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Phase field modelling of microstructure evolution

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Research group: Thermodynamics in materials engineering

Content

- Introduction on the phase field method
- Phase field simulations of grain growth
  - Zener pinning
  - Thermal grooving
- Outlook

Phase field method

- van der Waals, Cahn-Hilliard (1958), Hohenberg and Halperin (1977)

- Microstructure evolution (started ± 20 years ago)
  - Solidification
  - Ordering reactions
  - Martensitic transformation

- Nowadays
  - Wide range of applicabilities
  - Quantitative aspects
    - Parameter determination
    - Numerical implementation

Role of microstructures in materials science

Chemical composition, temperature, pressure
+
Cooling rate, history

↓

Microstructure
Shape, size and orientation of the grains, mutual distribution of the phases

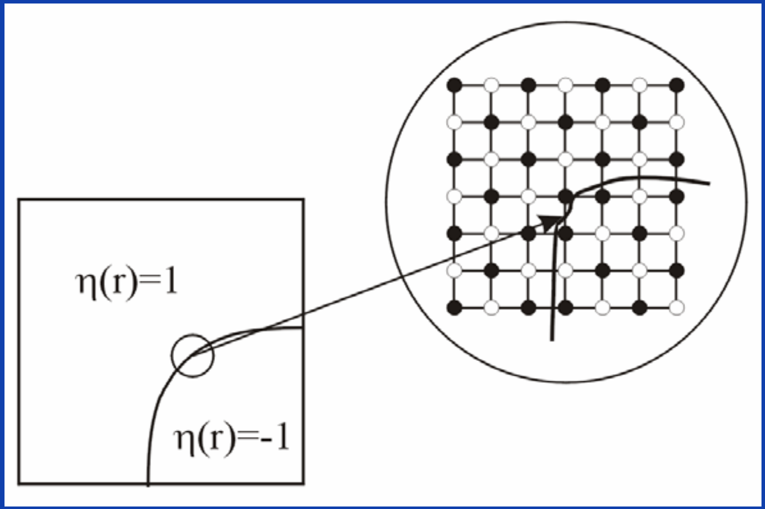
↓

Material properties

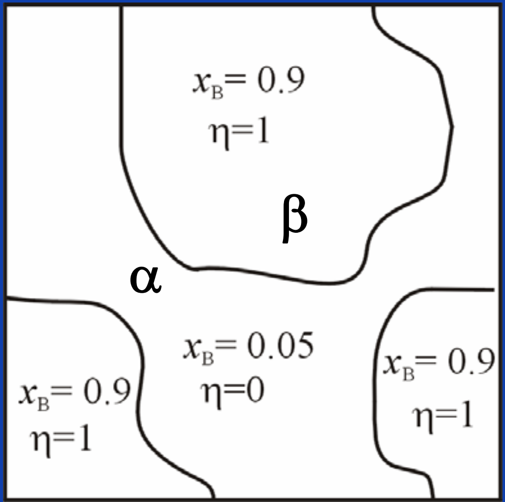
Strength, deformability, hardness, toughness, fatigue…

Representation of microstructures in the phase-field method

- **Field variables: continuous functions in space and time**
  - **Local composition** $x_B(\vec{r},t)$
  - **Local structure and orientation** $\eta_k(\vec{r},t)$



Anti-phase boundary



Binary alloy A-B

- ***Phase α: $\eta = 0$***
- ***Phase β: $\eta = 1$***

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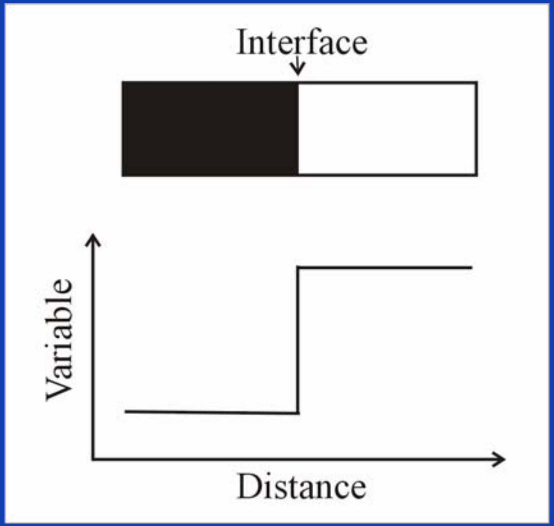
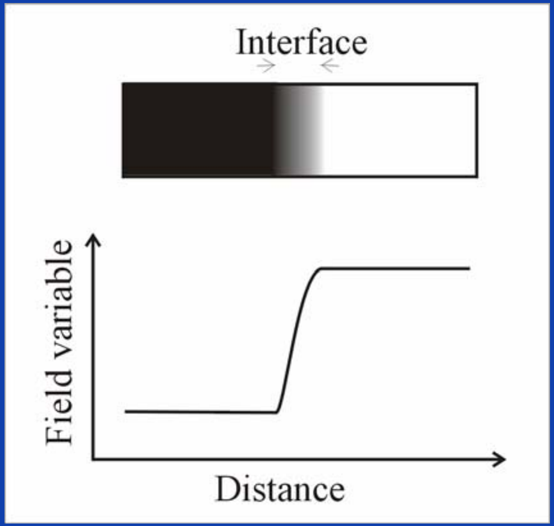
Diffuse-interface description

