Influence of grain boundary mobility on microstructure evolution during recrystallization

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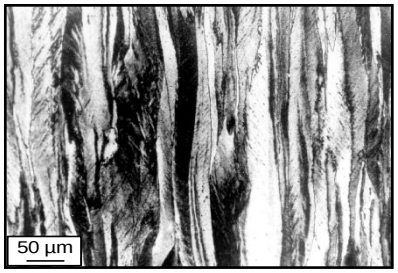
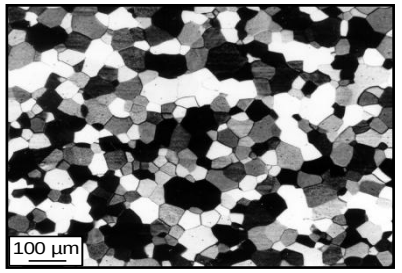
Motivation



deformed



recrystallized

- Recrystallization: change of microstructure as well as of the properties of crystalline materials.
- Experimental evidence for influence of low angle grain boundaries, but they are usually not taken into account.
- Recrystallization models discriminate between three different types of grain boundaries.
- Only few simulations investigated the effect of different grain boundary mobilities on the recrystallization behavior, but without taken into account a non-zero low angle grain boundary mobility.

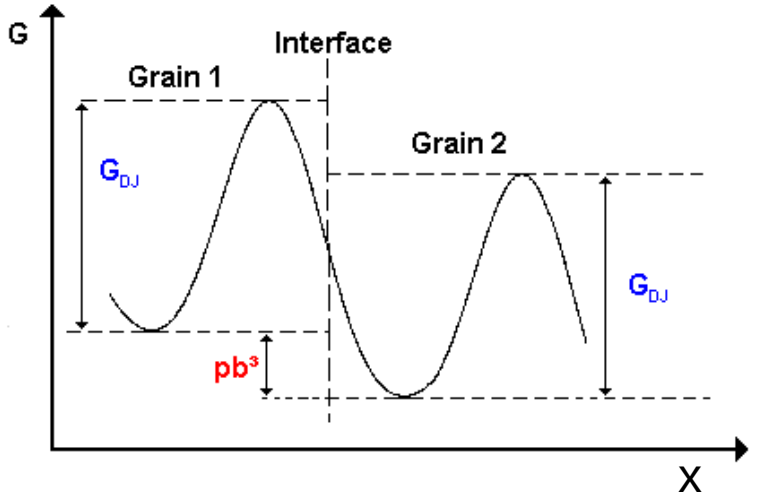
Investigation whether there is any influence of low angle grain boundaries on the microstructure and texture evolution during recrystallization.

- Attribute of each cell: orientation, dislocation density
- State: „recrystallized“ or „non-recrystallized“
- Switching rule: probabilistic formulation of the Turnbull equation

- Turnbull equation:

$$v = mp = m_0 \exp(-Q/kT)p$$

- New formulation with two contributions: $v = v_0 w$



$$\text{Deterministic part: } v_0 = \frac{kTm_0}{b^3}$$

$$\text{Probabilistic part: } w = \frac{pb^3}{kT} \cdot \exp\left(-\frac{Q}{kT}\right)$$

Model – the features

– simulation box 100x100x100 cells with 1x1x1µm^3 cell size

– Al single crystal with Cube orientation

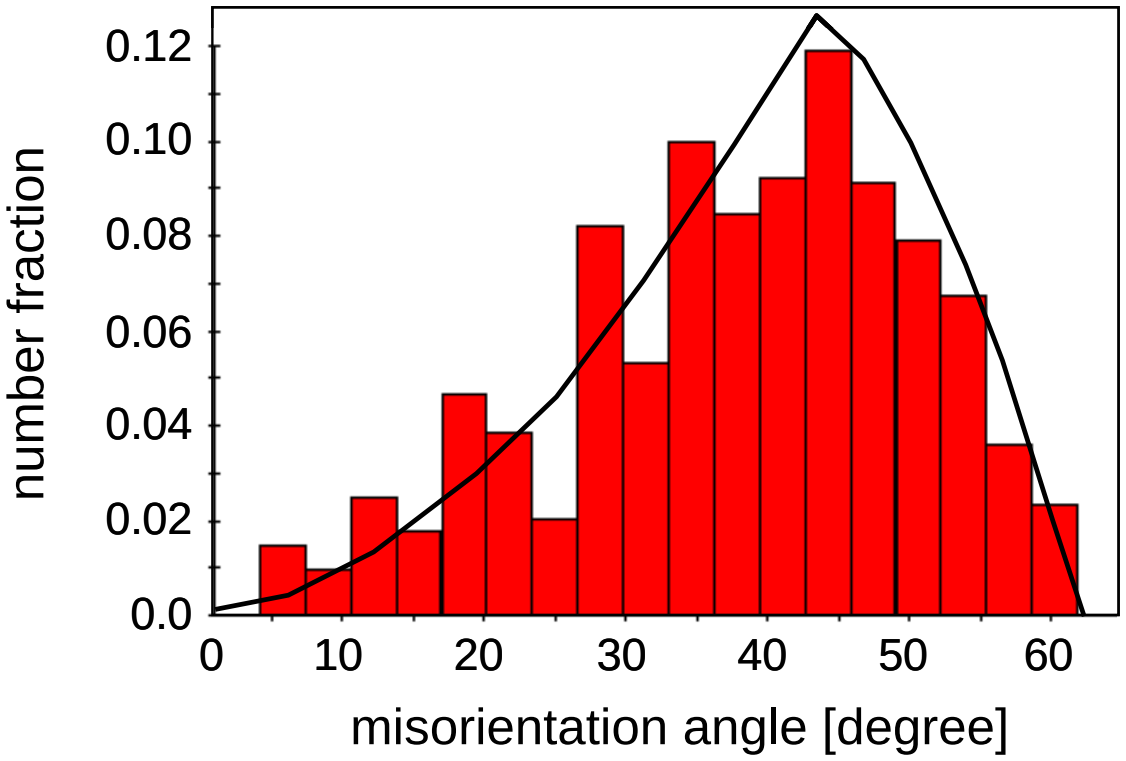
– nucleation takes place site saturated and randomly at t = 0

