17th Alemi Meeting

Modelling the kinetics of grain growth – Triple junctions and topology of grain arrangement

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  - Migration of grain boundaries meeting at triple junctions
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Motivation I: Materials at extreme conditions

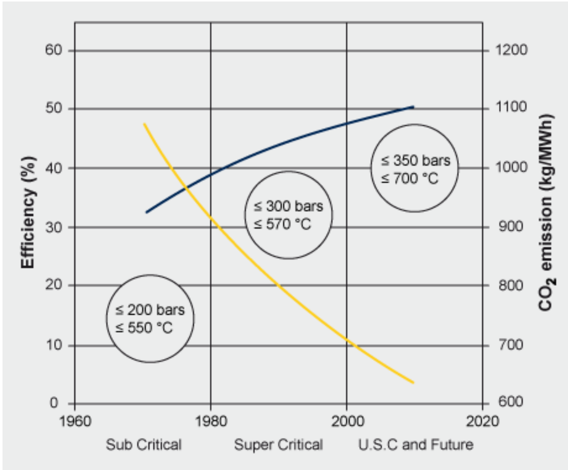
- Line pipe steels

turkstream.info

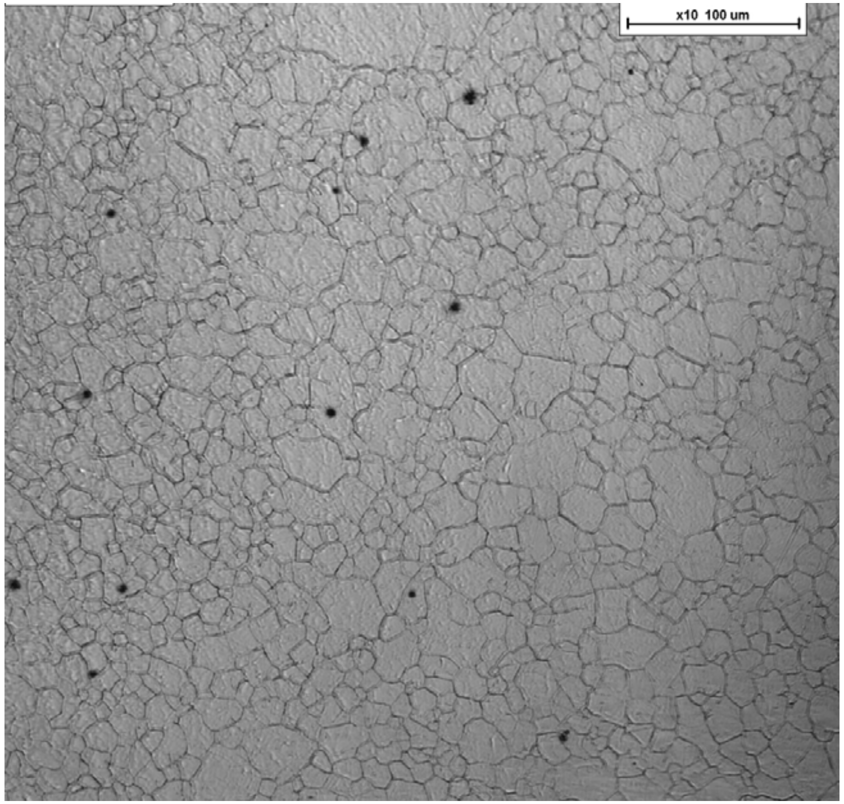
- Large steam turbines

(e.g. high temperature exposed, creep-resistant steels)

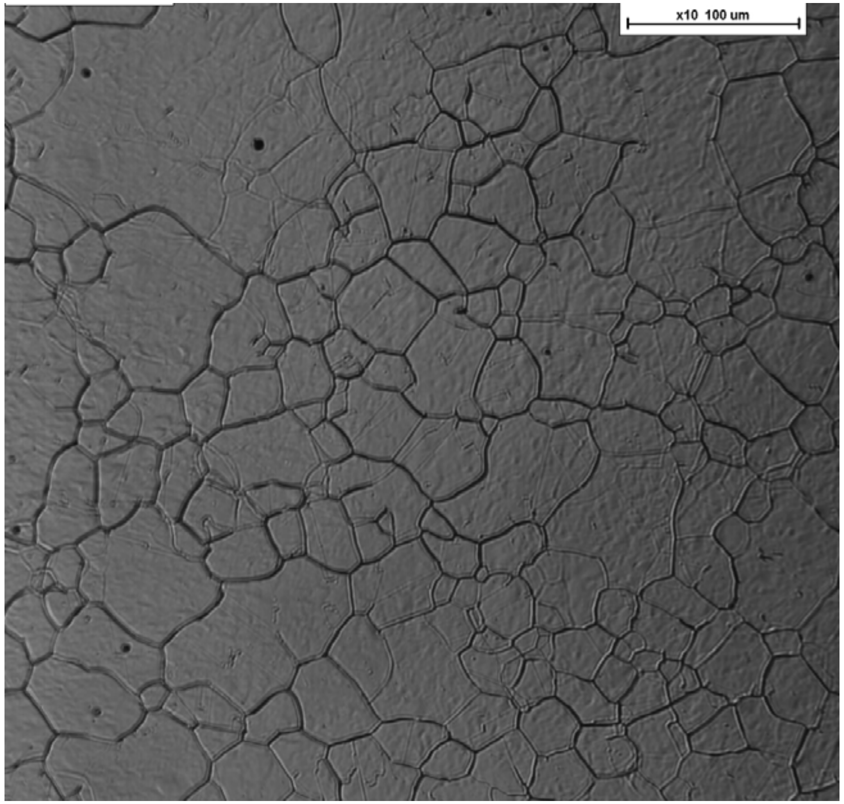
$$\eta_C = 1 - \frac{T_2}{T_1}$$



Motivation II: An example for grain growth



ϑ =1050°C at t = 243s



ϑ =1250°C at t = 183s

Mass fractions·100: w_{C} = 0.06, w_{Mn} = 1.65, w_{Nb} = 0.034, w_{Ti} = 0.012, w_{Mo} = 0.24, w_{N} = 0.005

Grain growth – a brief introduction

Grain growth in single phased materials

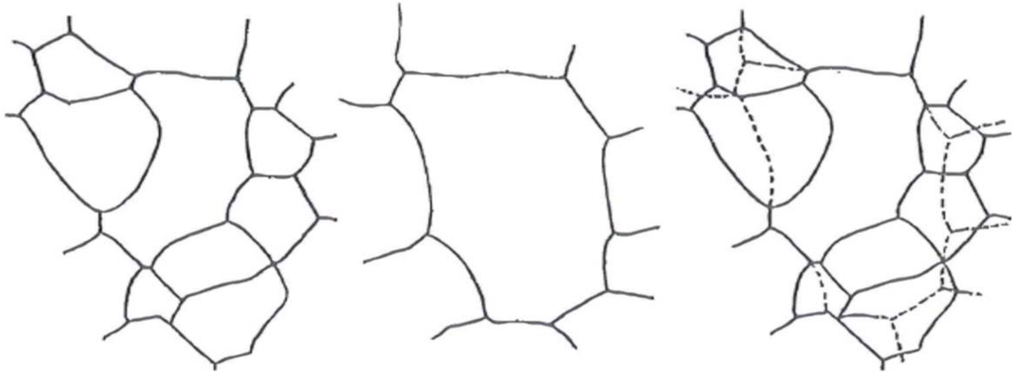
Curved grain boundaries tend to migrate to the center of the curvature.

Driving force: decrease in Gibbs energy due to reduction of grain boundary surface.