- **Sharp interface**



- Discontinuous variation in properties
- Requires tracking of the interfaces
- Simplified grain morphologies

- **Diffuse interface**



- Continuous variation in properties
- Interfaces implicitly given by local variations in field variables
- Complex grain morphologies

Thermodynamics and kinetics

- **Total free energy**

$$F = F_{bulk} + F_{surface} = \int_V f_0(x_i, \eta_k, T) + \frac{\kappa}{2}\sum_{k=1}^{p}(\nabla \eta_k)^2 + \frac{\varepsilon}{2}\sum_{i=1}^{C}(\nabla x_i)^2 dV$$

- **Evolution of field variables**
  - **Non-conserved field variables**

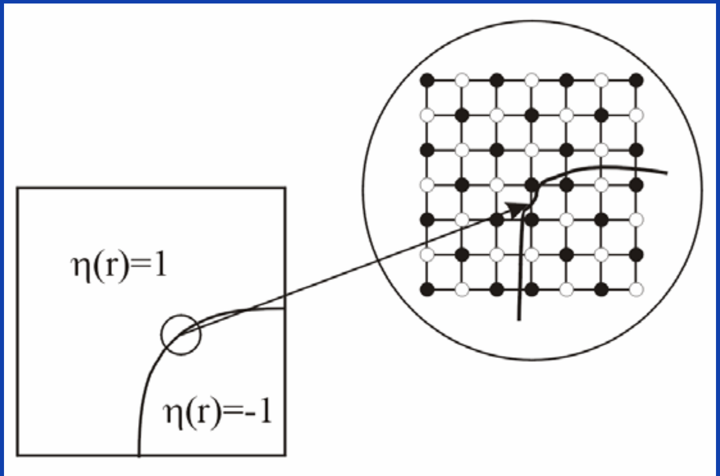
$$\frac{\partial \eta_k(\vec{r},t)}{\partial t} = -L \frac{\partial F(x_1,\ldots,x_C,\eta_1,\ldots,\eta_p)}{\partial \eta_k(\vec{r},t)} (+\xi(\vec{r},t))$$

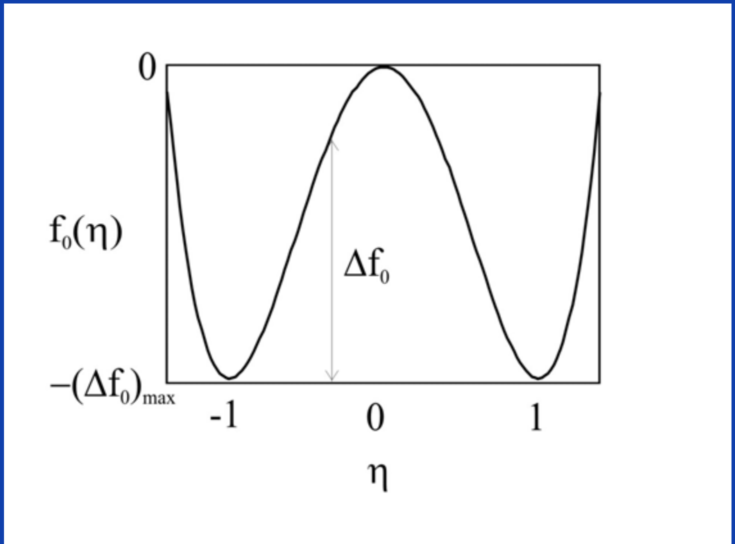
  - **Composition fields**

$$\frac{1}{V_m}\frac{\partial x_i(\vec{r},t)}{\partial t} = \vec{\nabla} M \cdot \vec{\nabla} \frac{\partial F(x_1,\ldots,x_C,\eta_1,\ldots,\eta_p)}{\partial x_i(\vec{r},t)} (+\xi(\vec{r},t))$$