– driving force results only from difference in stored energy

– constant dislocation density

Case 1:	**Case 2:**	**Case 3:**
HAGB: ΔH= 1.6eV and m_0=1.45×10^{12} µm/sMPa	HAGB: ΔH= 1.6eV and m_0=1.45×10^{12} µm/sMPa	HAGB: ΔH= 1.0eV and m_0=7.78×10^{8} µm/sMPa
LAGB: m=0	LAGB: ΔH=1.3eV and m_0=2.65×10^{10} µm/sMPa	LAGB: ΔH=1.3eV and m_0=2.65×10^{10} µm/sMPa

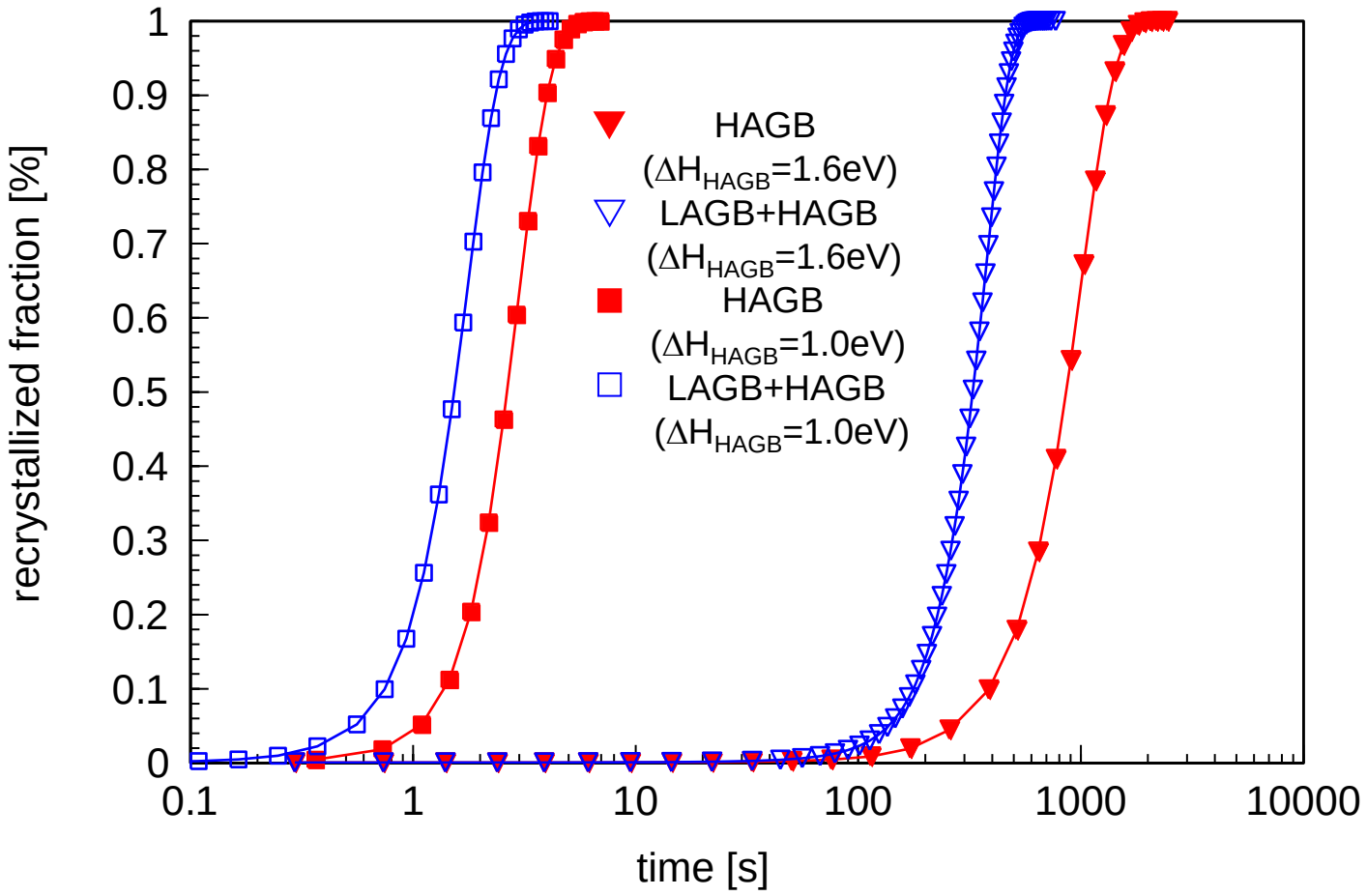
