Elle Latte

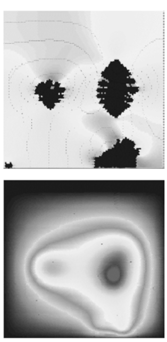
Lattice Spring Simulation

of

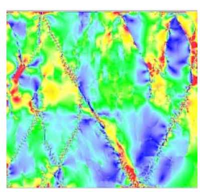
Visco-elasto-plastic Materials and Reaction-coupling

Contributions by Till Sachau, Anders Malthe-Sørenssen, François Renard, Renaud Toussaint, Bjørn Jamtveit, Jochen Arnold, Paul Bons, Marcus Ebner, Arzu Arslan

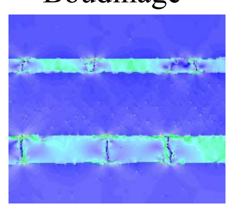
Phase Transitions



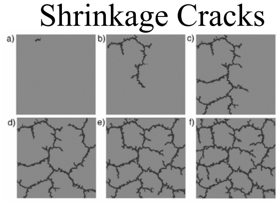
Fractures



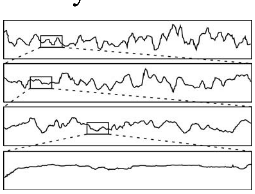
Boudinage



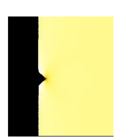
Shrinkage Cracks



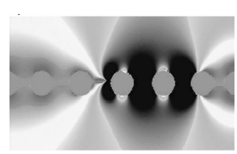
Stylolites



Grooves



Pressure Solution



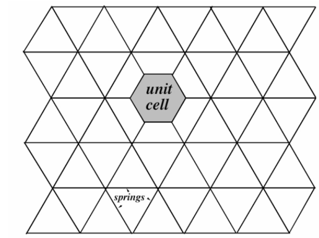
Lattice Spring and Particle Models

Calculation of normal forces on a node:

$$F_i = \sum_{(j)} \kappa \left(|x_i - x_j| - l \right) v_{i,j} + f_p$$

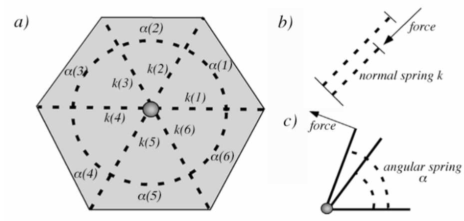
- constant: κ
- sum over neighbours: $\sum_{(j)}$
- distance between nodes: $|x_i - x_j|$
- equilibrium distance: l
- vector for direction: $v_{i,j}$
- extra force: f_p

Regular triangular grid



The equilibrium configuration of the spring network may be found using overrelaxation techniques.

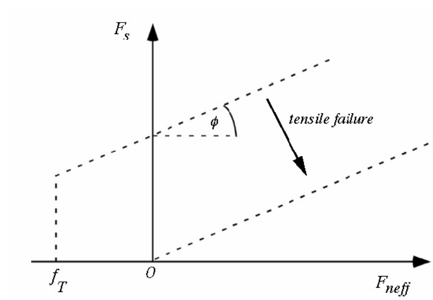
In order to vary the Poisson ratio and to treat random lattice one can also include angular springs.

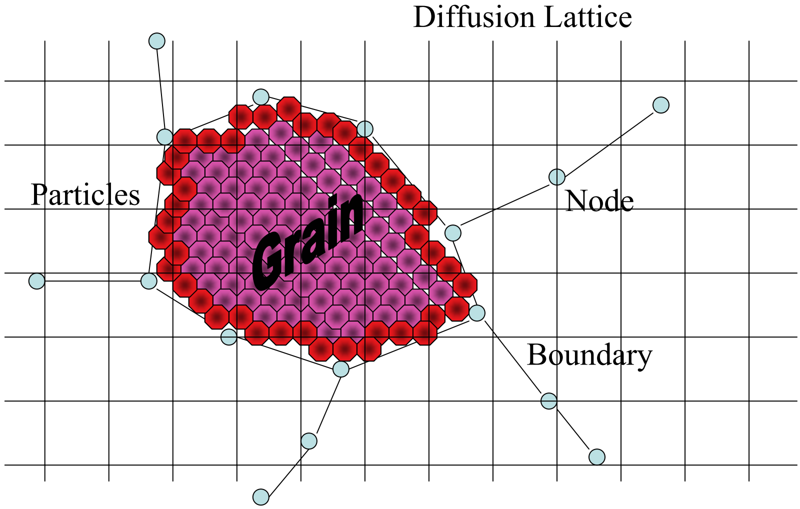


One strength of these models is that they can be used to model failure of material.
-> either particles slip past each other or springs or beams can break and the cohesion is lost.
Failure criterion is critical tensile strength for normal springs/contacts and a Mohr-Coulomb friction law for tangential forces/angular springs.