See . e.g [M. Hillert: Analytical treatments of normal grain growth: Materials Science Forum Vols 204-206 (1996) pp. 3-18.]

$$\mu \propto \gamma / r_{\mathrm{m}}$$

$$r_{\mathrm{m}}^2 - r_0^2 = kt$$



- Relation of curvature κ to mean grain size r_{m} ⇒ Steady state distribution
  (no topological information)
- Calculating migration of grain boundaries connected by triple junctions

Theory I: Gibbs energy and constraints

Gibbs energy G_i of grain boundary i per unit length L of the cylinder:

$$G_i = \int \gamma_i ds_i$$

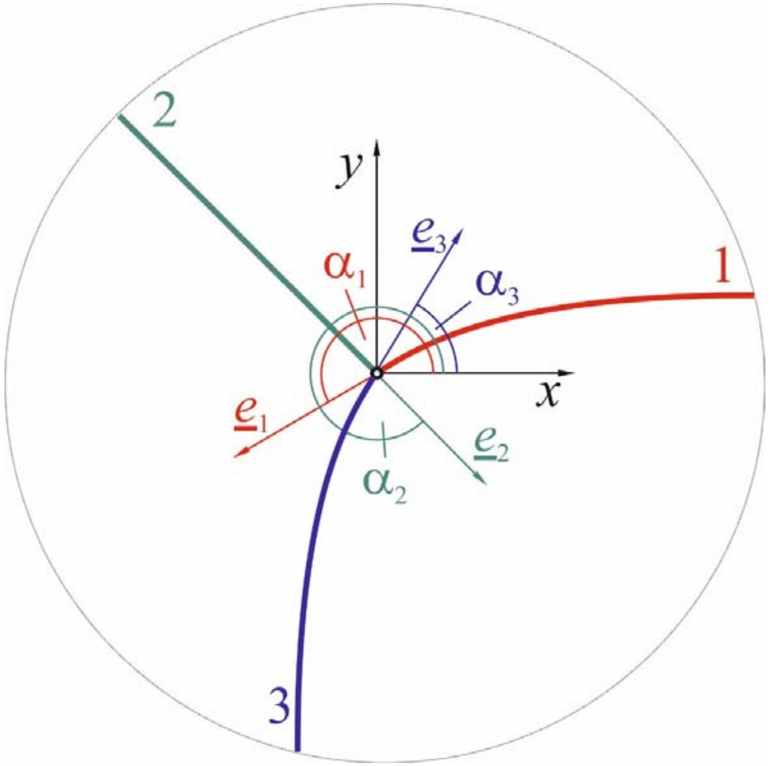
γ_i…specific grain boundary energy

Compatibility at triple junction

$$v_i^{\mathrm{n}} = \underline{v}_{\mathrm{T}} \cdot \underline{n}_i$$

Rate of change of length v_i^{t} of grain boundary i

$$v_i^{\mathrm{t}} = \underline{v}_{\mathrm{T}} \cdot \underline{e}_i$$



From: F. D. Fischer, J. Svoboda, K. Hackl: “Modelling the kinetics of a triple junction“, Acta Mater. 60 (2012) 4704-4711

Theory II : Rate of Gibbs energy and dissipation

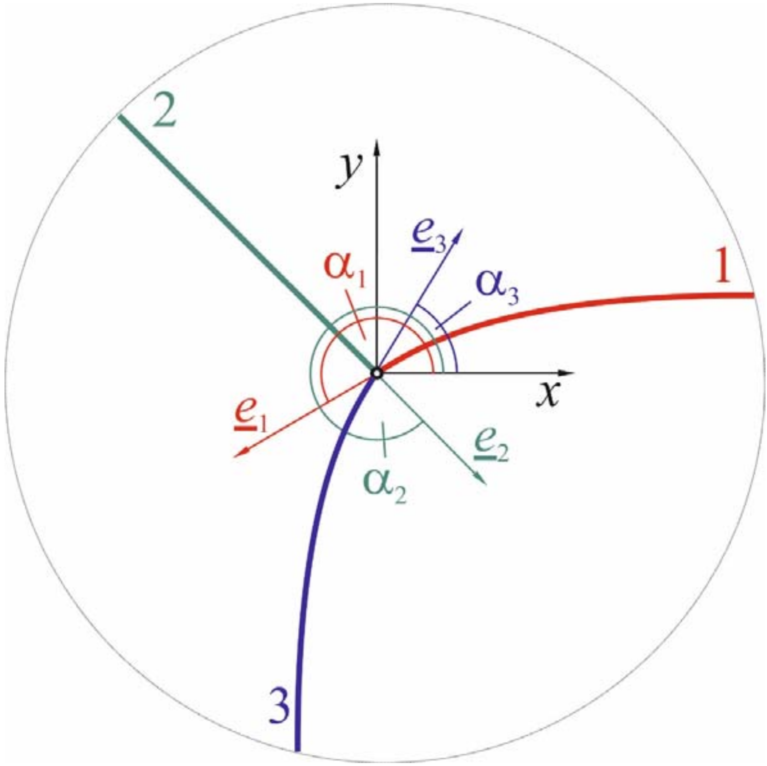
Rate of Gibbs energy $\dot{G}_i$ of grain boundary i

$$\dot{G}_i = \int_{S_i} \gamma_i \kappa_i(s_i) v_i^{\mathrm{n}}(s_i) ds_i + \gamma_i \underline{v}_{\mathrm{T}} \cdot \underline{e}_i$$

$$\dot{G} = \sum_{i=1}^{3} \dot{G}_i$$

Dissipation Q

$$Q = \sum_{i=1}^{3} \left(\int_{S_i} \frac{(v_i^{\mathrm{n}}(s_i))^2}{m_i} ds_i + \frac{v_{\mathrm{T}}^2}{m_{\mathrm{T}}} \right)$$



From: F. D. Fischer, J. Svoboda, K. Hackl: “Modelling the kinetics of a triple junction“, Acta Mater. 60 (2012) 4704-4711

Theory III

Lagrangian for the system

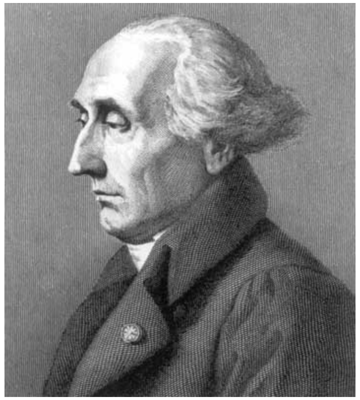
$$L = Q + \lambda(\dot{G} + Q) + \sum_{i=1}^{3} \beta_i [v_i^n - \underline{v}_T \cdot \underline{n}_i]$$

Variation or derivation with respect to the kinetic parameters $v_i^{\mathrm{n}}(s_i)$, v_i^{n}, $\underline{v}_{\mathrm{T}}$ yields the **evolution equations**:

$$v_i^n(s_i) = -m_T \gamma_i \kappa_i (s_i)$$

$$\underline{v}_T = -m_T \sum_{i=1}^{3} \gamma_i \underline{e}_i$$

$$v_i^n = -m_i \gamma_i \kappa_i$$



Joseph-Louis Lagrange

wikipedia.org

From: F. D. Fischer, J. Svoboda, K. Hackl: “Modelling the kinetics of a triple junction“, Acta Mater. 60 (2012) 4704-4711

