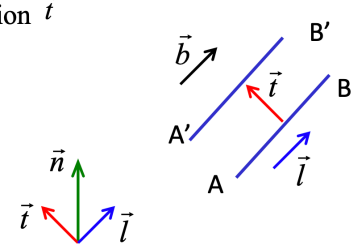
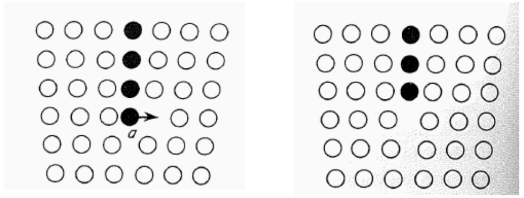


example:



$\uparrow \vec{t}$

$\otimes \vec{l}$ $\quad \leftarrow \vec{b}$ $\quad \vec{n} = \vec{l} \times \vec{t} \rightarrow$ $\quad \vec{b} \cdot \vec{n} < 0$

- positive climb
  crystal shrinks in direction parallel to slip plane
  results from compressive strain

in general, volume change due to climb is

$$\Delta V = \vec{b} \cdot \vec{l} \times \vec{t} = \vec{b} \times \vec{l} \cdot \vec{t}$$

Glissile and Sessile Interfaces

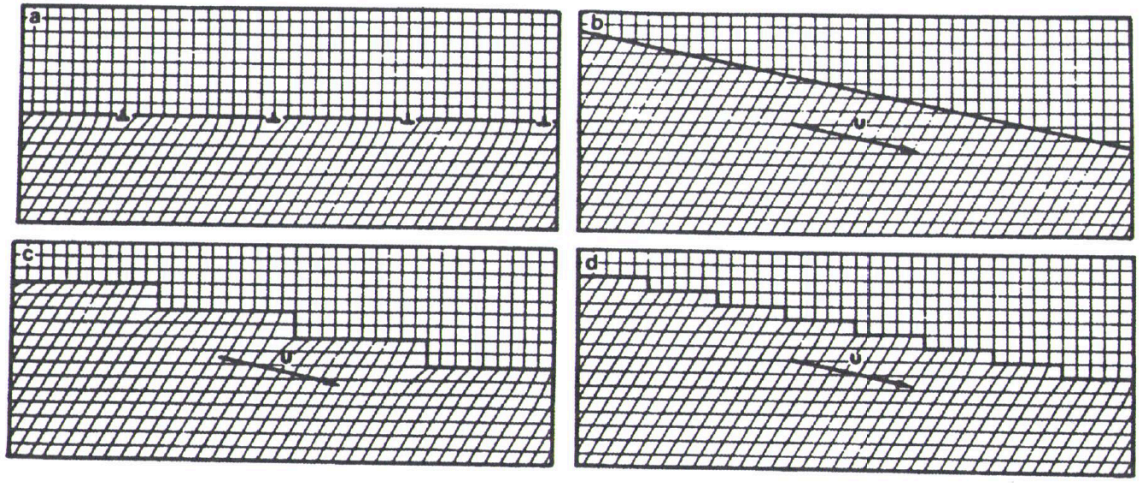


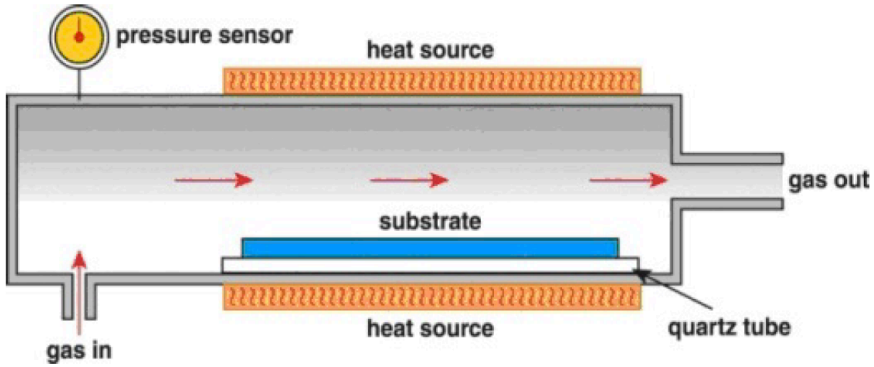
Figure 14.39. Possible interfaces for a transformation described by a shear e_{12} coupled with an expansion e_{11} in the shear plane. (a) The expansion is accommodated by a set of perfect lattice (misfit) dislocations. (b) The interface lies along an invariant line **u** and no dislocations are necessary. (c) The invariant line is resolved onto every other close-packed plane as in the f.c.c.–h.c.p. transformation where each ledge is an $a/6<112>$ partial dislocation. (d) The invariant line is resolved onto every close-packed plane as in an f.c.c.–b.c.c. transformation where each ledge contains an $a/12<112>$ partial dislocation. Reprinted with permission from [153] by Elsevier Science Ltd., Oxford, England.