-> failure under tension: $F_{neff} \leq f_T$

-> failure under shear: $F_s \geq \tan\phi F_{neff}$

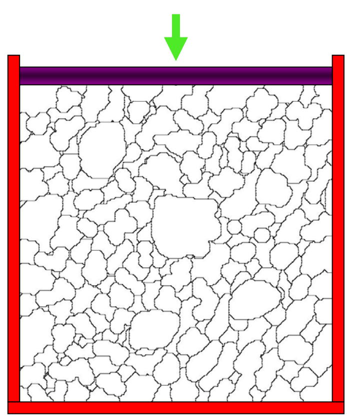




Particles of a grain have the same elastic Modulus

Springs of grain boundaries break easier

Get Elle Microstructure

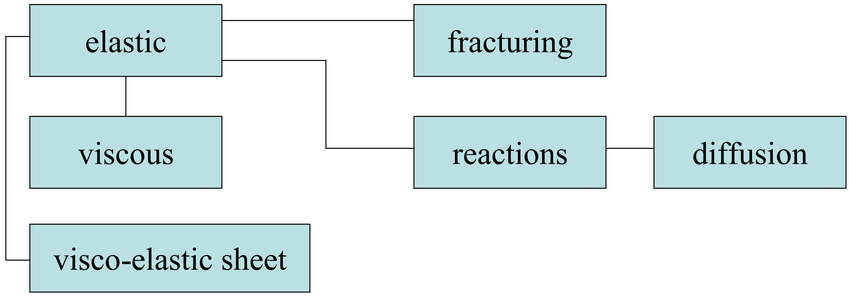


Boundary conditions: Particle walls, elastic walls, internal forces from fluid pressure, viscous layer.

Pure shear, simple shear, uniaxial compression/extension, variations.

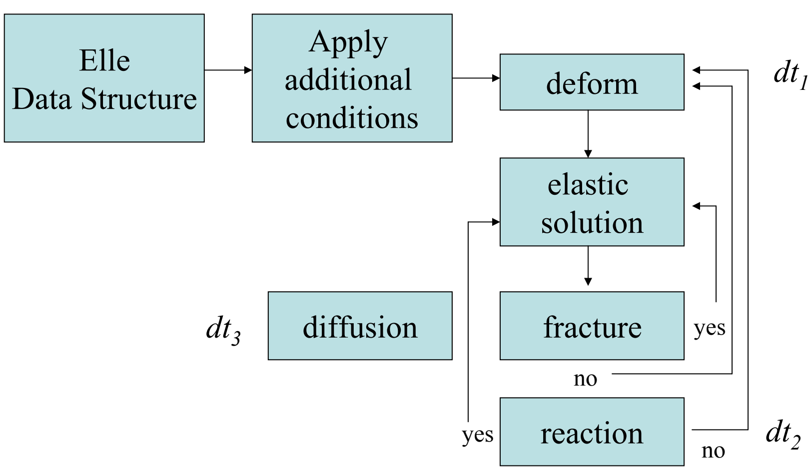
Internal Geometry from Elle, create layers, holes, heterogeneities

Moduls:



-> coupling is highly non-linear -> different time scales

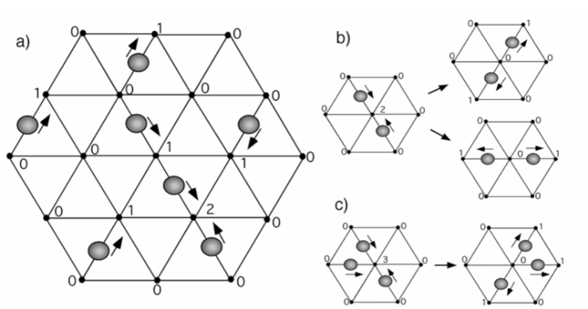
deformation step, reaction step, viscous step, diffusion step, fracturing step