Homogeneous free energy functional

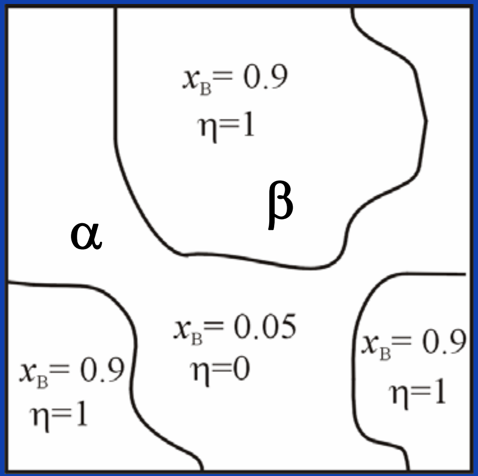
- **Anti-phase boundary**

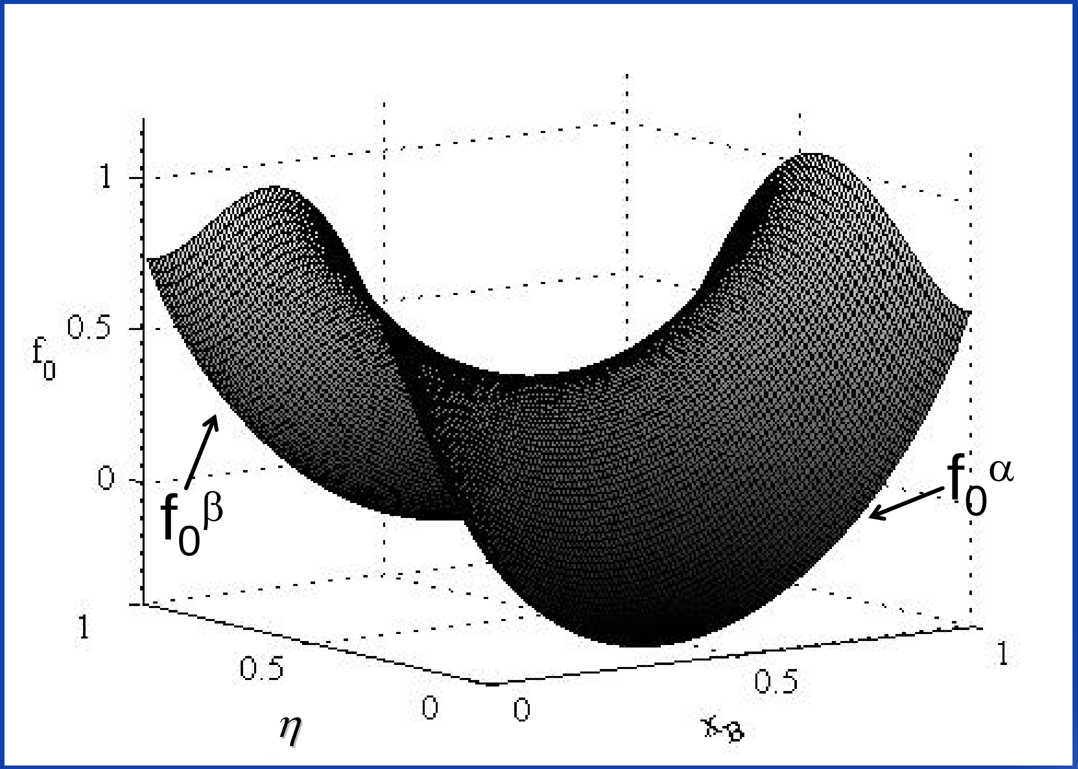




Homogeneous free energy

- **Two phase system**





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Major strengths of the phase-field technique

- **Complex morphologies + concurrent processes**

  - **Continuous field representation** $x_B(\vec{r},t)$, $\eta(\vec{r},t)$
  - **Several contributions to thermodynamic driving force**

$$F = F_{bulk} + F_{surface} + F_{elast} + F_{magn} + \ldots$$

  - **Kinetics**
    - **Mass diffusion**
    - **Heat diffusion (conduction)**
    - **Convection**

Quantitative aspects

- Parameter determination
  - Thermodynamic phase stabilities
  - Interfacial energy and mobility
  - Elastic energy
  - Orientation dependence
  - Solute diffusion