Nucleation



Nucleus distribution very similar for case 1, case 2 and case 3

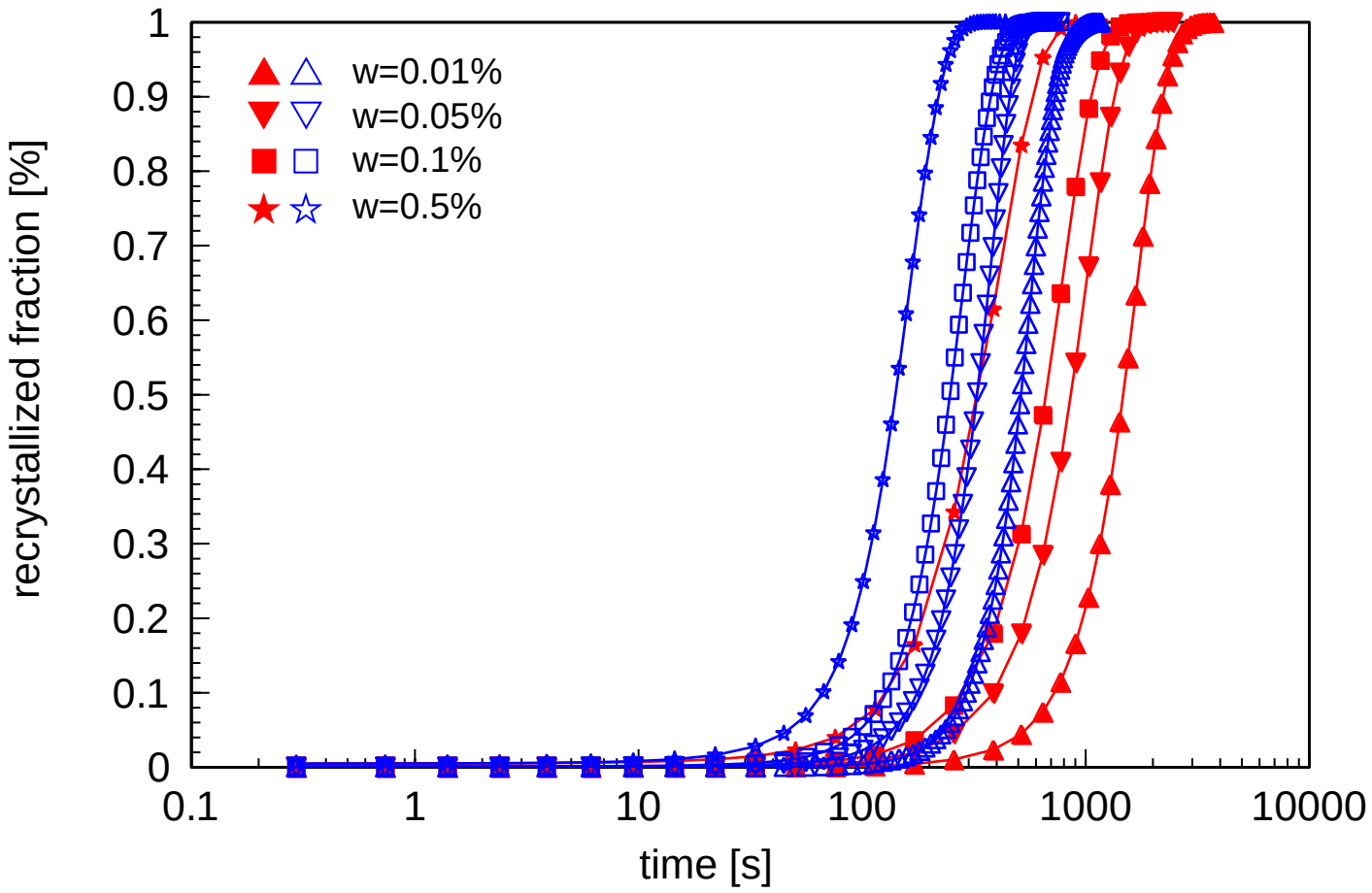
Initial fraction of LAGB in nucleus distribution: ~4.9%

Results – Kinetics: influence mobility



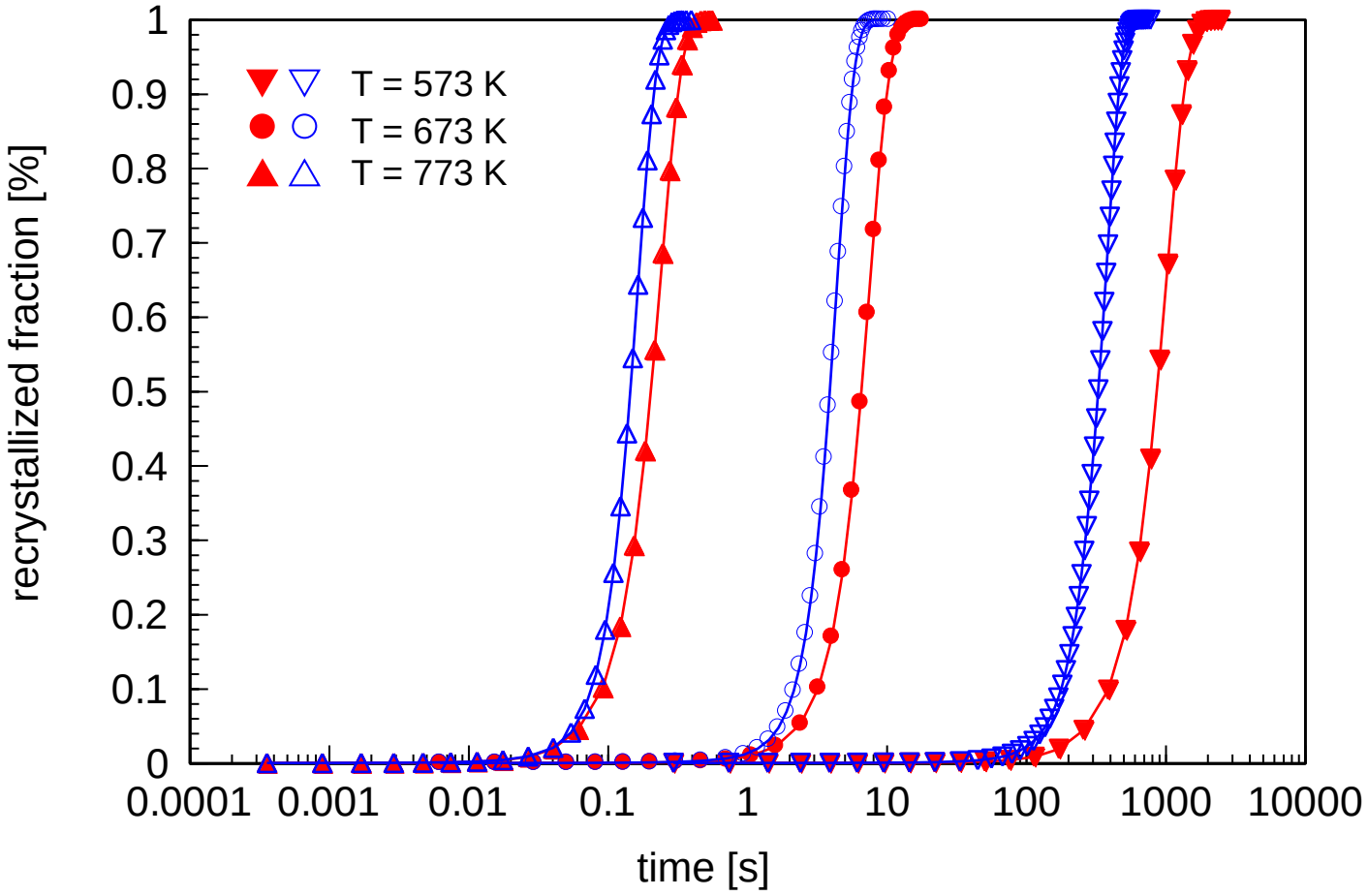
Influence of mobility for constant dislocation density $\rho=10^{14}m^{-2}$, number of nuclei w=0.05% and temperature T=573K.

