Grains, Interfaces, Nanomaterials
and how to model them

Maria Gokieli
ICM, University of Warsaw

Mathematics for Key Technologies and Innovation
Warsaw, 22 February 2008

In cooperation with

- M. Niezgódka

- T. Wejrzanowski

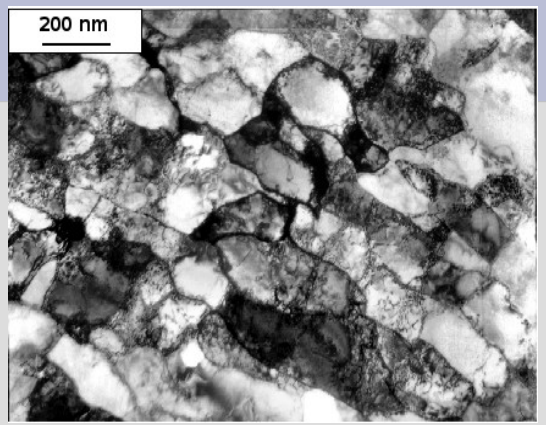
(Warsaw University of Technology)

- J. Piechota, W. Rudnicki, R. Sot, M. Szpindler

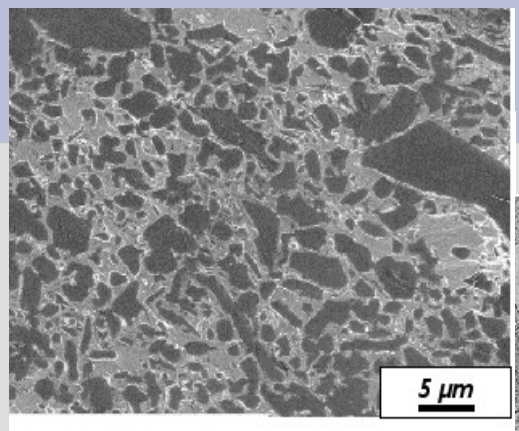
(ICM)

Materials with grained structure

Polycrystals (metals and alloys)

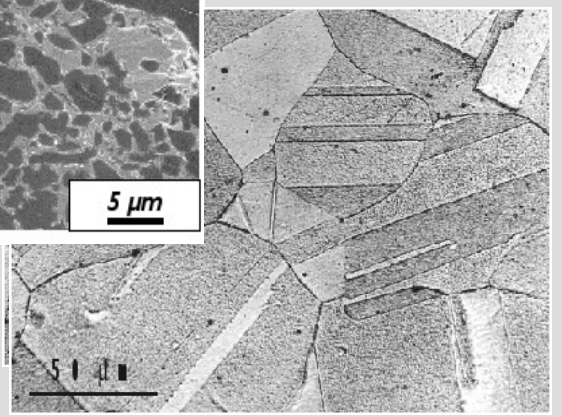


Fe[a]

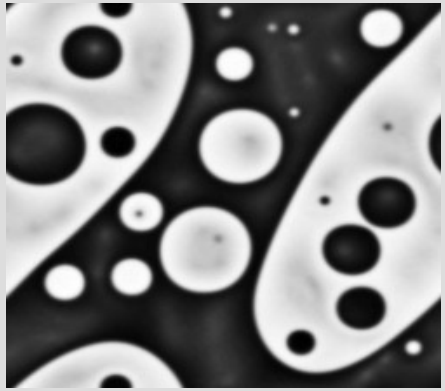


Al_2O_3-Ni [a]

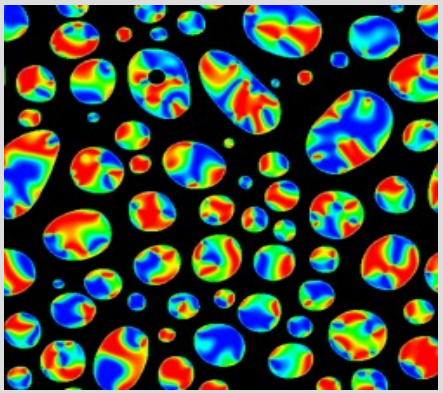
brass[a]



Mixtures



typical mixture[b]



liquid crystal[c]