- Lattice Gas automaton -> Experiment 1,2
- Fracturing -> Experiment 4
- Boudinage -> Experiment 11
- Dissolution grooves -> Experiment 12
- Stylolites -> Experiment 13
- Expanding Inclusions -> Experiment 18
- Mudcracks -> Experiment 19
- Visco-elastic deformation and fractures -> Experiment 20

- more experiments in the Latte interface -> Heat diffusion, solid-solid phase transition

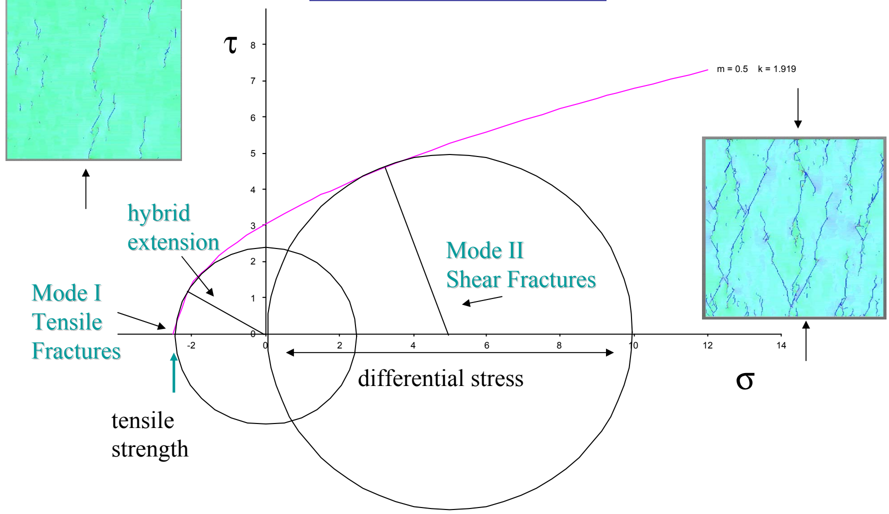
Lattice Gas Models are a class of cellular automata that can be used to model diffusion. Each site of the model represents for example a part of a fluid. The state of the site depends on the amount of fluid particles that are approaching the site. Momentum and mass are conserved in the model. Particles initially have a given velocity that may be random. How particles travel on the lattice depends now on their velocity and on collisions with other particles or boundaries.



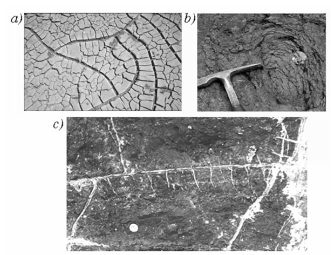
Particles travel on the triangular lattice. Numbers are states of sites -> how many fluid particles approach the site. Two or three particles may collide and will scatter in different directions. This may involve a Monte Carlo step in the case of two particles because there are two possible ways to scatter them.

General form of the failure envelope

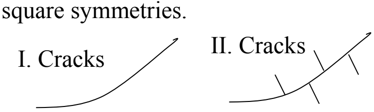
$$\tau = k(\sigma + \sigma_c)^m$$



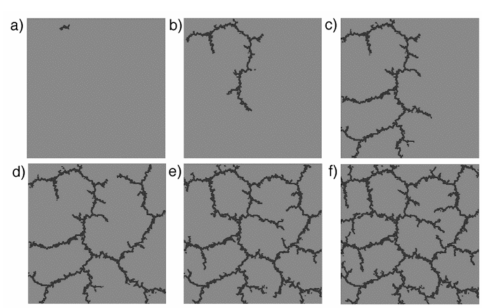
Mudcracks



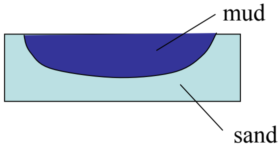
Shrinkage cracks in mud layers may form perfect hexagonal symmetries or more complex patterns because of age relations between cracks.
In addition cracks may form “egg-shell” patterns or square symmetries.



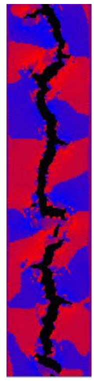
Progressive development of hexagonal mudcrack pattern in a lattice spring simulation. The initial nucleus of the crack branches and some crack branches start to curve.