HT-LSCM

High temperature laser scanning confocal microscopy

FERROUS METALLURGY
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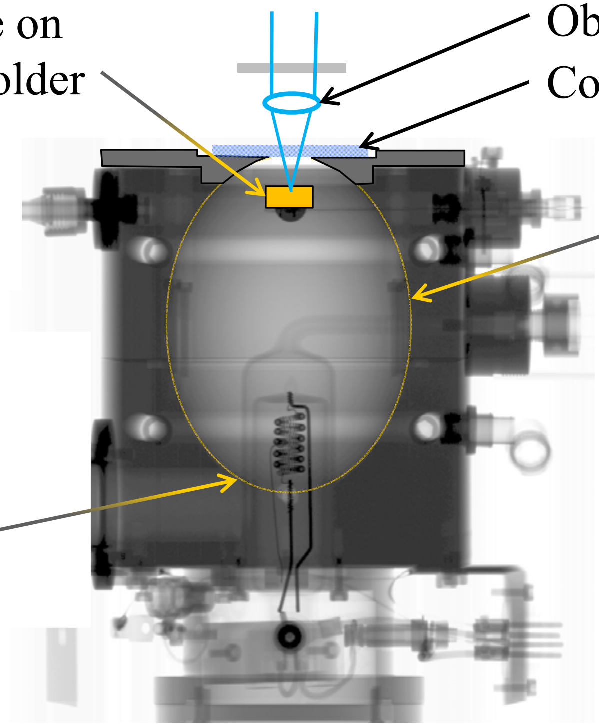
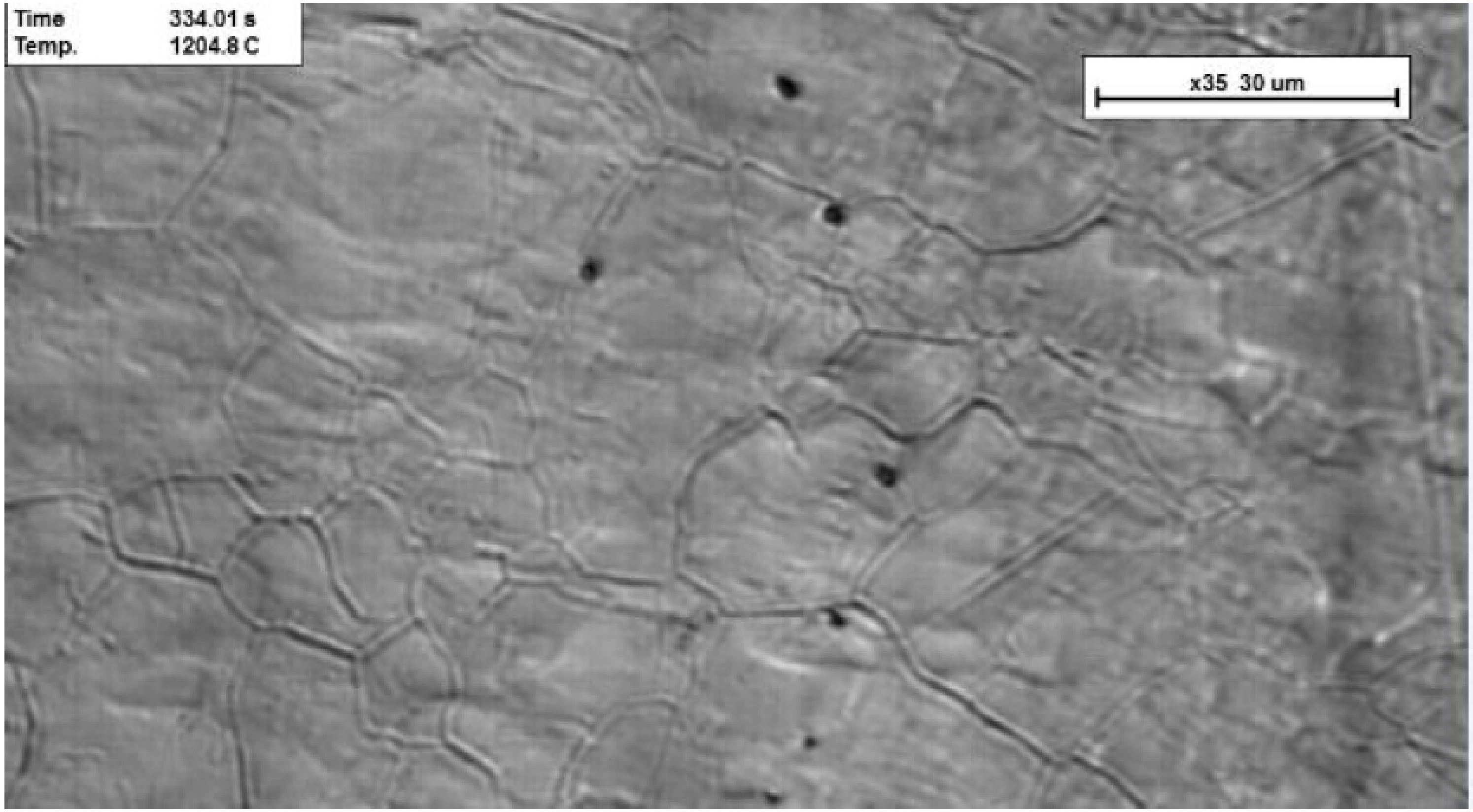


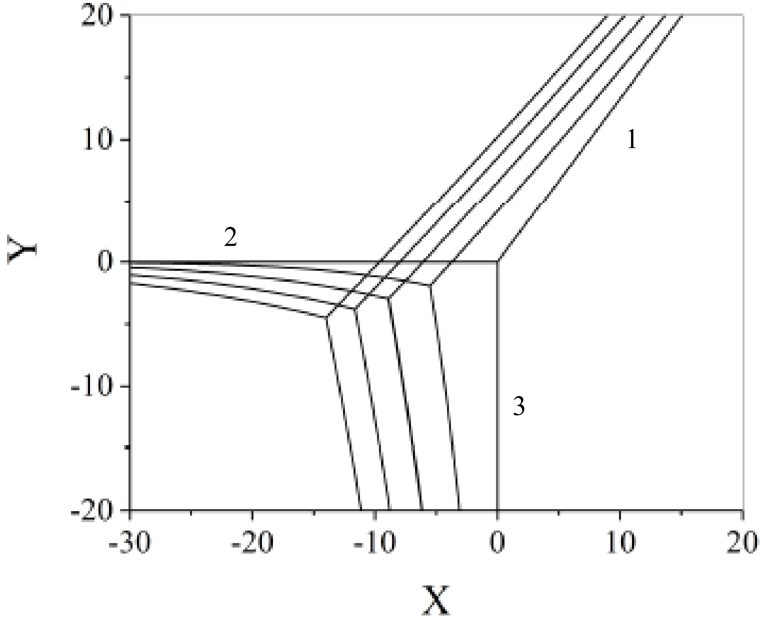
Temperatures up to 1650°C,
heating rates up to 50 K/s,
15 frames per second ⇒ dynamic processes.