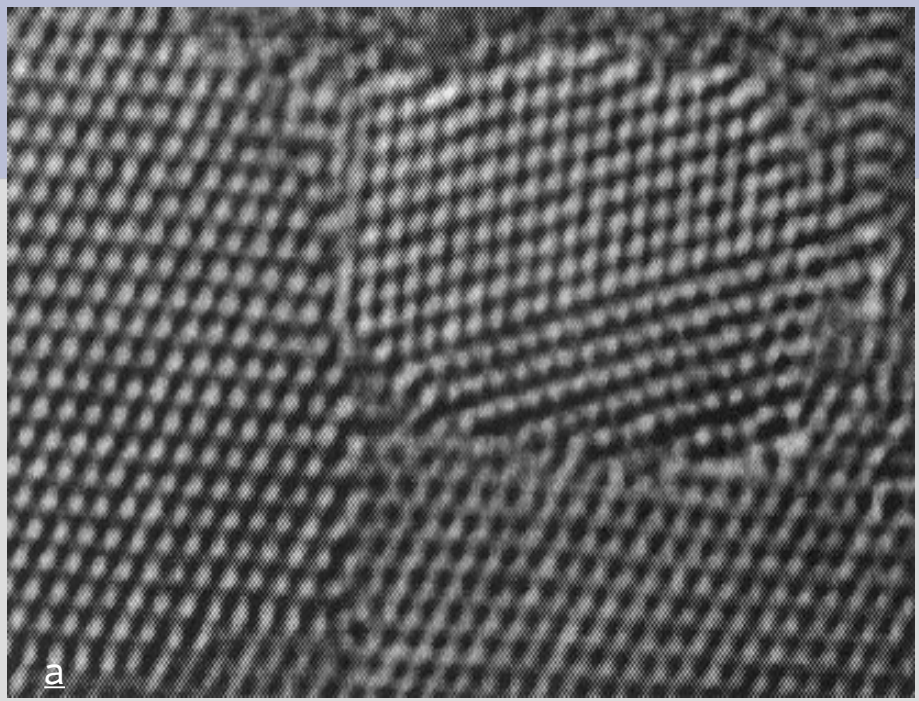
[a] courtesy of the Warsaw University of Technology

[b] Tanaka and Araki,Physical Review Letters 1998

[c] Tanaka and Araki,Physical Review Letters 2004

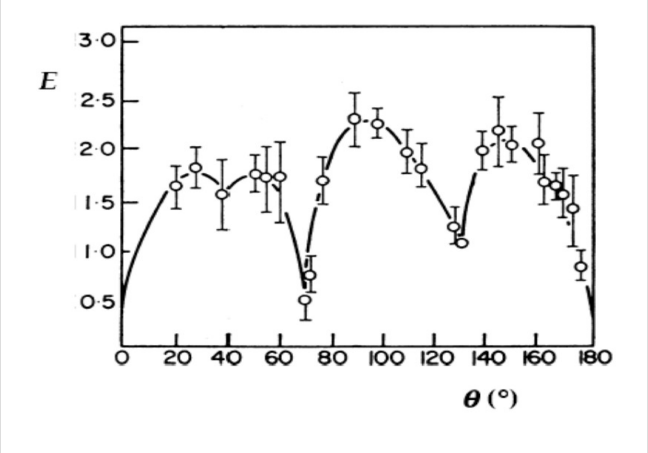
Grains and interfaces

In polycrystals, each grain is a crystal structure, rotated by some random angle.



[a]

Interface energy vs disorientation angle for Al



In alloys or mixtures, the other parameters determining grains are: composition and solid/liquid phase.

[a] University of Edinburgh, COSMIC laboratory, real image of a colloidal polycrystal