Glissile and Sessile Interfaces

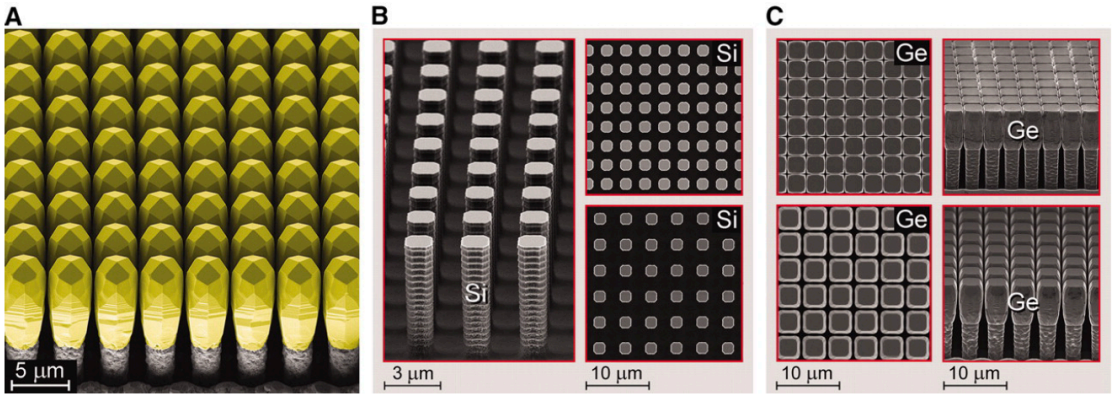
Thin Films in Modern Technology

Thin Films in Modern Technology

- Growth of thin films of materials allows extreme control of the structure of matter at the nano-scale
- On the lab. scale: molecular beam epitaxy (MBE)
  - Extremely ''clean'' conditions, exquisite control of all parameters
  - Batch operation, extremely slow, ultra-high vacuum
- On the industrial level: chemical vapor deposition (CVD)
  - ''Dirtier'' operation, but much simpler to operate

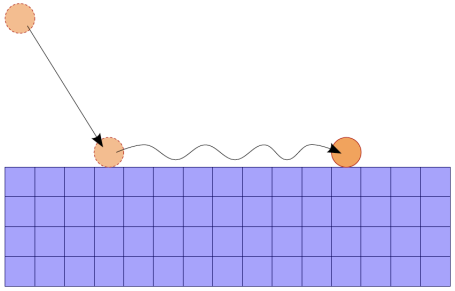


Thin Films – Morphology Control



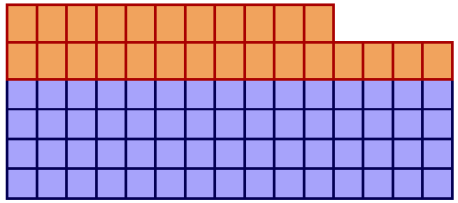
Strain-free Ge nanopillars grown by PECVD. [Falub et al., Science, 2012]