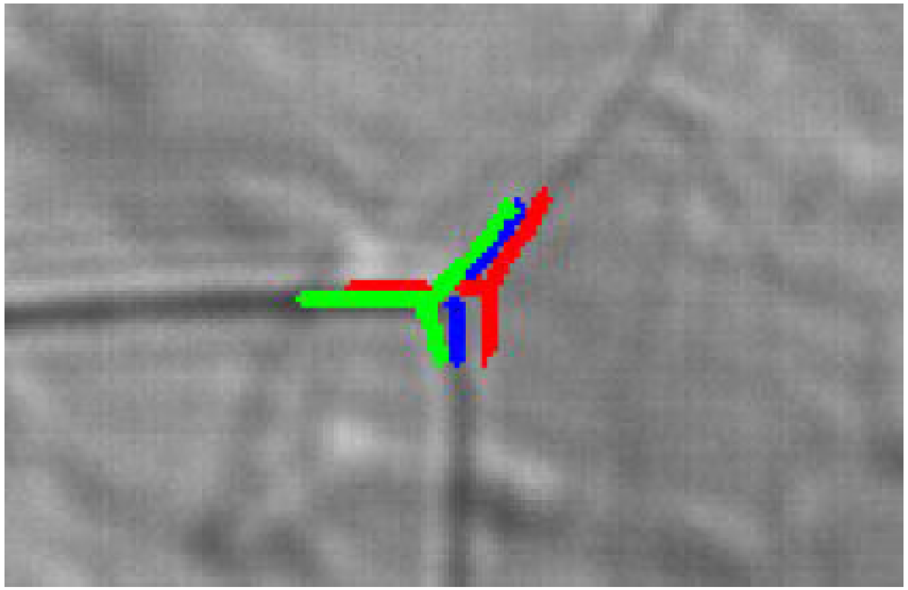
Radiographie Jördis Rosc/ÖGI

Austenite grain boundaries revealed by HT-LSCM



Motion of regions close to triple junctions I

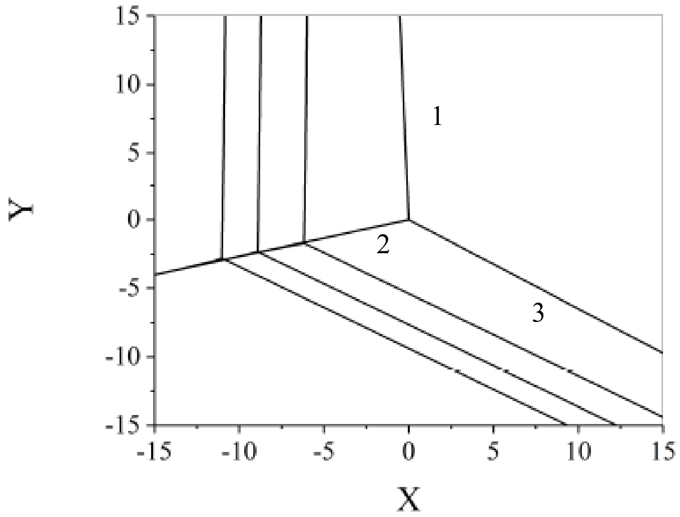


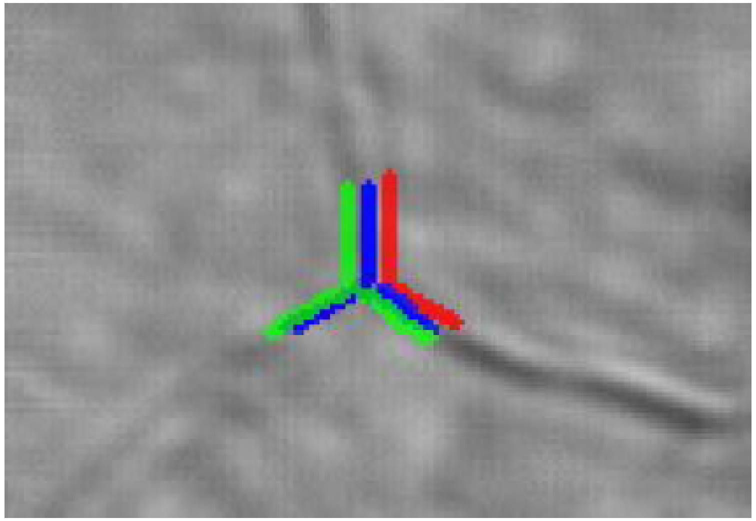


Temperature ϑ = **1204.8°C**, duration of the motion **8s**.

Best result: $\overline{M}_1 = 2, \ \overline{M}_2 = 0.267, \ \overline{M}_3 = 2.67, \ \overline{M}_t = 0.06$

Motion of regions close to triple junctions II

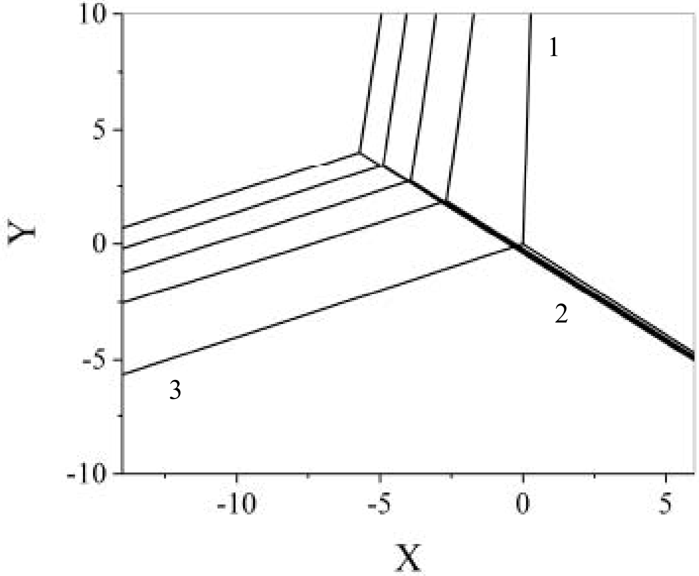


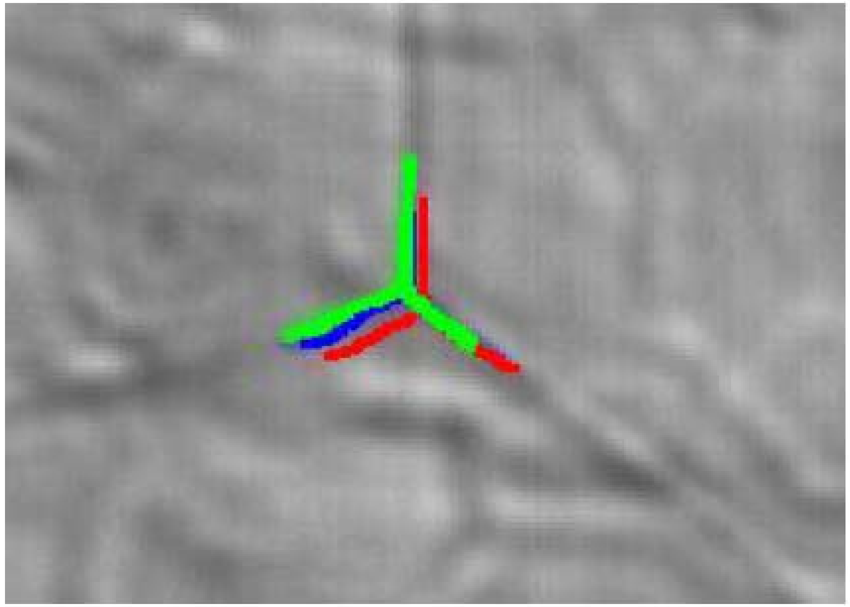


Temperature ϑ **= 1204.8°C**, duration of the motion **8s**.

Best result: $\overline{M}_1 = 0.33,\ \overline{M}_2 = 0.000067,\ \overline{M}_3 = 0.267,\ \overline{M}_t = 0.033$

Motion of regions close to triple junctions III





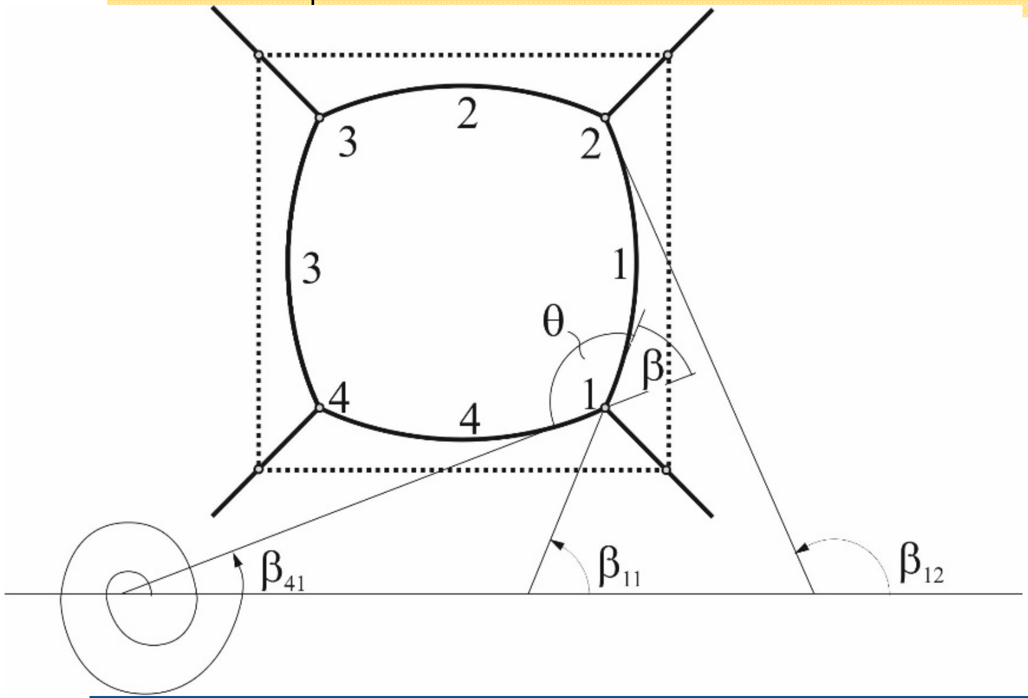
Temperature ϑ = **1204.8°C**, duration of the motion **8s**.