Results – Kinetics: influence number of nuclei



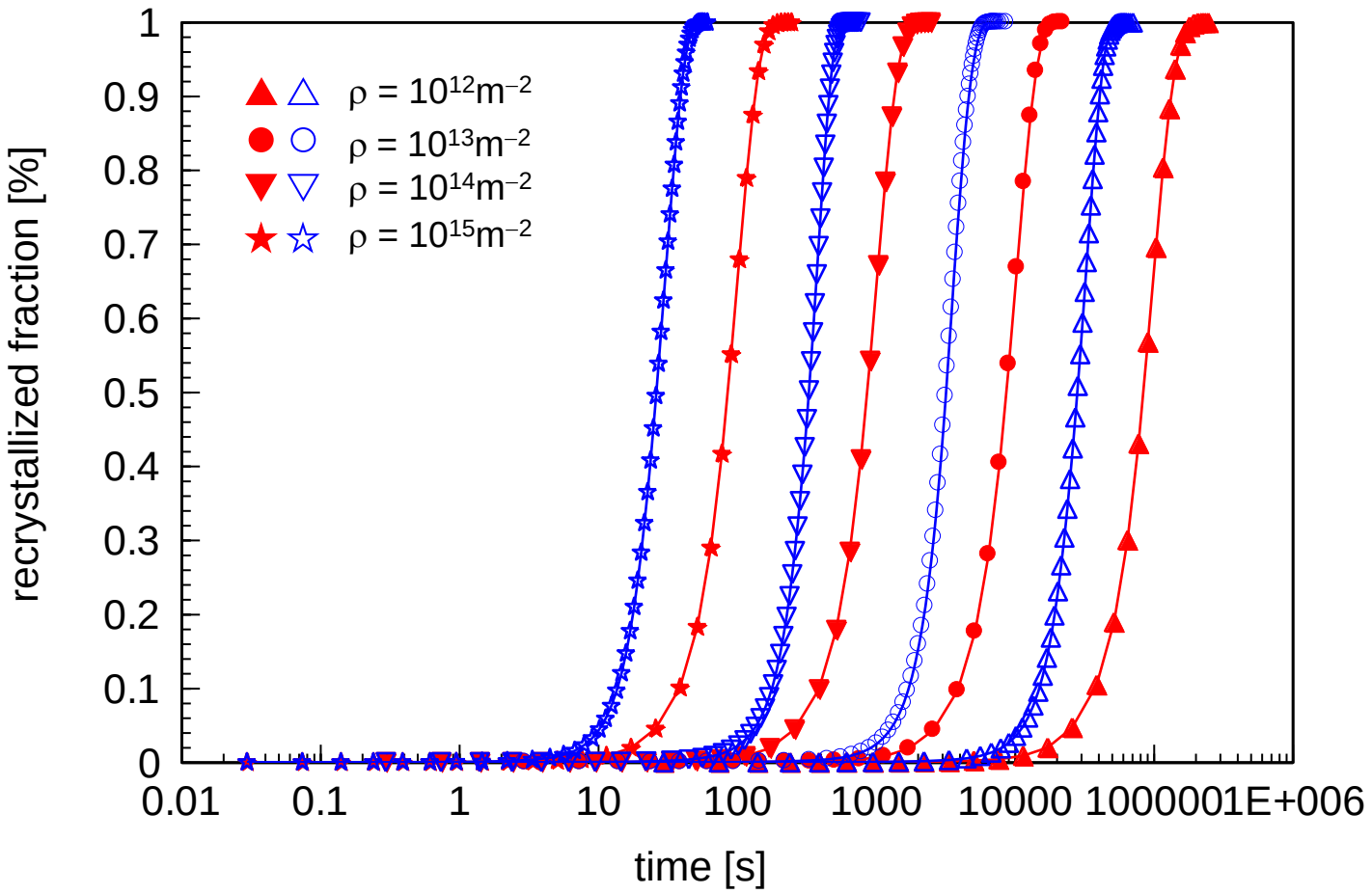
Influence of number of nuclei for constant dislocation density $\rho=10^{14}m^{-2}$ and temperature T=573K.