Mudcracks that grow in channels

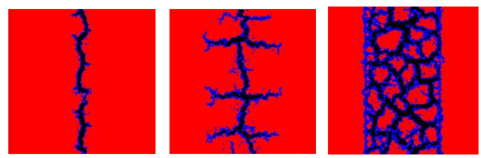


Mud channel between ripples



Direction of the main tensile stress flips -> wavy cracks develop!

Variation in shrinking velocity across channel and a variation in attachement to sand at the base (elastic sheet attached to viscous sheet)

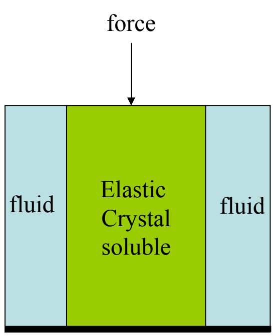


waves squares hexagons

A variation of elastic constants and strength of attachement produces different patterns.

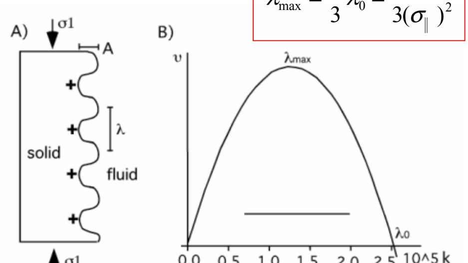
Example of surface and elastic forces that generate waves

A salt crystal surface in contact with a saturated solution is in equilibrium with the solution. If we stress the crystal it is out of equilibrium and dissolves. How does it come back to equilibrium ? Can we see patterns on the crystal surface ?



Setup of a stressed crystal in contact with a solution

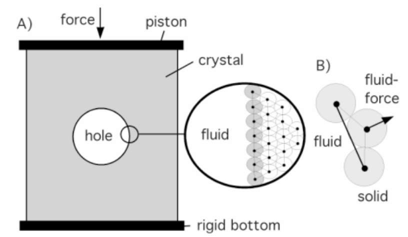
$$\lambda_{max} = \frac{4}{3}\lambda_0 = \frac{4\pi\gamma E}{3(\sigma_{\parallel})^2}$$



$(k = 2\pi/\lambda)$

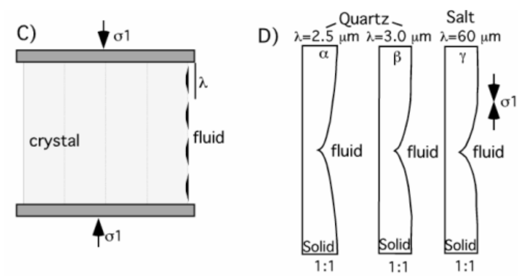
Elastic energy drives dissolution, surface energy in grooves will drive precipitation -> competing forces that scale differently. Therefore there is a certain wavelength of grooves that will grow fastest, that is grooves with a certain wavelength will preferably develop.

Use a lattice spring model, calculate elastic stresses and surface energy.

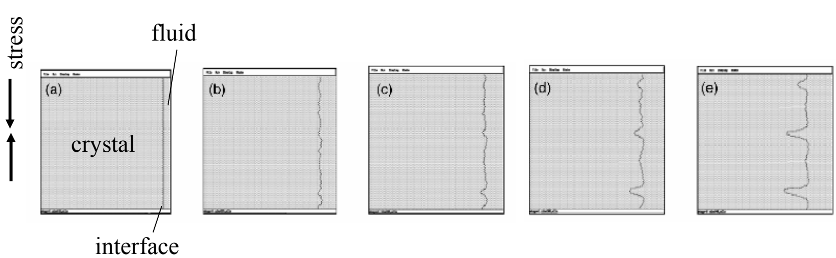


$$D_r = k_r V_s \left\{ 1 - \left[\exp\left(-\frac{\Delta \psi_s}{RT} \right) \right]^{\frac{1}{2}} \right\}$$

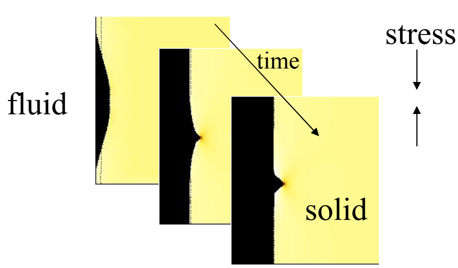
Linear rate law: dissolution is a function of the changes in elastic and surface energy -> dissolve particles and take them off the lattice -> coupling between dissolution and elastic and surface forces.