Best result: $\overline{M}_1 = 3,\ \overline{M}_2 = 0.3,\ \overline{M}_3 = 3,\ \overline{M}_t = 0.06$

Theory IV

Rate of area change $\dot{A}$

$$\dot{A} = m_{\mathrm{gb}}\gamma\left[(\beta_{11}-\beta_{n1})+(\beta_{22}-\beta_{12})+(\beta_{33}-\beta_{23})+..+(\beta_{nn}-\beta_{(n-1)n})\right]$$



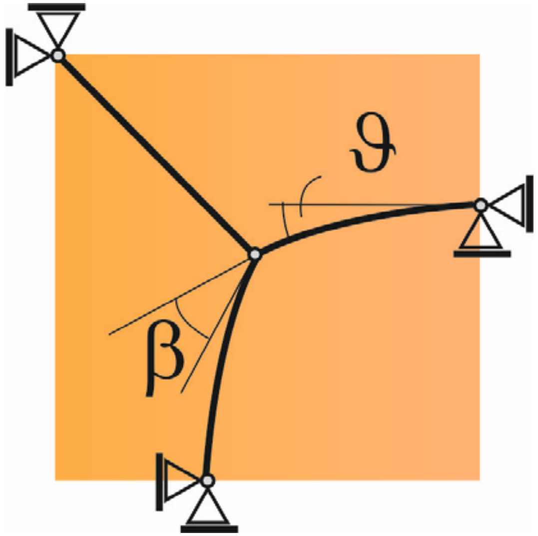
From: W. W. Mullins, Two dimensional motion of idealized grain boundaries, J. Appl. Phys. 27 (1956) 900-904