Results – Kinetics: influence temperature



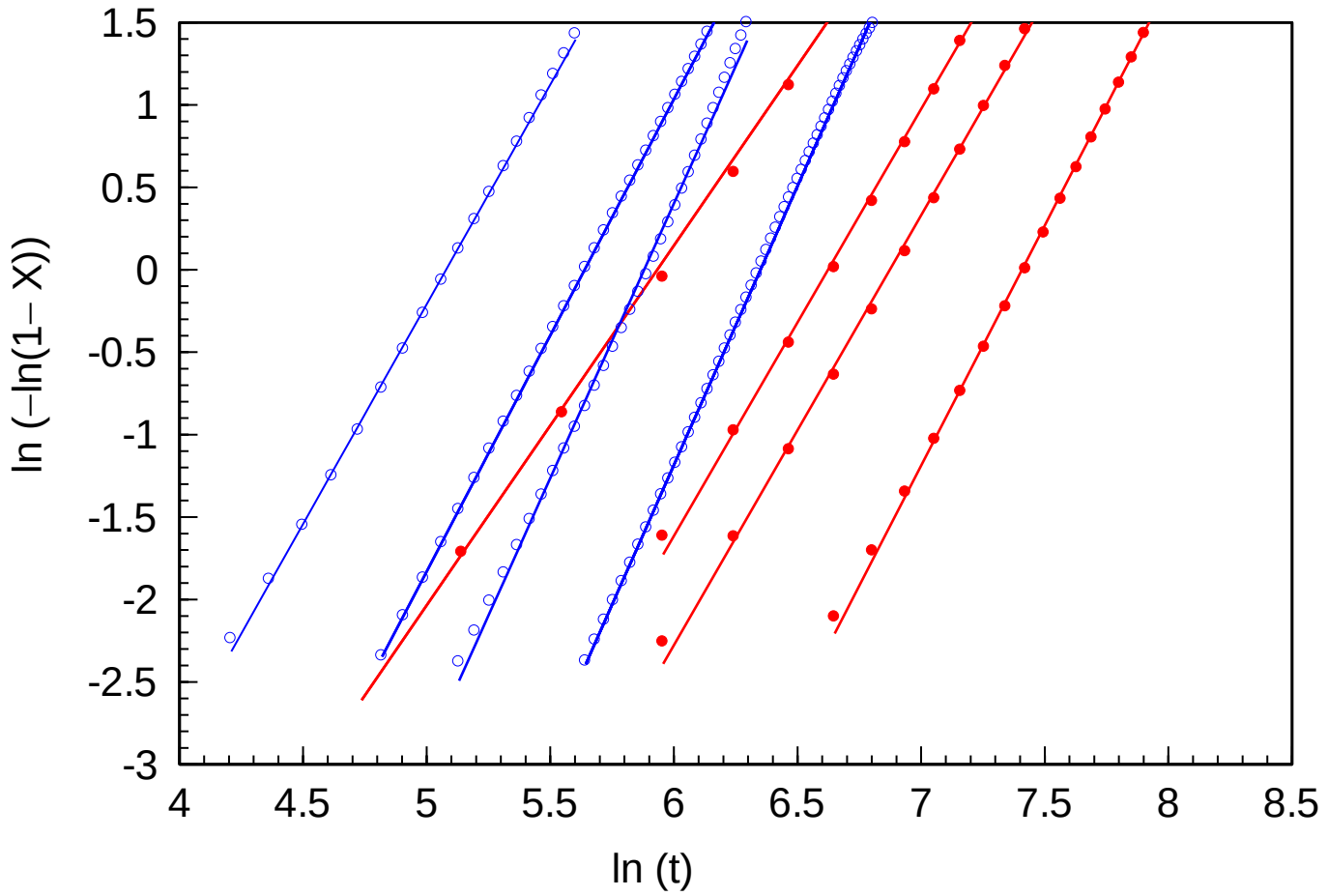
Influence of temperature for constant dislocation density $\rho=10^{14}m^{-2}$ and number of nuclei w=0.05%.

Results – Kinetics: influence dislocation density



Influence of dislocation density for constant number of nuclei w=0.05% and temperature T=573K.

Results – Kinetics: Avrami exponents



Determination of Avrami exponent q from Avrami plot based on:

$$\ln\left(-\ln\left(1-X\right)\right) = q \cdot \ln t + \ln k_0$$

Results – Kinetics: Avrami exponents

Mobile LAGB and HAGB	Only mobile HAGB
$\rho=10^{14}m^{-2}$;T=573K;w=0.01%; **q=3.30**	$\rho=10^{14}m^{-2}$;T=573K;w=0.01%; **q=2.91**
$\rho=10^{14}m^{-2}$;T=573K;w=0.05%; **q=3.30**	$\rho=10^{14}m^{-2}$;T=573K;w=0.05%; **q=2.74**
$\rho=10^{14}m^{-2}$;T=573K;w=0.1%; **q=2.89**	$\rho=10^{14}m^{-2}$;T=573K;w=0.1%; **q=2.74**
$\rho=10^{14}m^{-2}$;T=573K;w=0.5%; **q=2.72**	$\rho=10^{14}m^{-2}$;T=573K;w=0.5%; **q=2.68**
$\rho=10^{14}m^{-2}$;T=673K;w=0.05%; **q=2.82**	$\rho=10^{14}m^{-2}$;T=673K;w=0.05%; **q=2.75**
$\rho=10^{14}m^{-2}$;T=773K;w=0.05%; **q=3.09**	$\rho=10^{14}m^{-2}$;T=773K;w=0.05%; **q=2.70**
$\rho=10^{12}m^{-2}$;T=573K;w=0.05%; **q=3.28**	$\rho=10^{12}m^{-2}$;T=573K;w=0.05%; **q=2.68**
$\rho=10^{13}m^{-2}$;T=573K;w=0.05%; **q=3.17**	$\rho=10^{13}m^{-2}$;T=573K;w=0.05%; **q=2.79**
$\rho=10^{15}m^{-2}$;T=573K;w=0.05%; **q=3.21**	$\rho=10^{15}m^{-2}$;T=573K;w=0.05%; **q=2.75**