- Numerical solution of a set of coupled partial differential equations

- Width of the interface

Phase field simulations of microstructural evolution

Experiments, atomistic simulations and thermodynamic models

Crystal structure, phase stabilities, interfacial properties (energy, mobility, structure,anisotropy), diffusion properties

↓

Phase field simulations

Morphological evolution of the grains at the mesoscale during solidification, precipitation, solid-state phase transformations, grain growth,…

↓

Models that predict macroscopic material properties

Strength, deformability, hardness, toughness, fatigue…

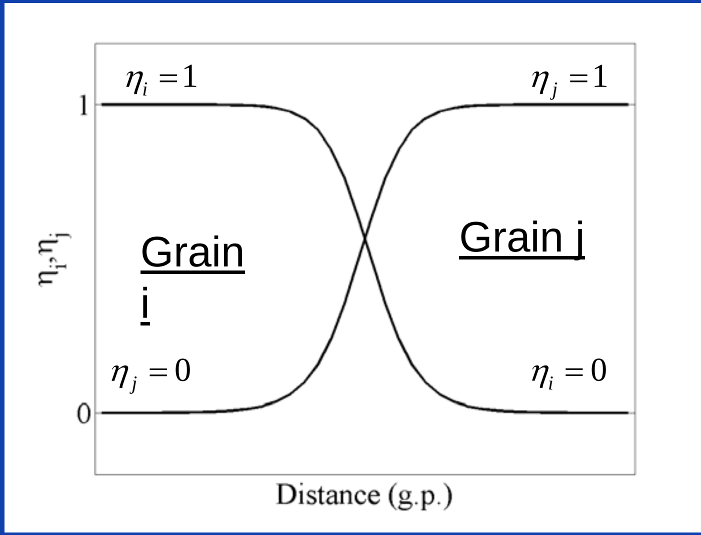
Phase field simulations of grain growth

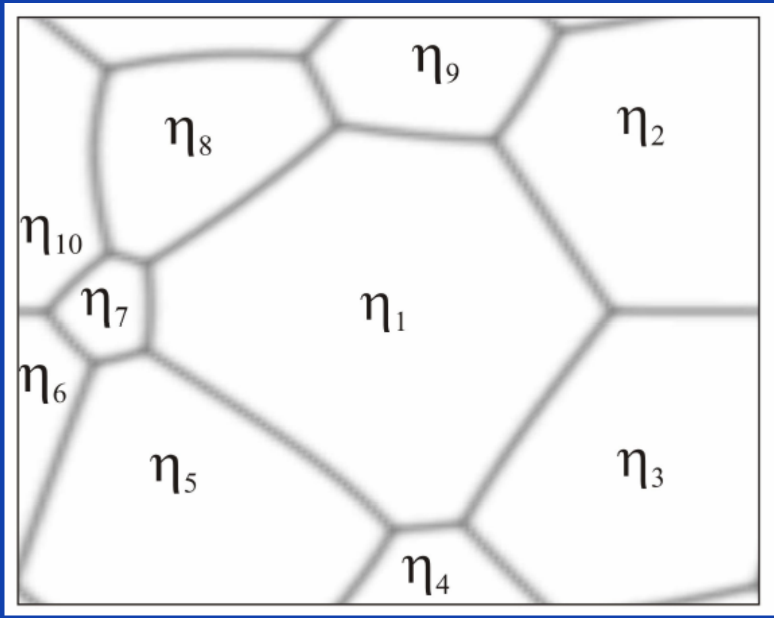
- **Polycrystalline microstructure (L.Q. Chen 1994):**

$$\eta_1, \eta_2, \ldots, \eta_i(\vec{r}, t), \ldots, \eta_p$$

- **Grain i of matrix-phase**

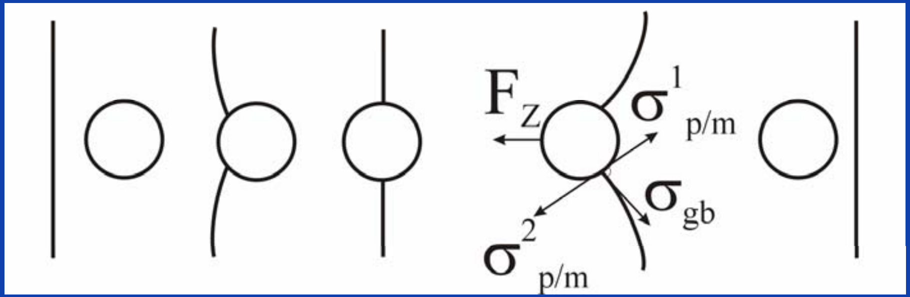
$$(\eta_1, \eta_2, \ldots, \eta_i, \ldots, \eta_p) = (0, 0, \ldots, 1, \ldots, 0)$$