Comparison of infinite and finite grains

Rate of area change $\dot{A}$ for n-sided polygons

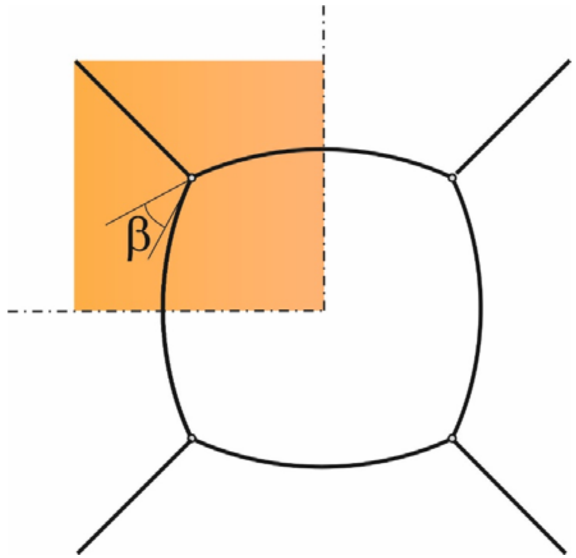
Case I: Infinite grains

$$\dot{A}_1 = m_{gb}\gamma\left[n\beta - (2\pi - n\vartheta)\right]$$



Case II: Finite grains

$$\dot{A}_2 = m_{gb}\gamma(n\beta - 2\pi)$$

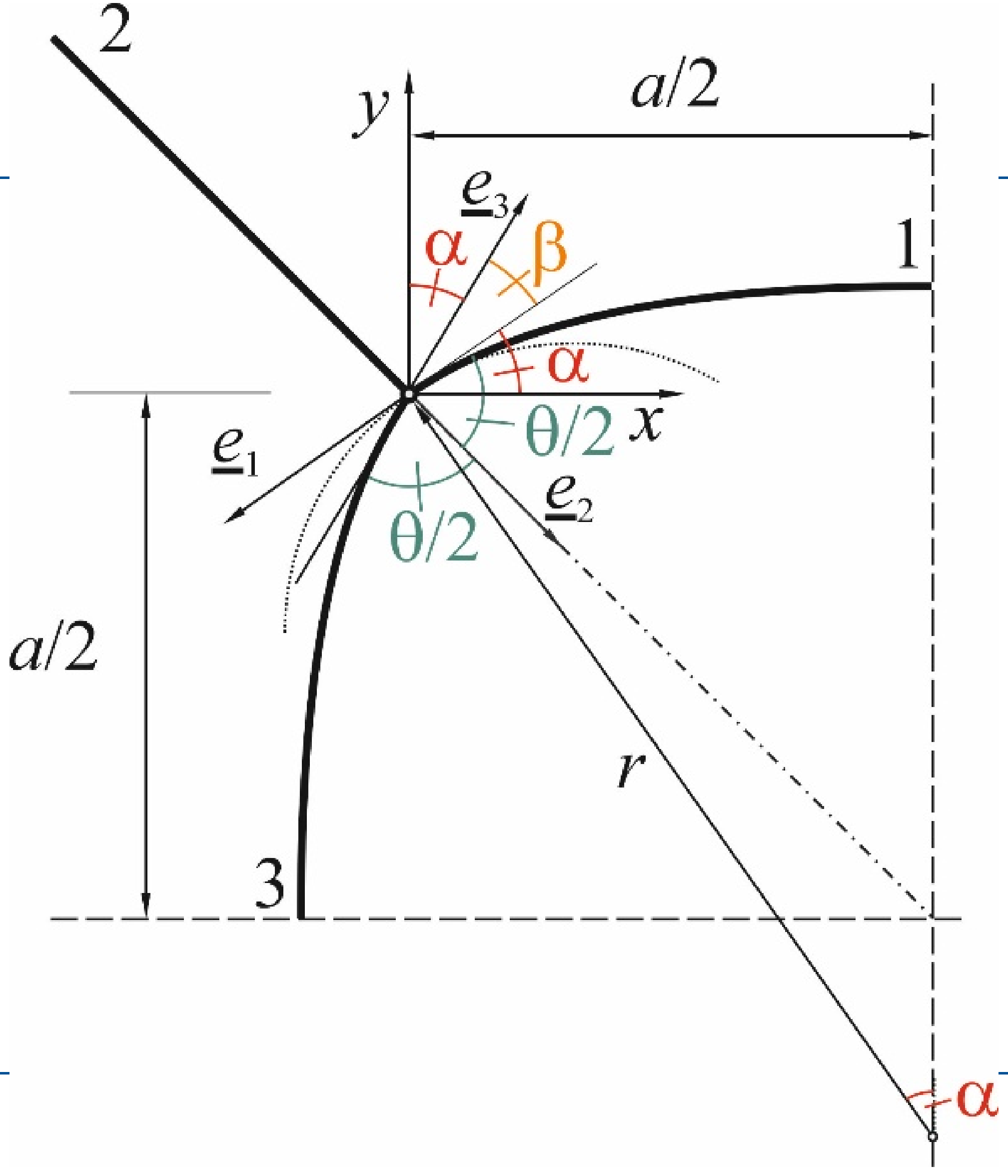


Normalized quantities

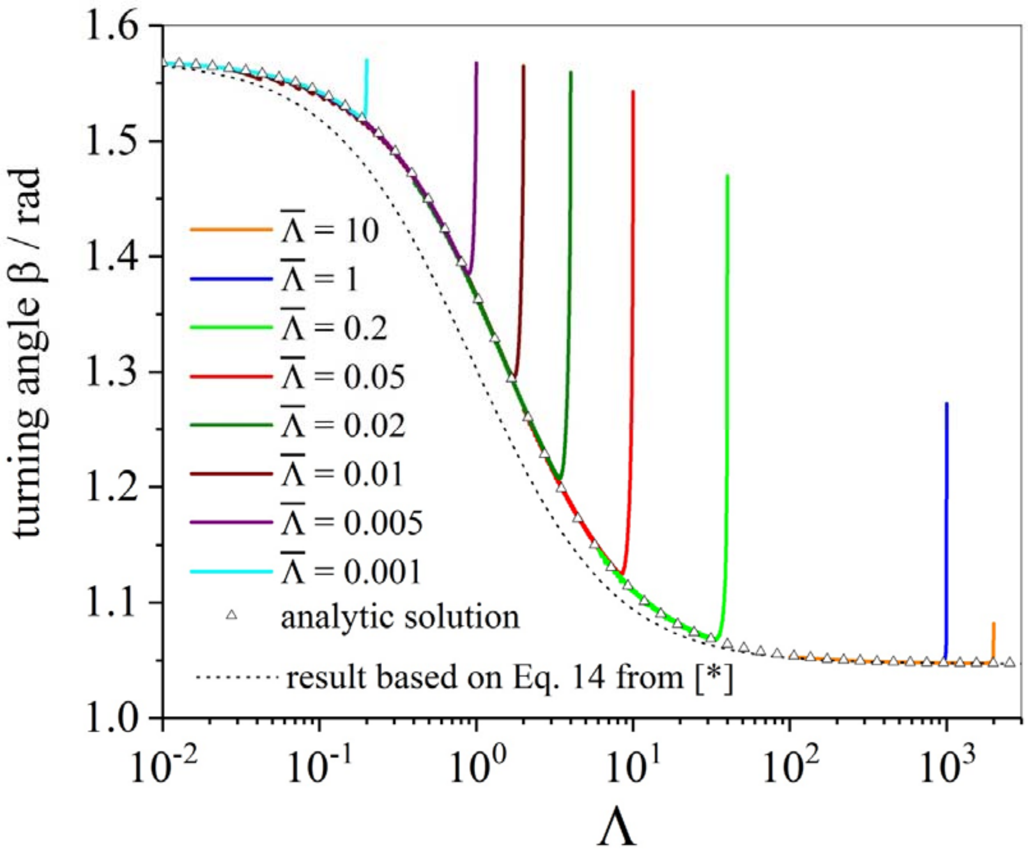
$$\overline{\Lambda} = \frac{\Lambda}{a} a_0 = \frac{m_T}{m_{gb}} a_0$$

$$\Lambda = \frac{m_T a}{m_{gb}}$$

$$\tau = \frac{A_0}{m_{gb} \gamma}$$



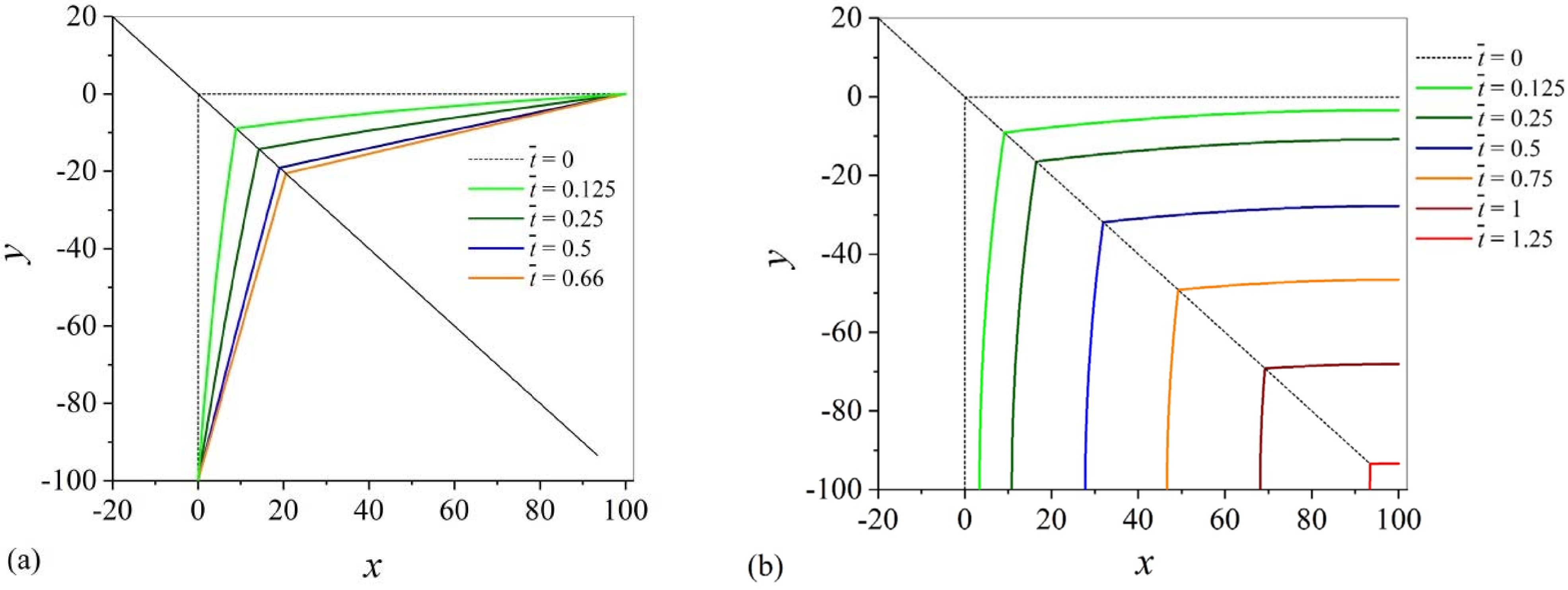
Shrinkage of a quadratic grain I



$$\Lambda = \frac{m_T a}{m_{gb}}$$

[*] L.A. Barrales-Mora, G. Gottstein, L.S. Shvindlerman, Effect of a finite boundary junction mobility on the growth rate of grains in two-dimensional polycrystals, Acta Mater. 60 (2012) 546–555.