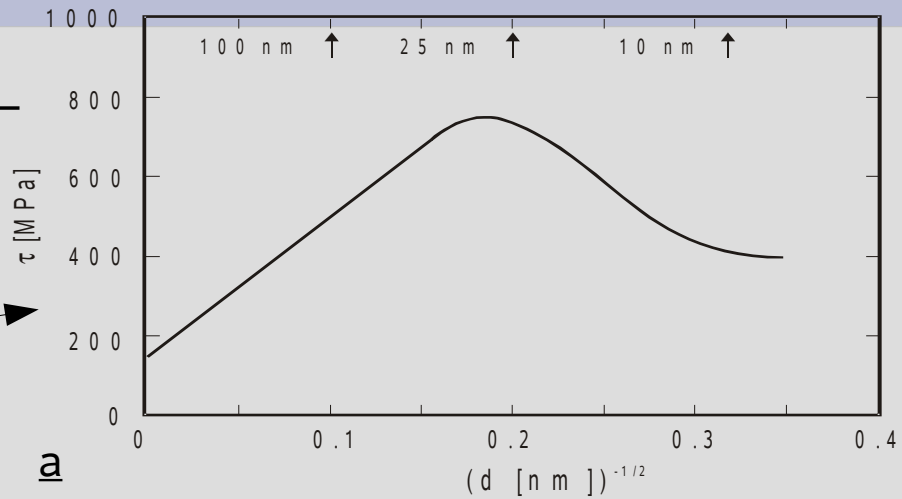
Challenge: nanomaterials

For metals and alloys, small grains are an advantage as for material's properties. E.g.:

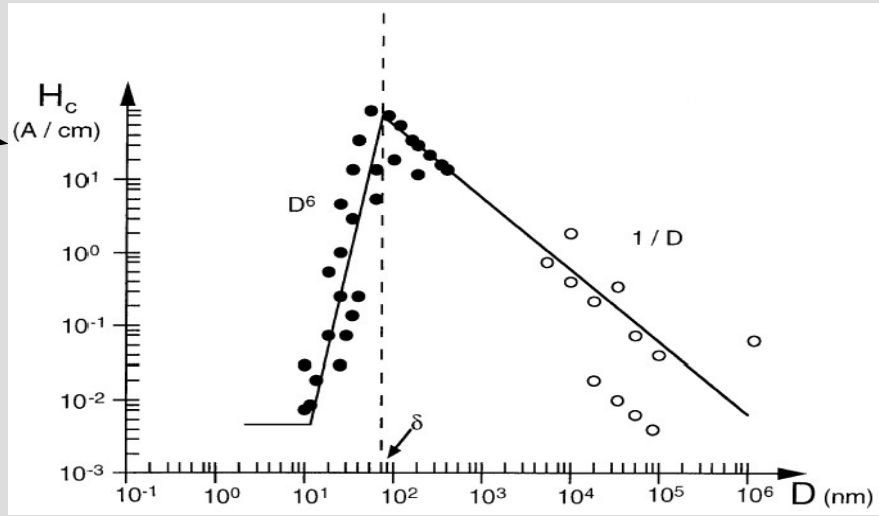
- plasticity limit (resistance to deformations)

- magnetic properties

But they are very unstable: interfaces are regions of much higher internal energy.



a



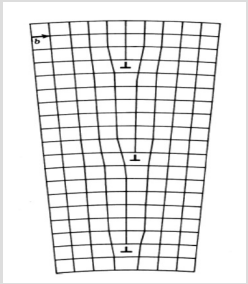
b

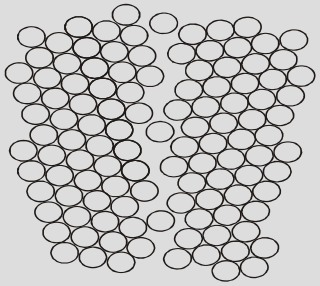
[a] E. Artz, Acta Metallurgica 1998

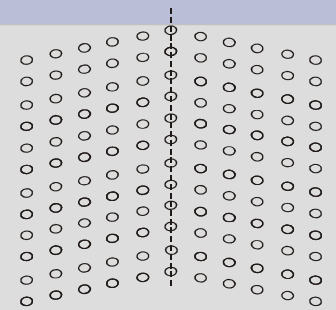
[b] Masumura, Hazzledine, Pande, Acta Materialia 1998

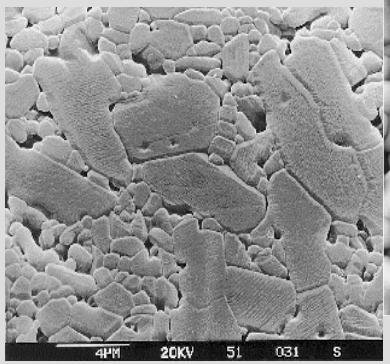
Other micro parameters known to influence structural stability