The initial structure is a so-called "cusp instability". It is not stable because stresses at the tip increase while the cusp grows into the crystal -> dissolution is enhanced.



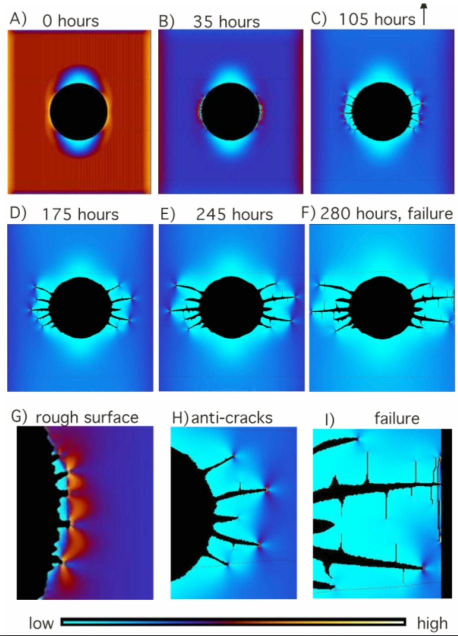
Random fluctuations -> Bifurcation -> preferred wavelength

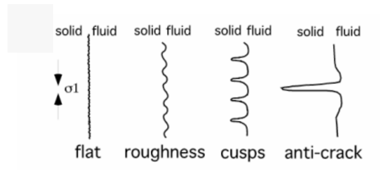


-> but we are not in equilibrium, so what happens now ??

If we insert a predefined wavelength on the crystal a groove develops -> non-linear behaviour, not predictable by linear stability analysis.

The instability may develop “anti-cracks” -> crack-like structures that grow perpendicular to the main compressive stress.

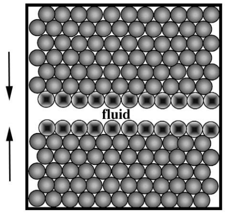




The structures develop anti-cracks and go through a coarsening, some of the initial anti-cracks win and grow further into the crystal whereas others loose and disappear.

Example-> dynamic scaling of stylolites in simulations

σ1



Two rocks are pressed together. Dissolution at the contact is a function of elastic and surface energy and contact stress:

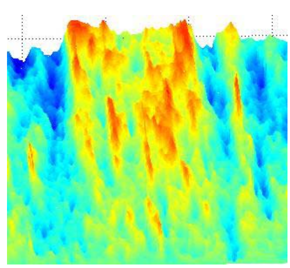
$$D_r = k_r V_s \left[1 - \exp\left(-\Delta P_n V_s - \Delta \psi_s \Big/ RT \right) \right]$$

The heterogeneity is called “noise”. In this case the noise is quenched -> frozen into the system at the beginning

Stresses are calculated with a *Lattice Spring Model*.

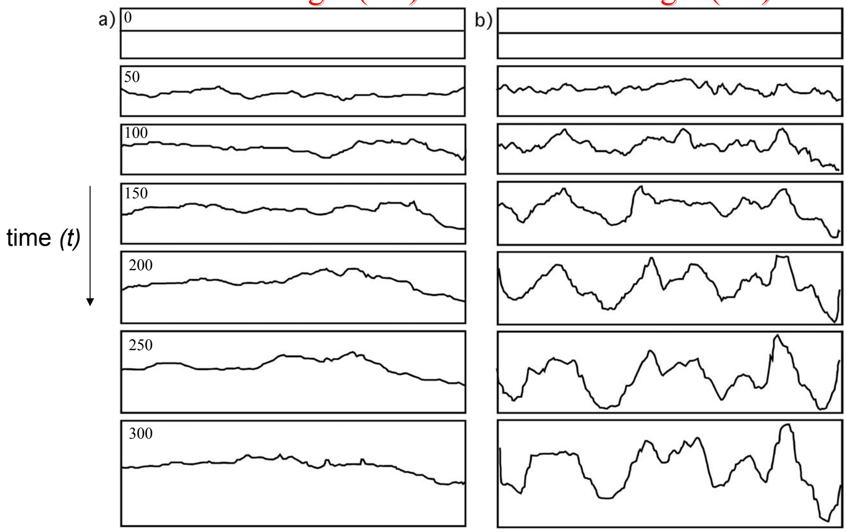
Heterogeneities in the rock are induced by a variation of dissolution constants -> Monte Carlo part of the model.