Growth Models for Thin Films

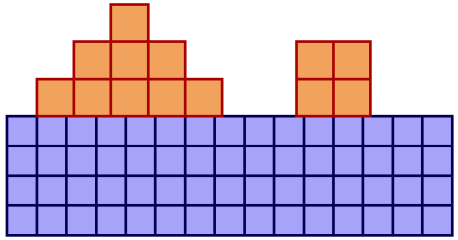


Growth Models for Thin Films

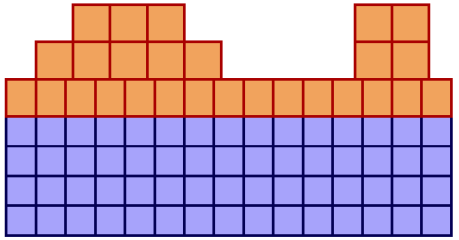
Frank-Van der Merwe



Volmer-Weber



Stranski-Krastanov



Growth Models for Thin Films

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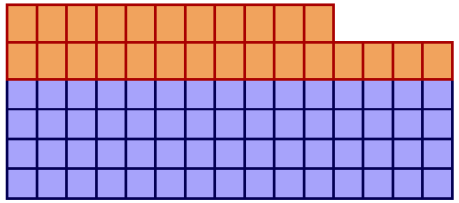
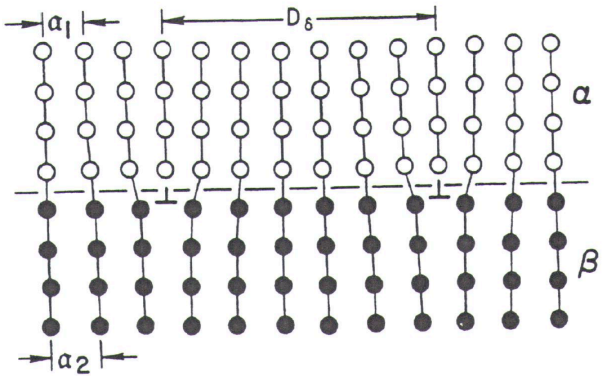
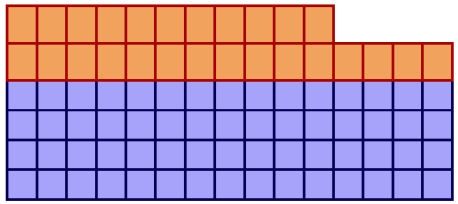