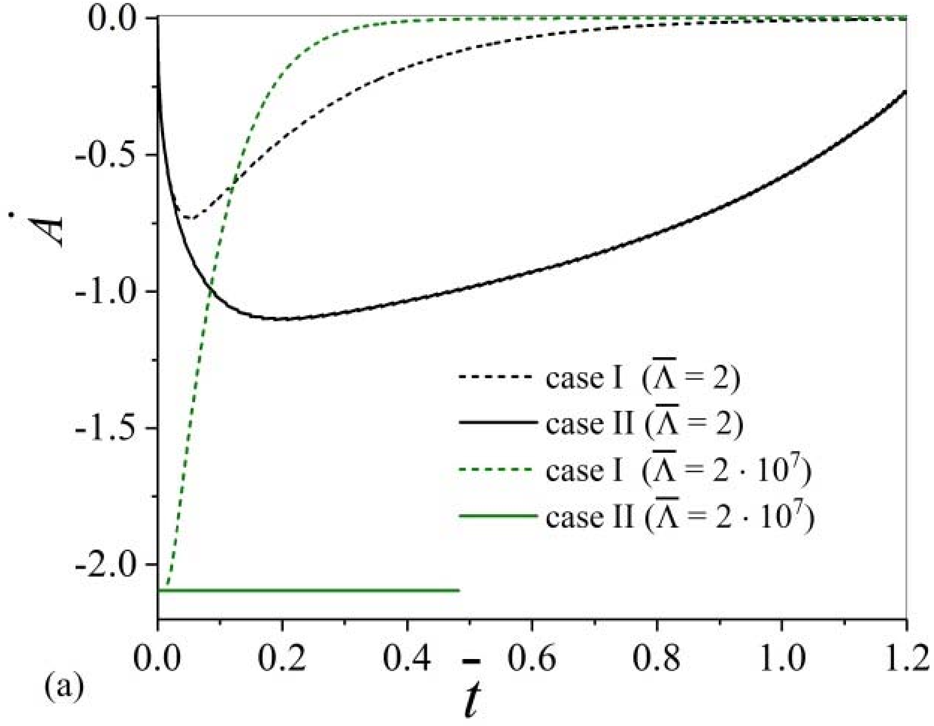
Shrinkage of a quadratic grain II

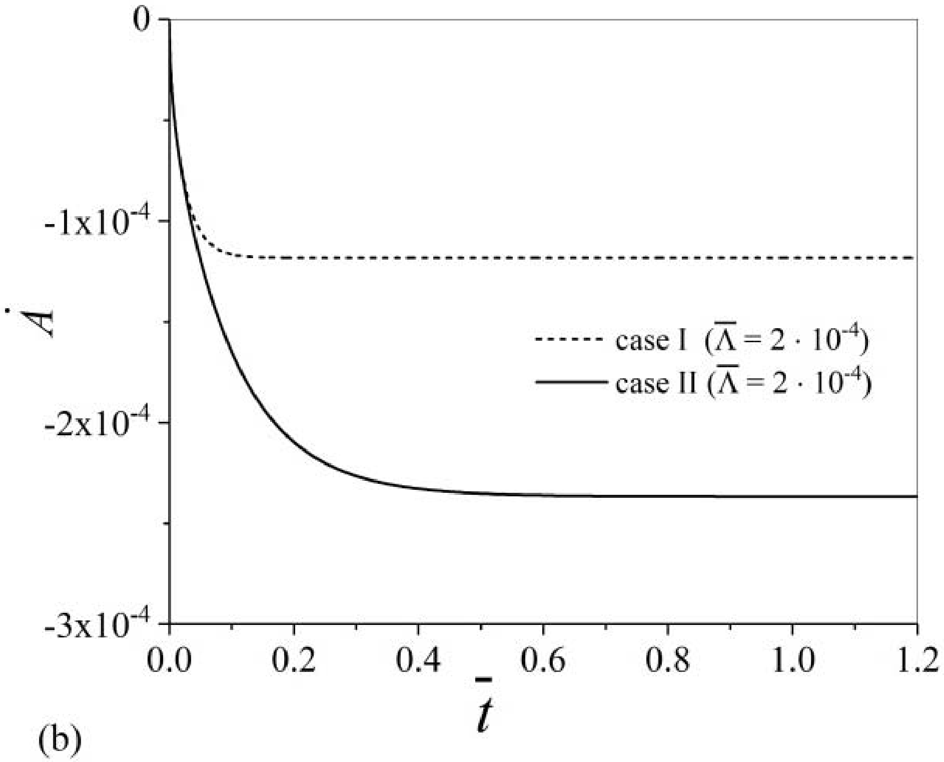


(a) Case I: Infinite grain

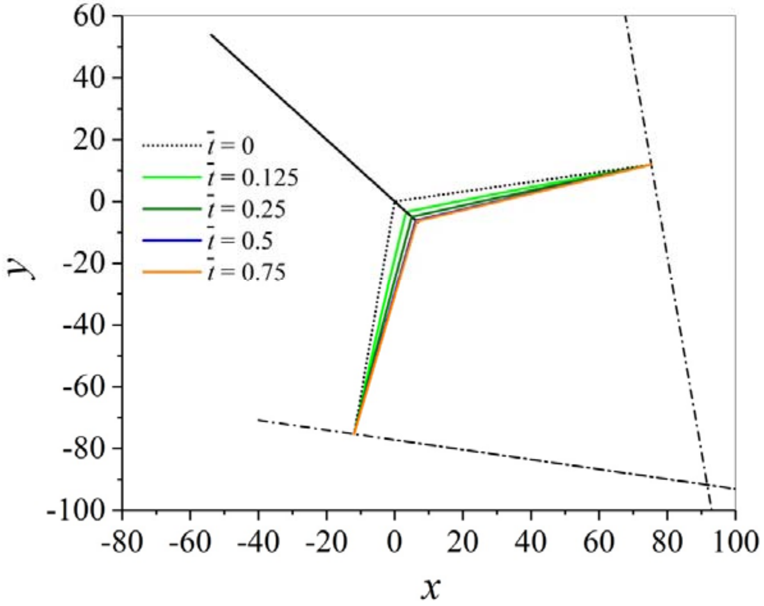
(b) Case II: Finite grain

Shrinkage of a quadratic grain III

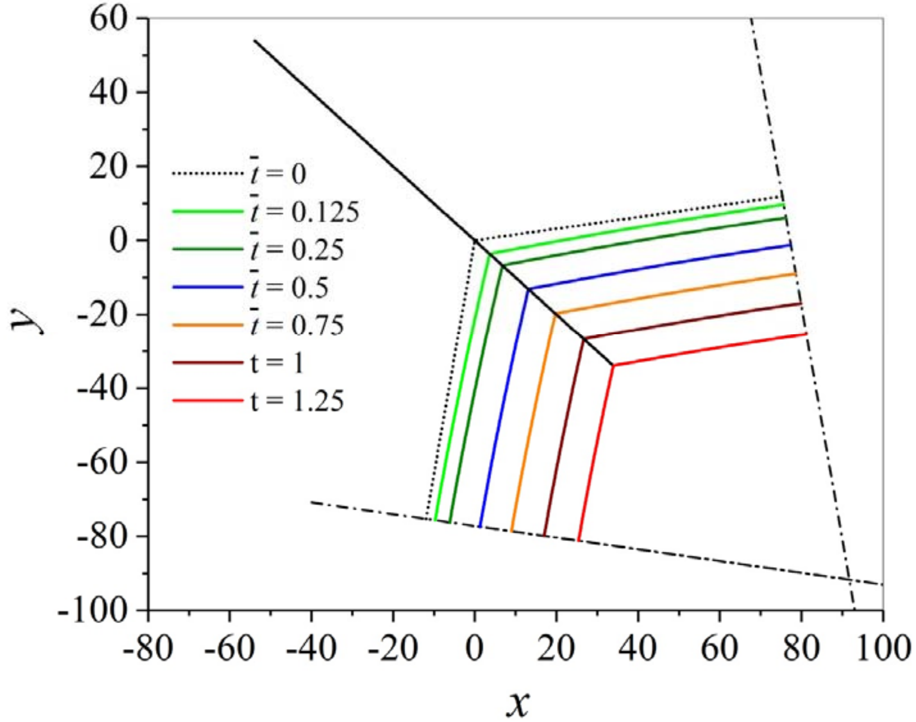




Shrinkage of a pentagon

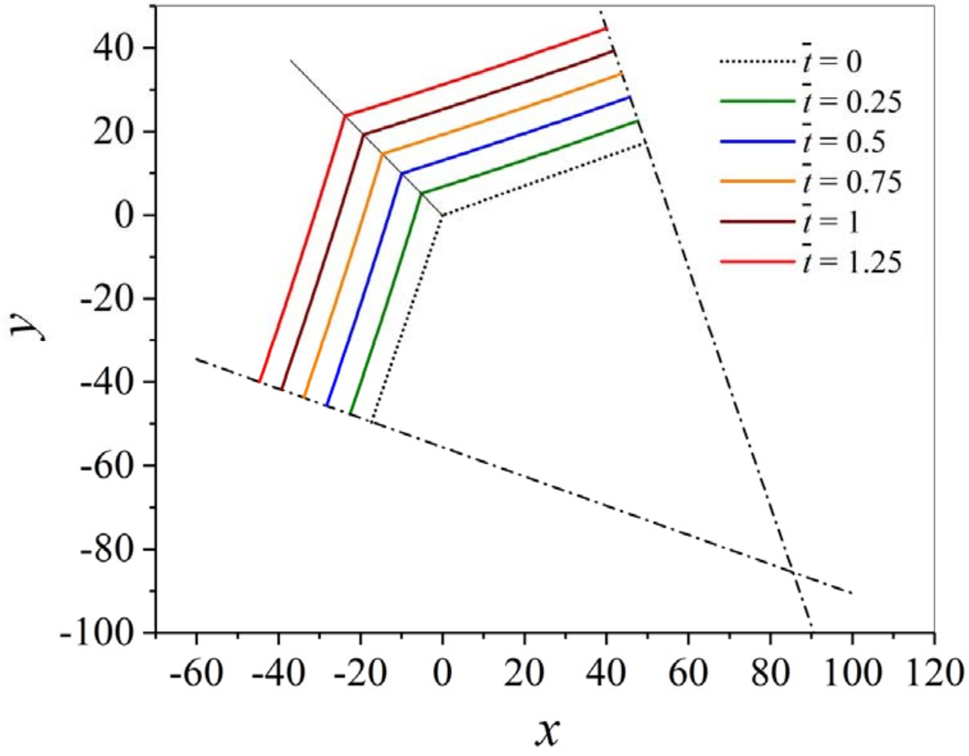


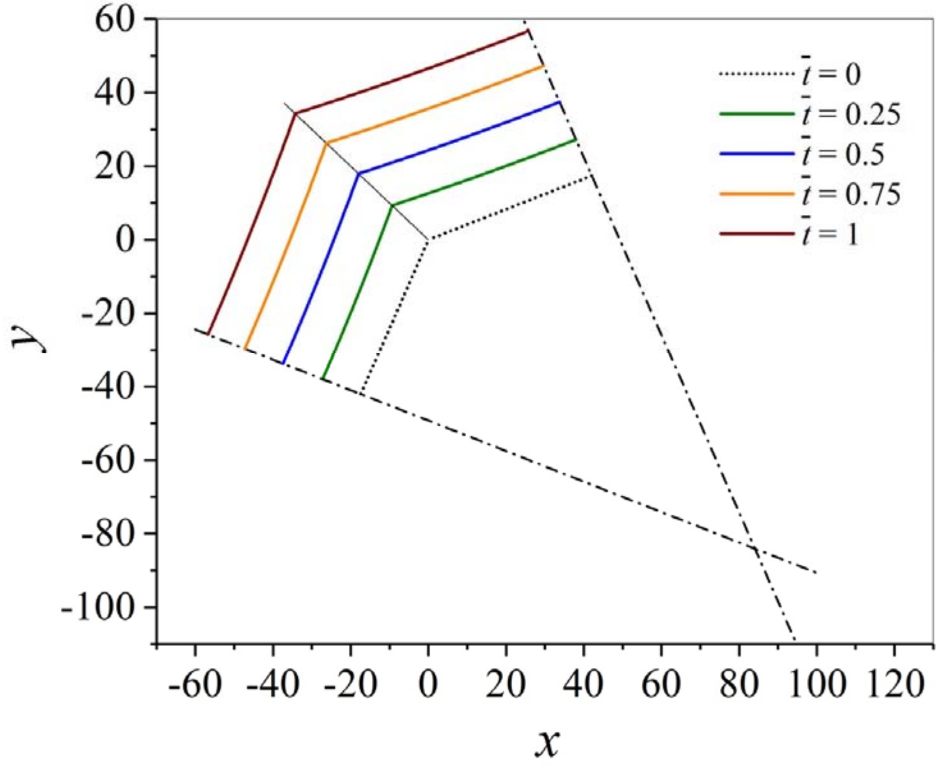
(a) Case I: Infinite grain



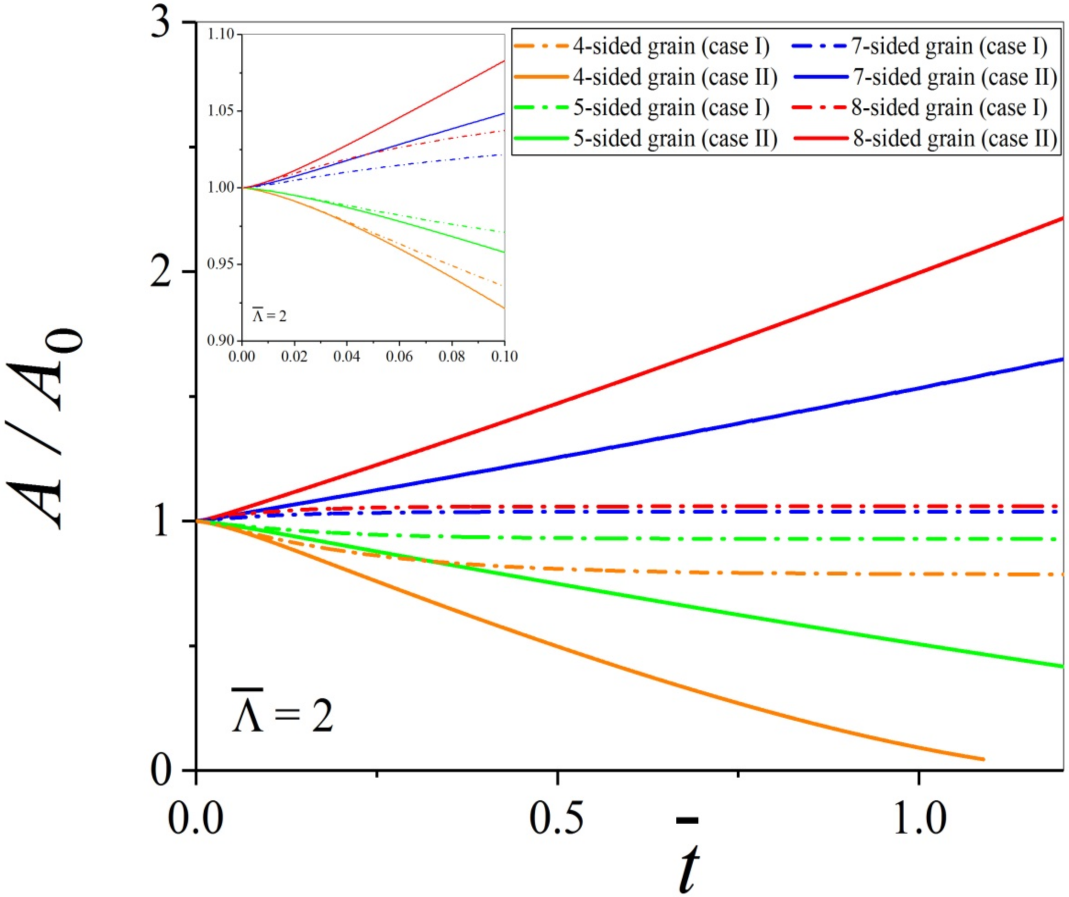
(b) Case II: Finite grain

Growth of a heptagon and an octagon





Growth or shrinkage of n-sided grains



Conclusions and Outlook

- ***2dim-grain growth by motion of triple junctions***
  - Motion of triple junction – comparison to in-situ experiments
  - Influence of the topology
  - Initially quadratic grain
    - Change of the turning angle
    - Dependence on the ratio $\overline{\Lambda}$
  - Growth and shrinkage of n-sided grains

- ***Outlook***
  - Comparison to in-situ micrographs – influence of alloying elements on migrating grain boundaries

Thank you for your attention!