Zener pinning

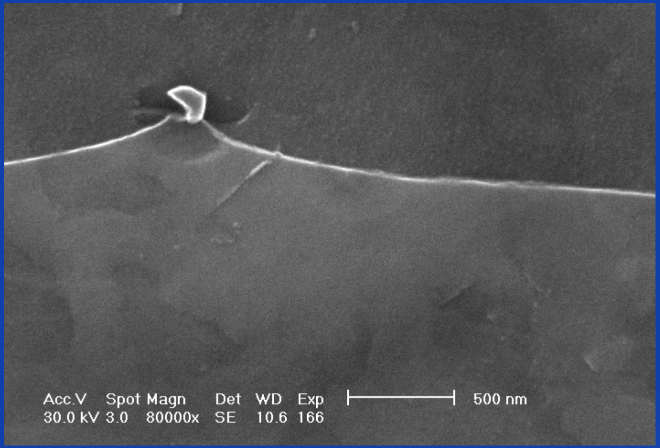
- Mechanism for controlling grain size
  - E.g. *NbC, AlN, TiN,... in HSLA-steels*



- Zener relation for limiting grain size

$$\frac{\overline{R}_{\lim}}{\overline{r}} = K \frac{1}{f_V^b}$$

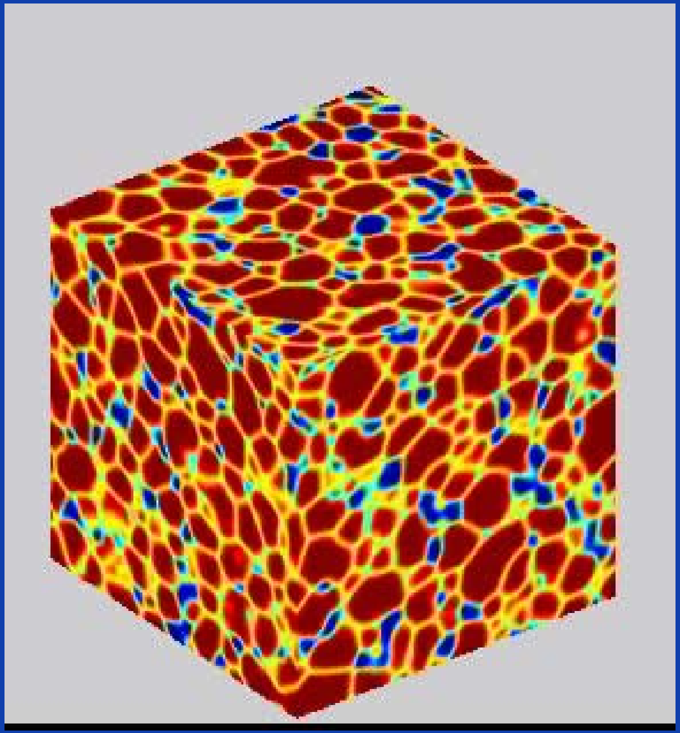
- Influence of
  - Shape of the particle
  - Interfacial properties of particles
  - Particle-grain boundary correlation
  - Initial distribution
  - Evolution particles