We can look at scaling properties in time and space



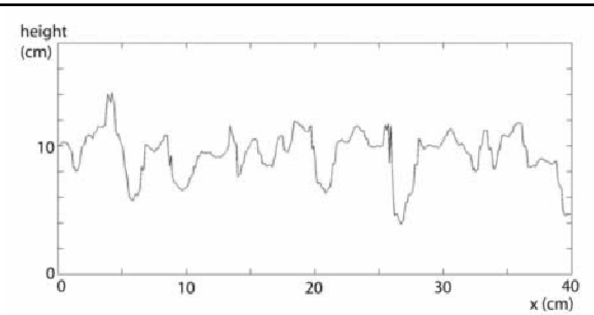
How does the amplitude of the stylolite grow ?
-> self-affine time series!

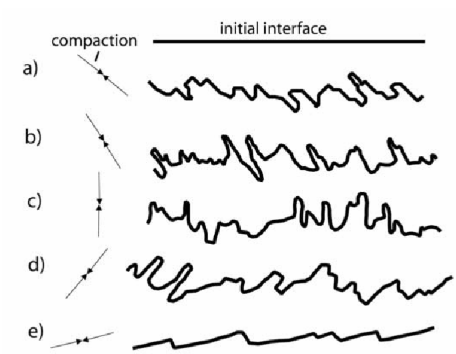
0.02m length (1:1) | 2m length (1:1)



Early saturation

Growth non-linear, but no saturation





Characterize the width of the interface (Amplitude of the roughness) with a RMS function (Root Mean Square).

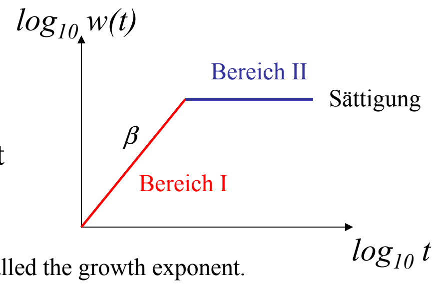
$$w(L,t) \equiv \sqrt{\frac{1}{L}\sum_{i=1}^{L}\left[h(i,t)-\bar{h}(t)\right]^2}$$

Where w is the width, L the system size, t the time and h the height of point i on the surface.

Typically the dynamic roughening of interfaces develops two distinct scaling regimes -> first regime follows a power law (self-affine time series), in the second regime the roughness growth saturates -> the amplitude stays constant!

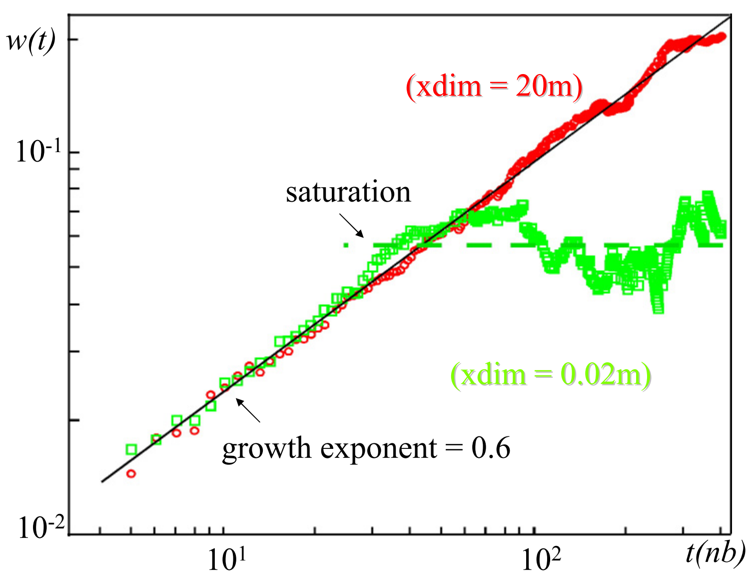
Regime I: $w(L,t) \sim t^{\beta}$

Regime II: w stays constant

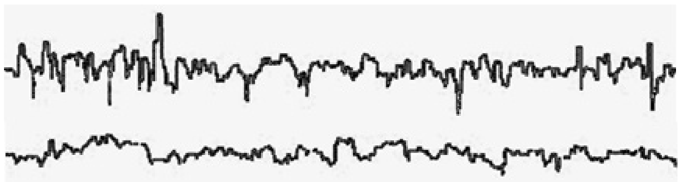


The exponent β of the first regime is called the growth exponent.