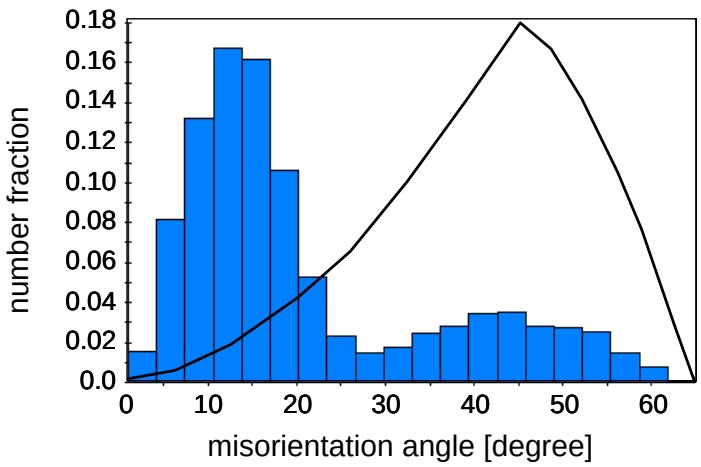
$>q_{theo}=3$ site saturated nucleation but different growing rates

$\sim q_{theo}=3$ site saturated nucleation and constant growing rate

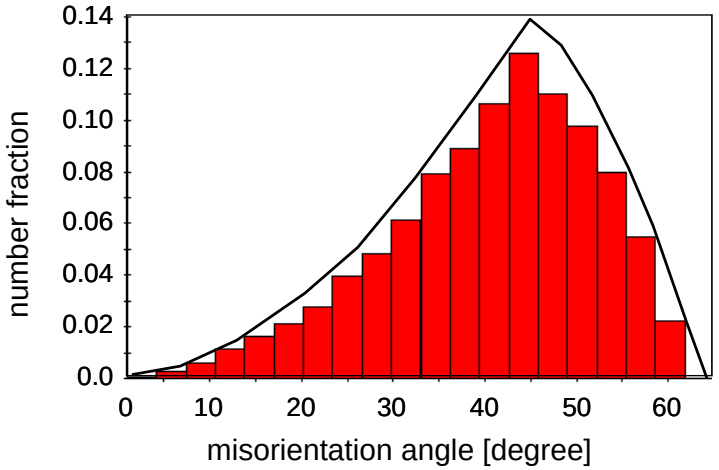
Obviously, recrystallization in LAGB case is much faster than recrystallization in HAGB case.

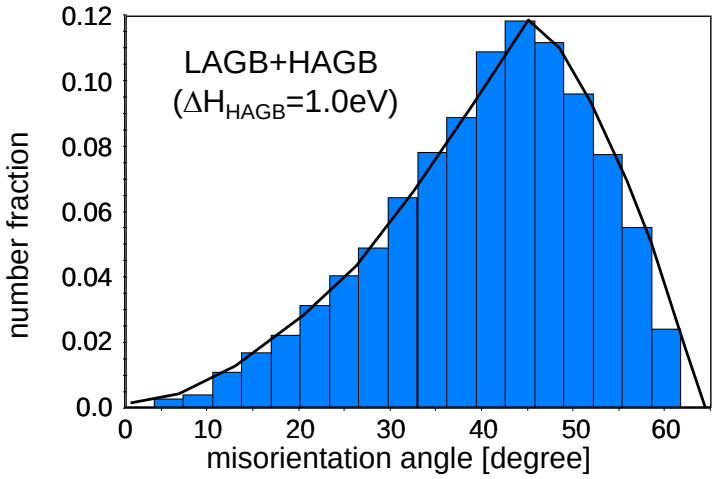
Results – Fractions of grain boundaries

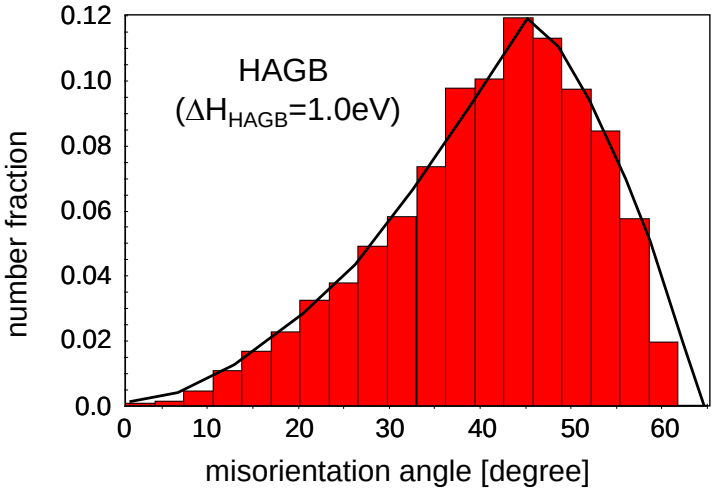
LAGB+HAGB
(ΔH_{HAGB}=1.6eV)



HAGB
(ΔH_{HAGB}=1.6eV)