MnS precipitate in low-C steel

Zener pinning

- **3D phase field simulation**



Grain orientations: $\eta_1, \eta_2, ..., \eta_i(\vec{r}, t), ..., \eta_p$

Particles: $\eta_i = 0, \forall i$

Conserved variable: $\phi(\vec{r}, t)$

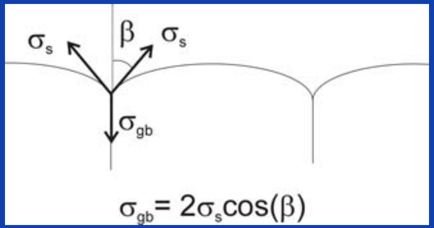
$\Rightarrow$ Grain size distribution

$\Rightarrow$ Limiting grain size

$\Rightarrow$ Number of particles on grain boundary

Thermal grooving

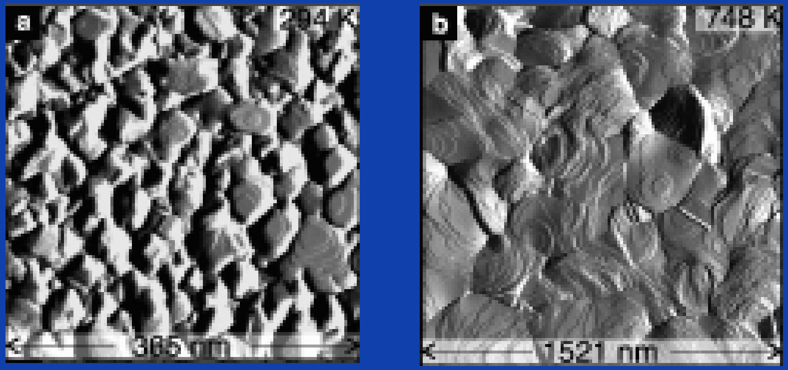
- Surface tension



- Formation mechanism
  - Bulk diffusion, surface diffusion, evaporation/condensation
  - Groove shape

- Drag effect on grain growth in thin films

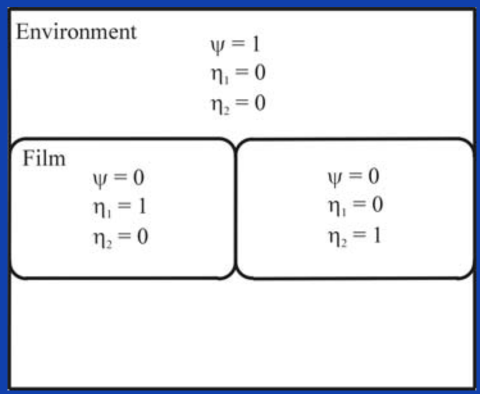
- Abnormal grain growth induced by orientation dependence of surface energy
  => huge grain size

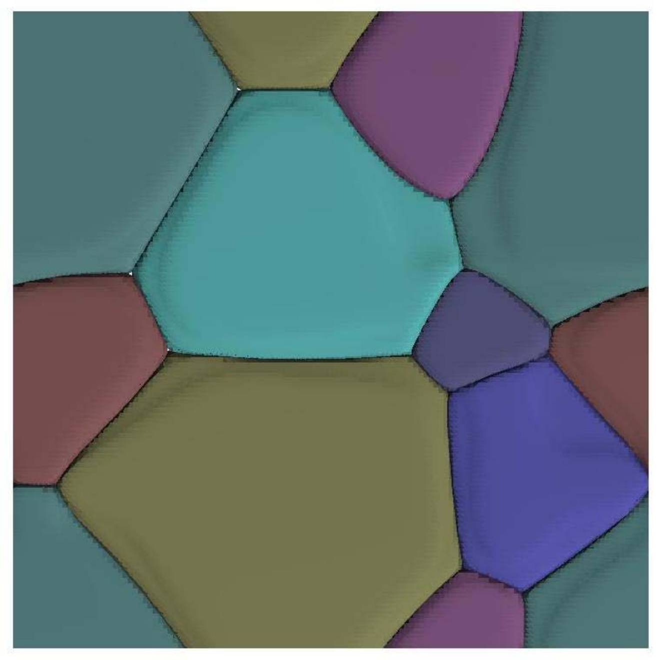


In-stiu STM image for a gold film (Rost et al. 2003)

Thermal grooving

- **3D phase field simulation of surface grooving**
  - **System geometry**





  - **Model**
    - **Grains** $\eta_1, \eta_2, \ldots, \eta_i(\vec{r}, t), \ldots, \eta_p$
    - **Conserved variable** $\psi(\vec{r}, t)$
  - **Application**
    - **Onset of abnormal grain growth**

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Outlook

- Quantitative simulations for multi-component and multi-phase materials
  - Model refinement
    - Easy coupling with thermodynamic databases
    - Individual parameters for interfacial energy
  - Physical characteristics

- Extension of the grain growth model
  - Stability of the particles
  - Surface properties of the particles

Outlook

- Phase field simulations for Ag-Cu-Sn
  - Multi-phase/multi-component
  - Elastic energy
  - COST 531, COST MP0602 → input parameters
- Phase field simulations for oxidic systems
  - Ions with multiple valence, e.g. Fe^{2+}/Fe^{3+}
  - Slags, ceramics

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End

- Thank you for your attention!
- More information: *http//nele.studentenweb.org*

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