A smaller stylolite shows also the second regime, the roughness saturates.

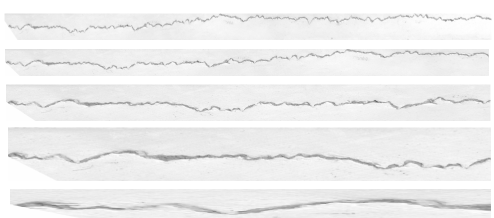


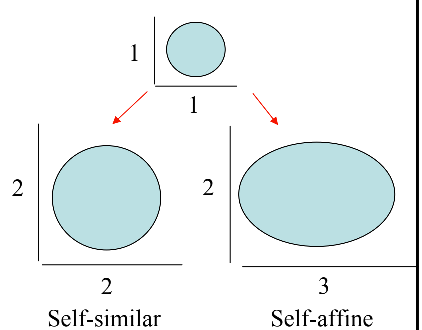
Scaling of the roughness



Self-affine space series

Rescale the images-> different scaling in x and y -> *anisotropic rescaling*





$$y(x) \sim b^{-\alpha} y(bx)$$

Where α is the roughness exponent -> if we blow up a function *y(x)* with a factor *b* horizontally we must blow it up with a factor b^{α} vertically !
For a rough interface with a height *h* this equation means that if two points on the surface are separated by a distance *l* their difference in height Δh scales as:

$$\Delta h \sim l^{\alpha}$$

-> another power law…

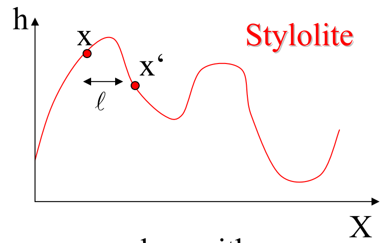
Desribe the roughness with a height-height corellation function for a given time step

Height-height correlation function (h is height of point at position x)

$$C(\ell) \equiv \left[\left\langle \left(h(x) - h(x') \right)^2 \right\rangle_x \right]^{1/2}$$

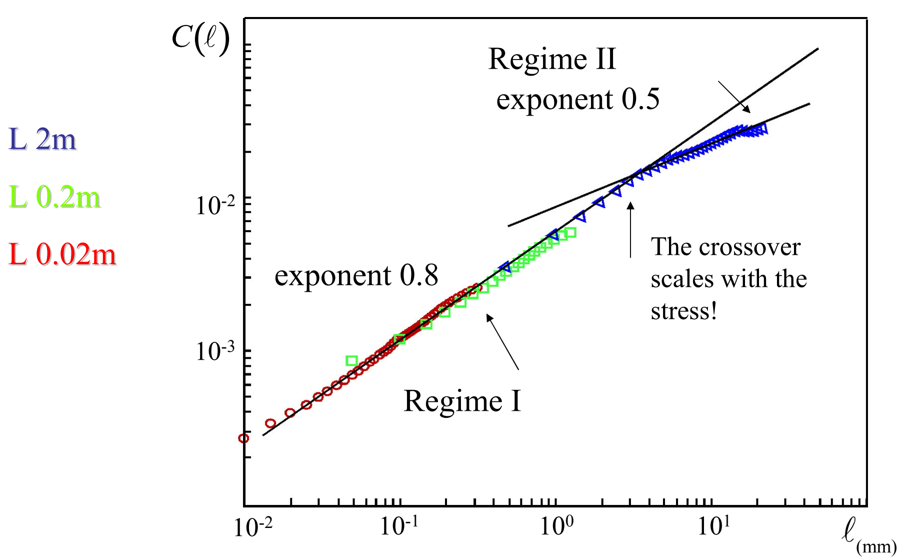
where $\left[|x - x'| = \ell \right]$

The roughness exponent is defined by: $C(\ell) \approx \ell^{\alpha}$



-> the rouhness should follow a power law with an exponent α, the roughness exponent

We find two self-affine scaling regimes, one regime is dominated by elastic energy and the second regime is dominated by surface energy.



What else?

Hydrofractures

-> release of fluids/melts in stressed systems

Reaction-Diffusion systems coupled with fracturing

-> Heat diffusion, thermal shrinking and fracturing

-> Stylolite dissolution coupled with diffusion, precipitation and porosity reduction

Large scale rift dynamics

-> gravity, visco-elasticity, brittle-ductile transition

-> 3D?

+ random lattice and remeshing....