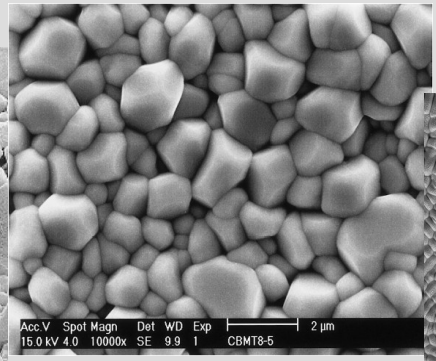
- Interface characteristics
- Grains' form
- Grain's form, size,orientation distribution

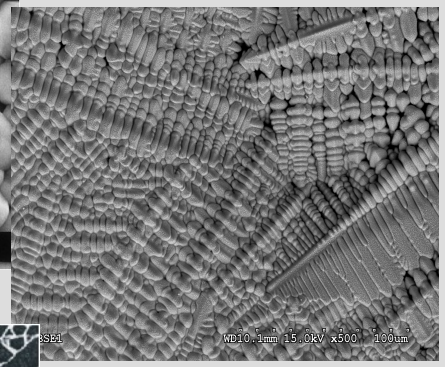


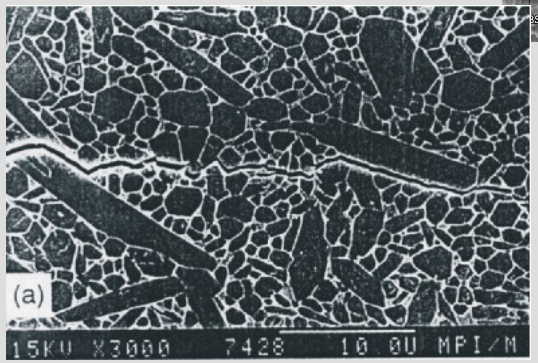












Images: courtesy of the Warsaw University of Technology

Phenomena involved in the micro-structure evolution

- Metals:

crystallization, grain growth and rotation

- Alloys:

phase separation, grain growth and rotation, diffusion along interfaces

- Mixtures:

phase separation, diffusion, reaction

Mathematical models: micro scale

We used two stochastic models, each containing:

- a crystallization part (geometrical or 'real')
- an energy functional, defining the energy of each atom with its nearest interactions and orientation dependence, e.g.

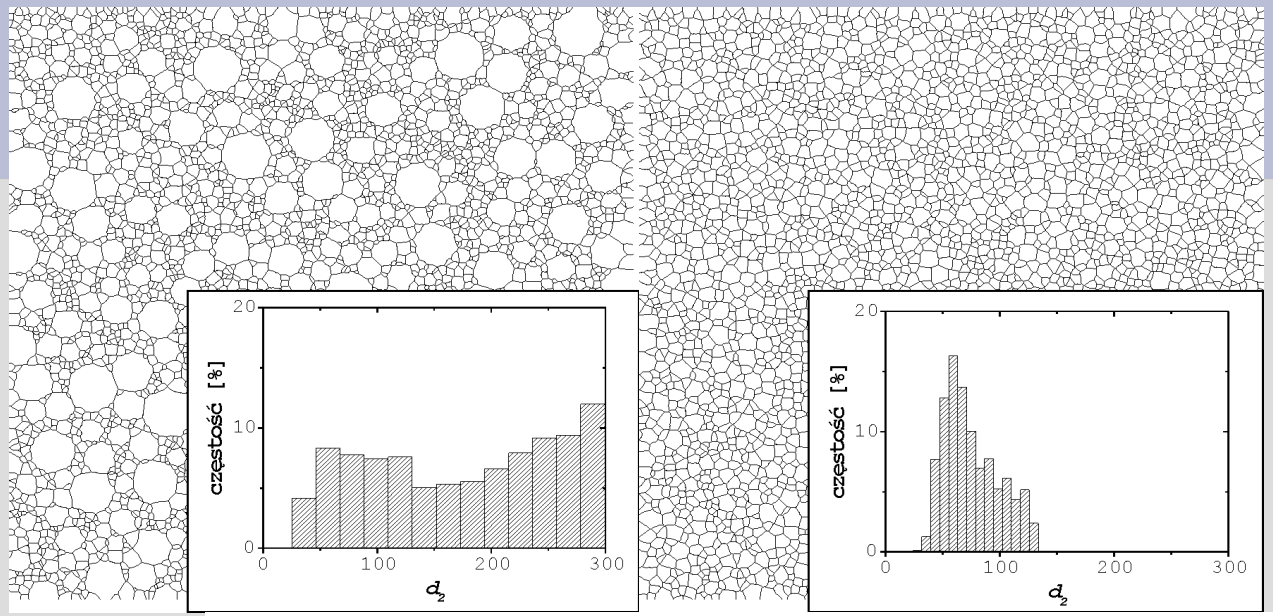
$$E = -c\left[m + \frac{1}{4}\sum_i f(\theta - \theta_i)\cdot n_i\right]$$