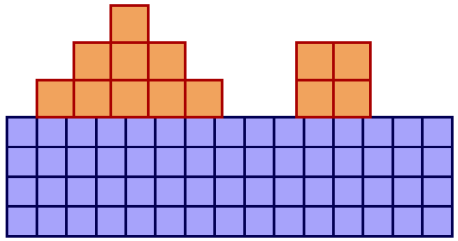


Growth Models for Thin Films: First Explanation

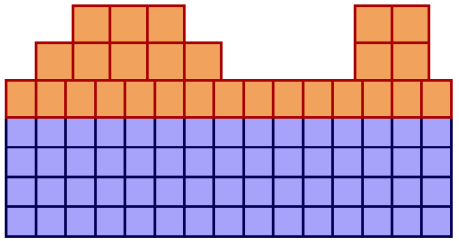
Frank-Van der Merwe



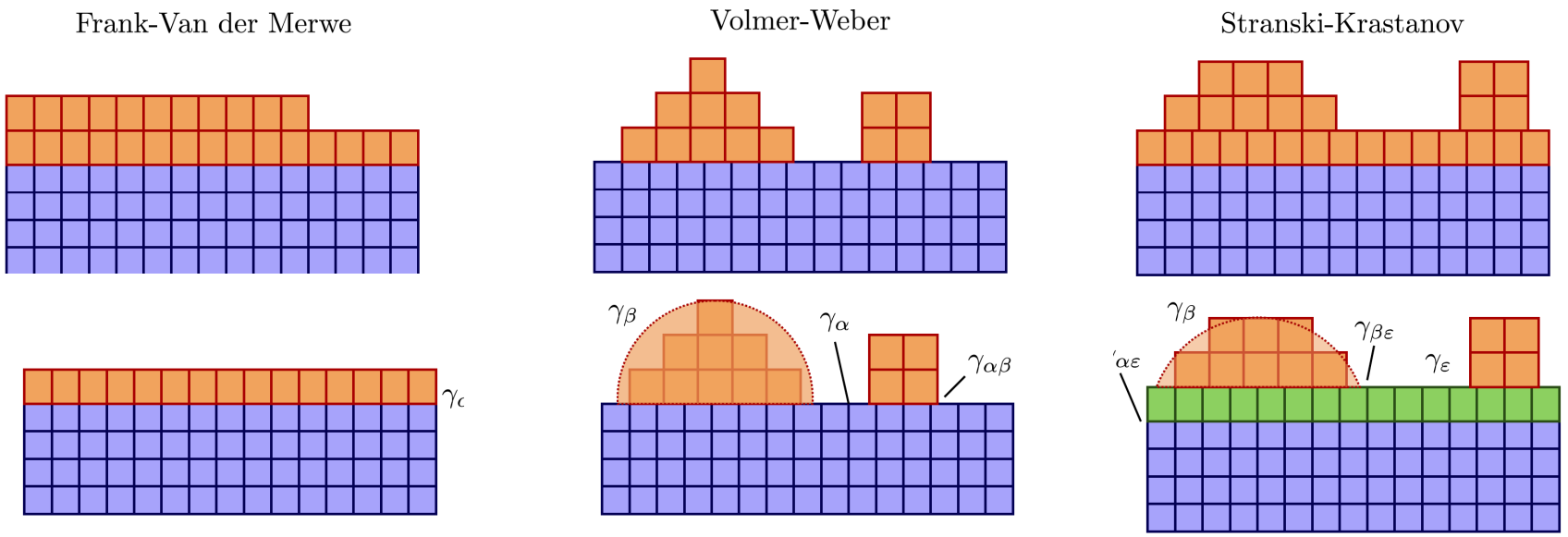
Volmer-Weber



Stranski-Krastanov



Growth Models for Thin Films: Second Explanation



- Let's look at these from a macroscopic point of view: Recall Young's equation $\gamma_\beta \cos\theta = \gamma_\alpha - \gamma_{\alpha\beta}$
  - 3D Island (VW) growth corresponds to finite contact angle: $\gamma_{\alpha\beta} + \gamma_\beta > \gamma_\alpha$
  - Layer-by-layer (FM) growth corresponds to $\theta = 0$: $\gamma_{\alpha\beta} + \gamma_\beta \leq \gamma_\alpha$
  - Stranski-Krastanov growth is harder to explain based on macroscopic surface energies. If we consider the strained film as a different material ε, it must be that $\gamma_{\alpha\varepsilon} + \gamma_\varepsilon \leq \gamma_\alpha$, and $\gamma_{\beta\varepsilon} + \gamma_\beta > \gamma_\varepsilon$

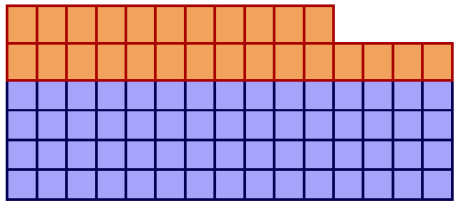
Strained and Unstrained Growth

$$E_{el} = e^2 C_5 L_f$$

$$C_5 = 2\mu_f \frac{1+\nu_f}{1-\nu_f}$$

Growth Models for Thin Films: Third Explanation

Frank-Van der Merwe



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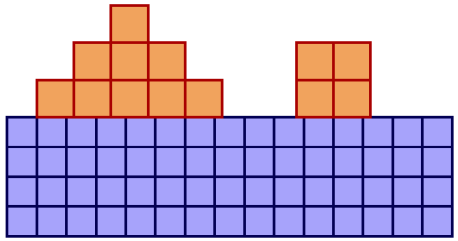

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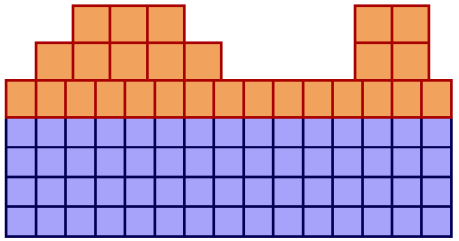


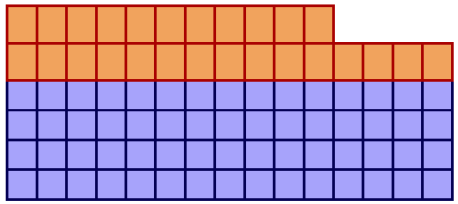
$$\mu(n) = \mu_\infty + [\varphi_a - \varphi'_a(n) + \varepsilon_d(n) + \varepsilon_e(n)]$$

$$\frac{d\mu}{dn} > 0$$

$$\frac{d\mu}{dn} < 0$$

Growth Models for Thin Films: Third Explanation

Frank-Van der Merwe



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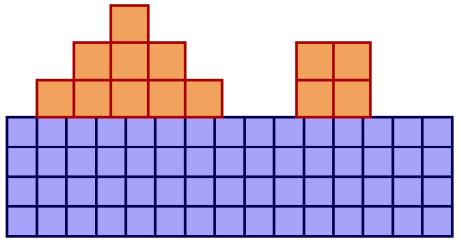

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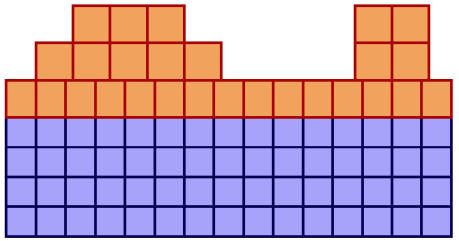