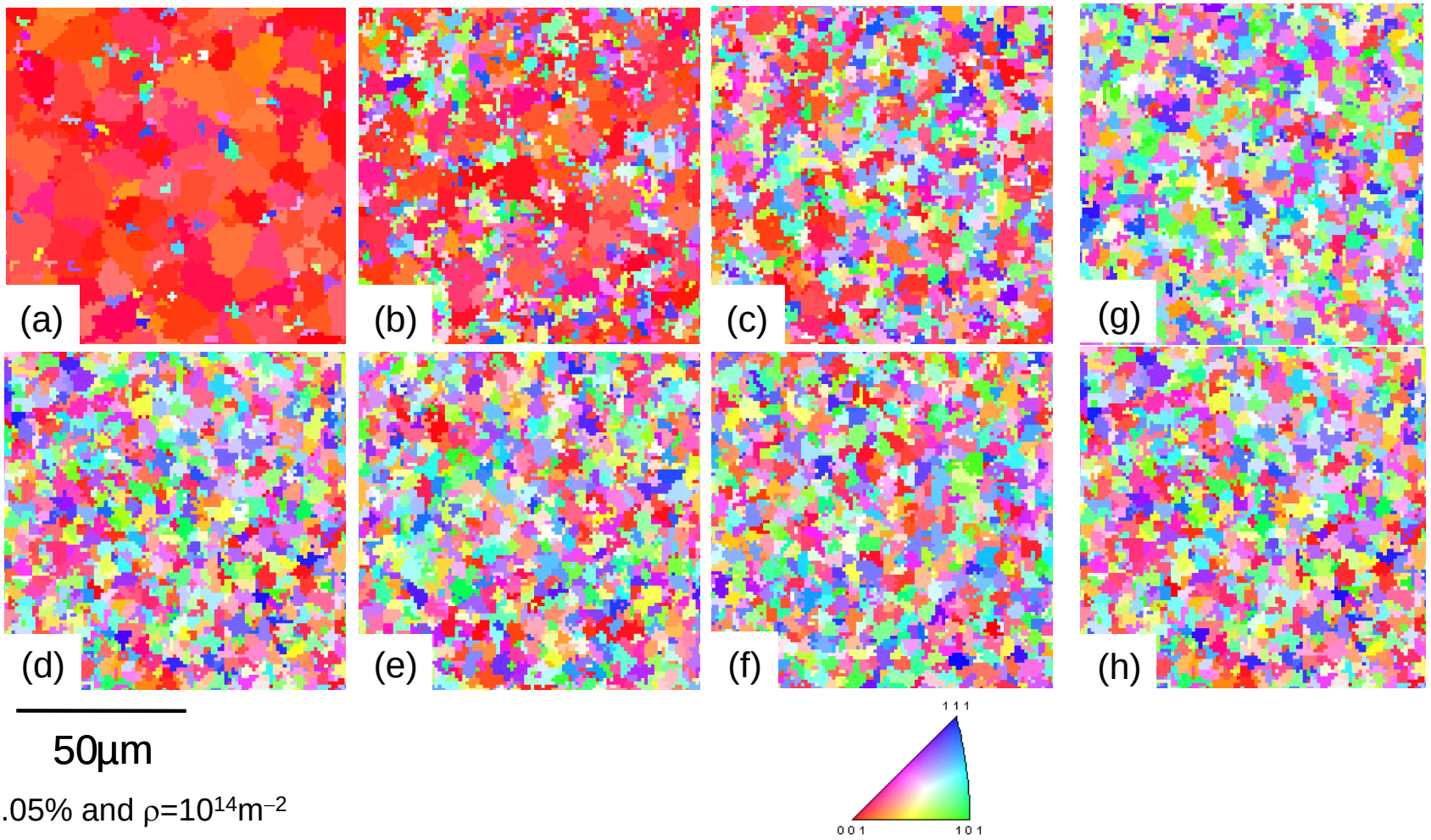






Initial dislocation density for these simulations: $\rho=10^{14}m^{-2}$, number of nuclei w=0.05% and T=573K.
The Mackenzie distribution is plotted as solid line and gives the distribution for a completely random [illegible] ribution.

Results – Microstructure evolution



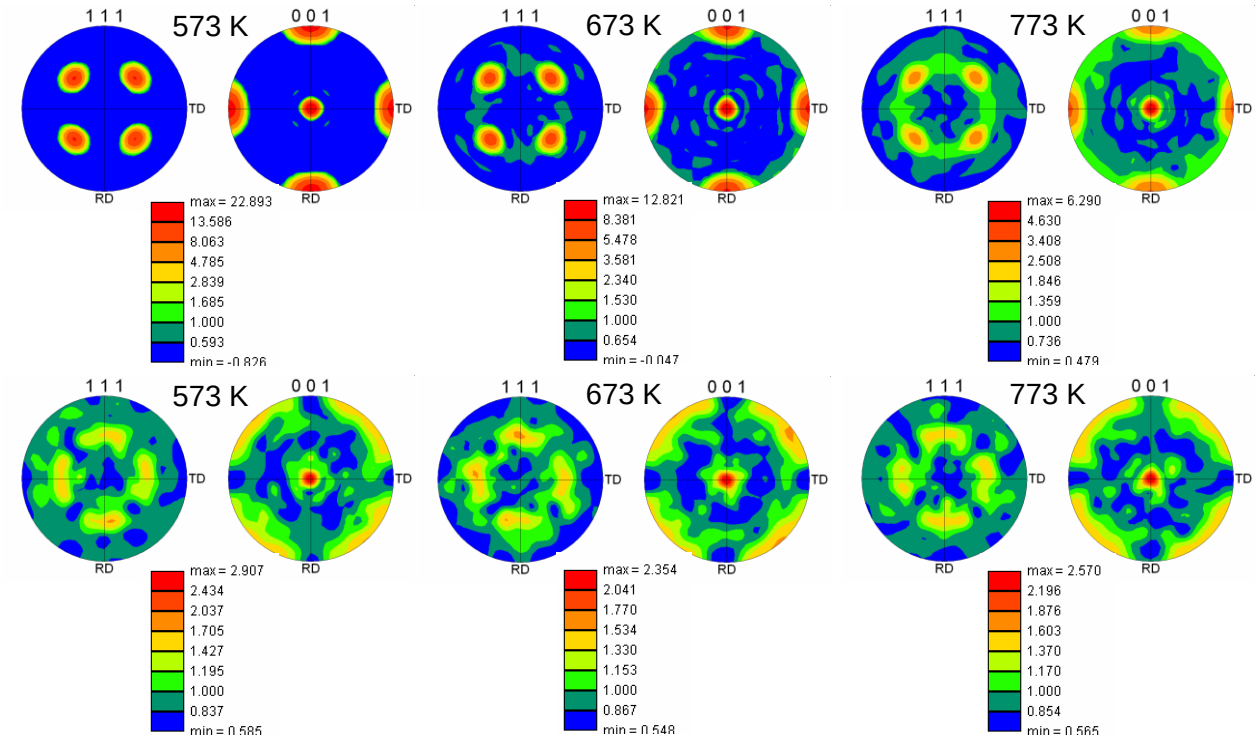
w=0.05% and $\rho=10^{14}m^{-2}$

(a) $m_{LAGB}>0$ and $m_{HAGB}>0$ at 573 K. (b) $m_{LAGB}>0$ and $m_{HAGB}>0$ at 673 K. (c) $m_{LAGB}>0$ and $m_{HAGB}>0$ at 773 K.