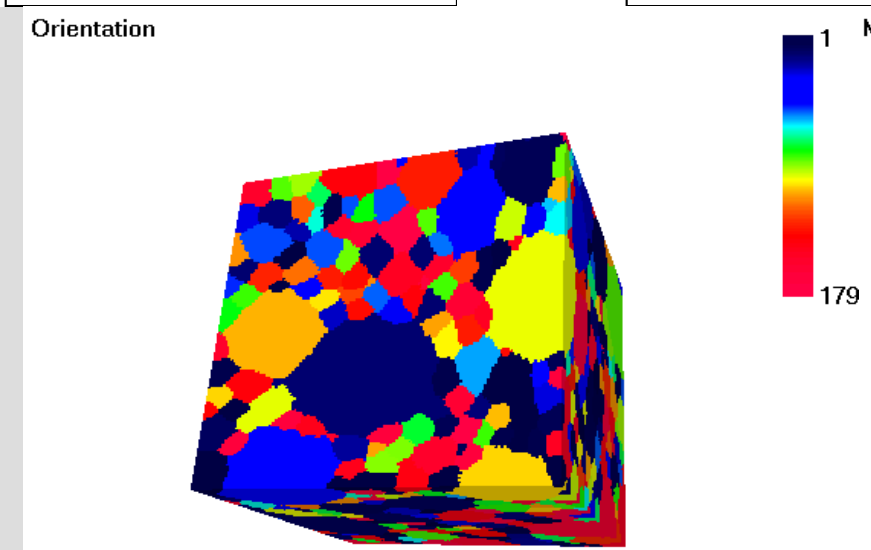
number of neighbours in same grain

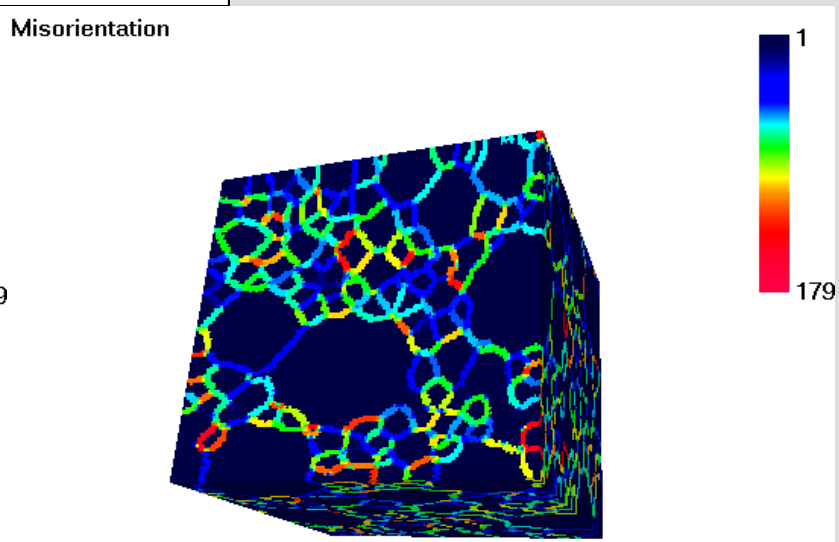
number of neighbours in grain of orientation ϑ_i