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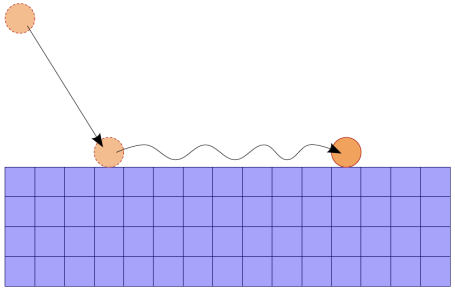
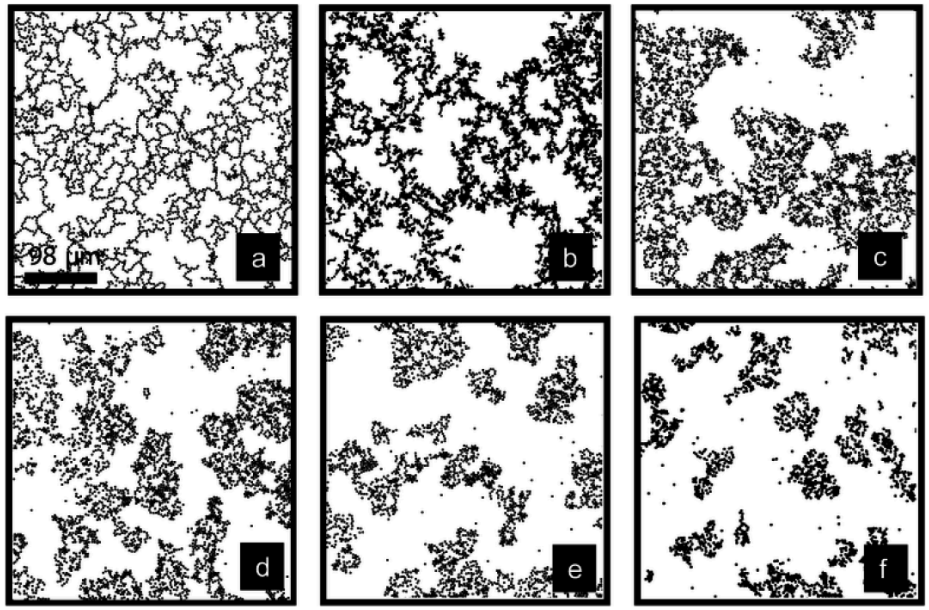


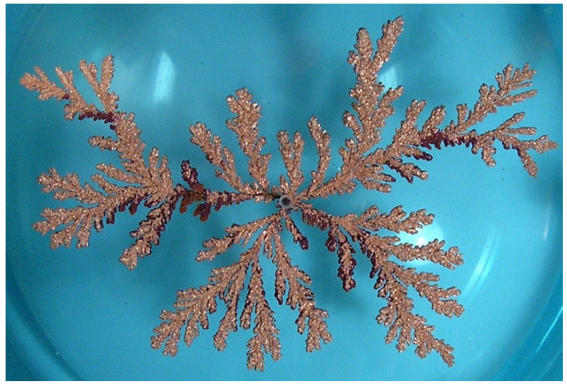
Diffusion Limited Aggregation

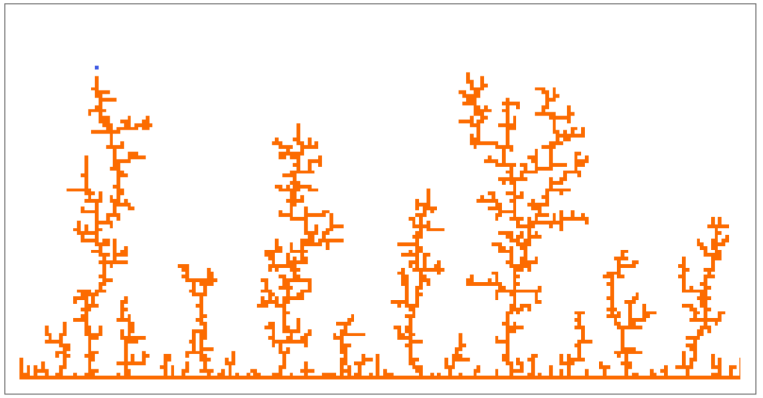


Flow-induced aggregation of colloids. [Massachaele et al., Soft Matter, 2011]

Diffusion Limited Aggregation

- Growth regimes discussed this far assume local equilibration between atom attachments
- The opposite case is a "stick where you hit" grow mode - strongly out of equilibrium structure
- Diffusion-limited aggregation





Conclusions