- a classical Metropolis probability of atom's jump

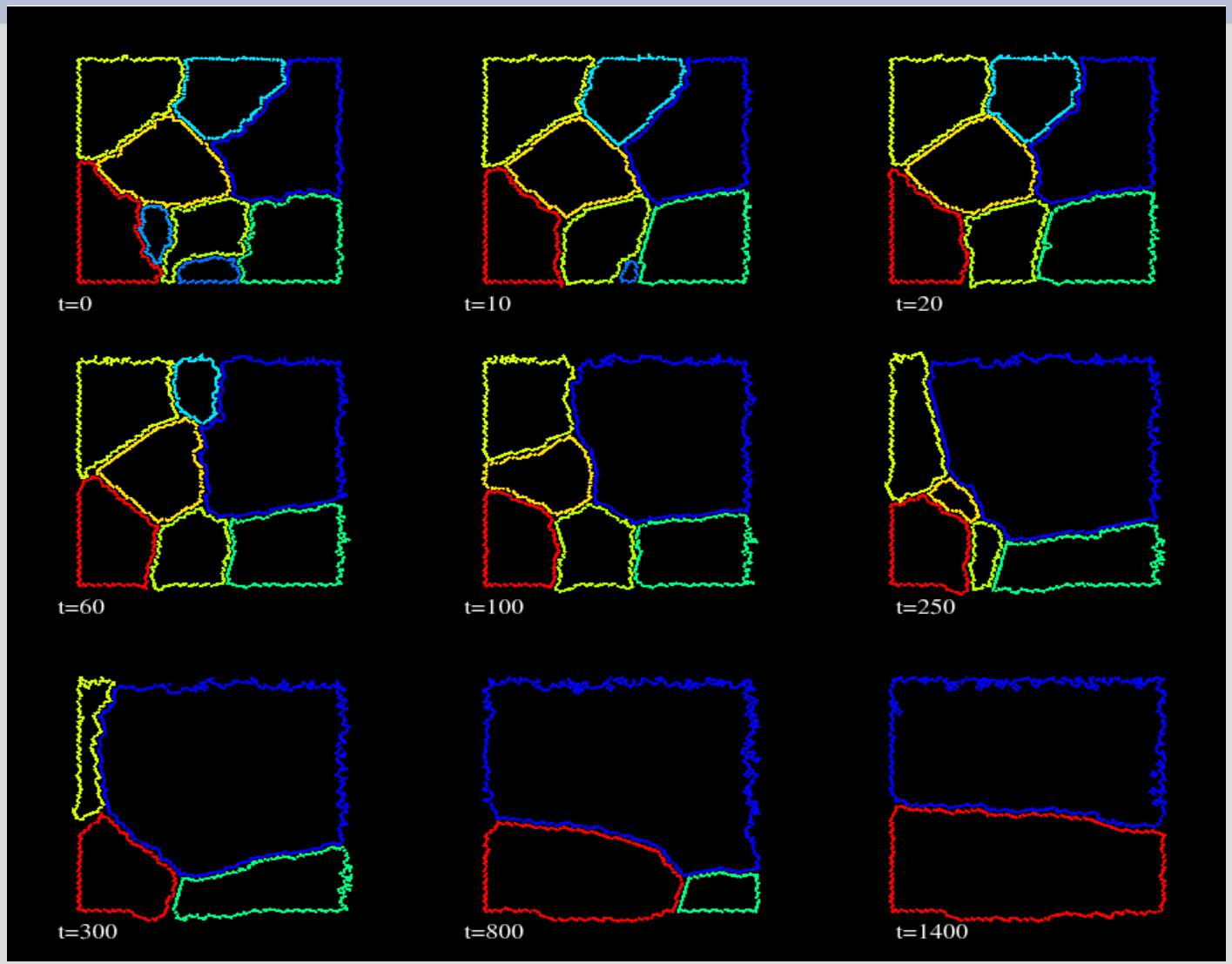
Micro simulations - data







Micro simulations: example of evolution



Mathematical models: systems of coupled PDEs

Cahn-Hilliard	reaction-diffusion mean curvature	total variation flow

Used model: Kobayashi-Warren-Carter 2000

θ - orientation, η - measure of structure order

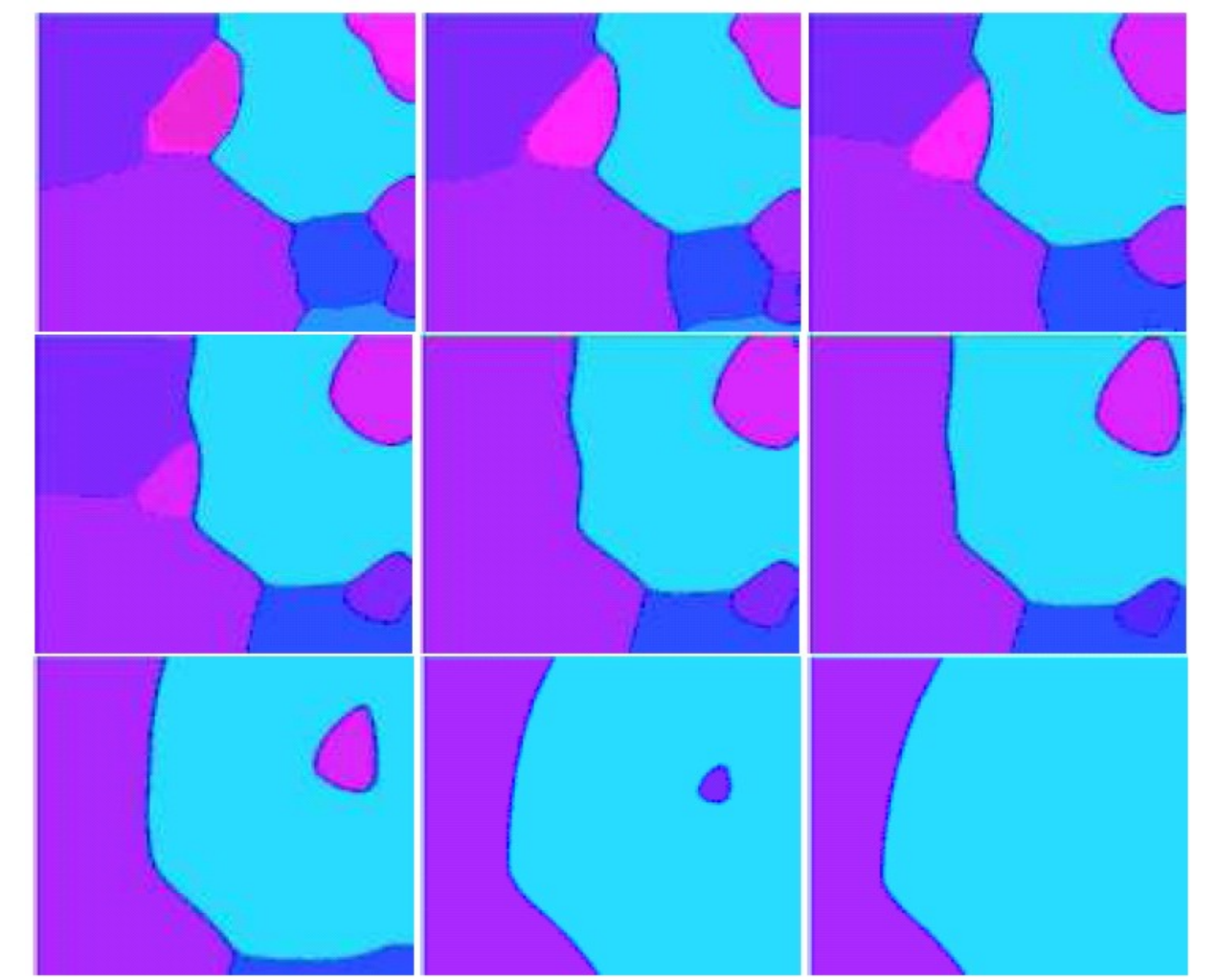
$$\begin{cases} \tau_1 \eta_t = \nu^2 \Delta\eta + a^2(1-\eta) - 2s\, m(\eta)\,|\nabla\theta| \\ \tau_2 \eta^2 \theta_t = s\,\nabla\left[\eta^2 \dfrac{\nabla\theta}{|\nabla\theta|}\right] + \kappa^2 \Delta\theta \end{cases}$$

κ, ν, a, $s > 0$ – free energy parameters, m – given function

Macro simulations on data from the experiment

We determined the free energy parameters for aluminium from micro and *ab initio* modelling.

Time scaling parameters are still to be determined.



Conclusions

- choosing the right model is choosing the right scale, variables, parameters, potentials, equations and numerics
- parameters: reality vs numerics
- domain's geometry: domains with thin parts should be studied. The nano structure is obtained in very fine wires.