(d) $m_{LAGB}=0$ and $m_{HAGB}>0$ at 573 K. (e) $m_{LAGB}=0$ and $m_{HAGB}>0$ at 673 K. (f) $m_{LAGB}=0$ and $m_{HAGB}>0$ at 773 K.

At T=573 K: (g) $\Delta H_{LAGB}/\Delta H_{HAGB}=1.3eV/1.0eV$. (h) $m_{LAGB}=0$ and $\Delta H_{HAGB}=1.0eV$.

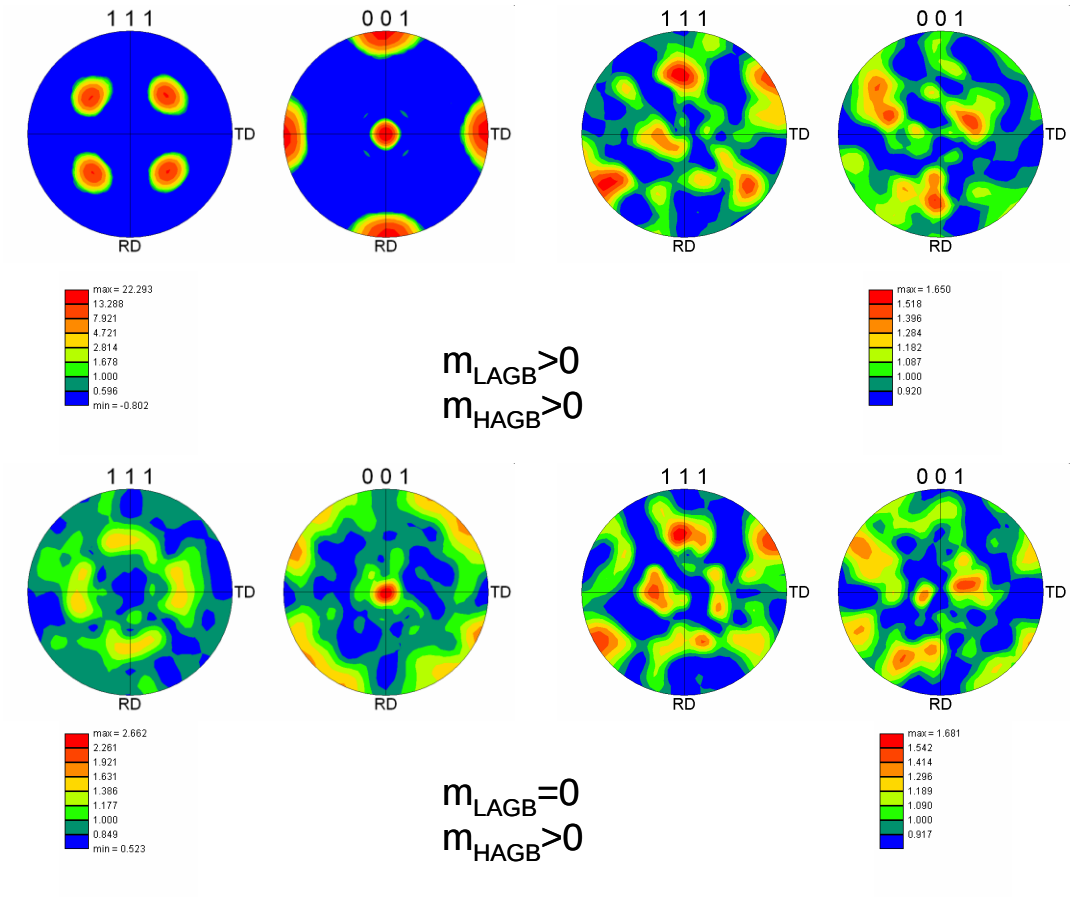
Results – Texture evolution



Pole figures for fully recrystallized Al single crystals with initial Cube orientation and w=2%.

Upper row: Predicted textures at different temperatures for the case of mobile low and high angle grain boundaries:
Bottom row: Predicted textures at different temperatures for the case with only mobile high angle grain boundaries.
Initial dislocation density: $\rho=10^{14}m^{-2}$.

Results – Texture evolution: influence mobility



Upper row: Predicted textures for the cases of mobile low and high angle grain boundaries:
Left side: $\Delta H_{LAGB}/\Delta H_{HAGB}$=1.3eV/1.6eV; right side: $\Delta H_{LAGB}/\Delta H_{HAGB}$=1.3eV/1.0eV.

Bottom row: Predicted textures for the cases with only mobile high angle grain boundaries.
Left side: m_{LAGB}=0 and ΔH_{HAGB}=1.6eV; right side: m_{LAGB}=0 and ΔH_{HAGB}=1.0eV.

Initial dislocation density for these simulations: $\rho=10^{14}m^{-2}$, number of nuclei w=0.05% and T=573K.

Summary

- Results of 3D cellular automaton simulations were shown. Three cases were compared in order to study the influence of mobile low angle grain boundaries on the recrystallization behavior.
- The texture evolution shows an increasing randomization for the HAGB simulations. For LAGB simulations the texture remains stable up to 100% recrystallized fraction.
- The kinetics of recrystallization is faster for the LAGB simulations than for the HAGB simulations.
- The fraction of low angle grain boundaries is remarkably larger in the LAGB simulation case.
- The presented simulation results show that there is obviously an influence of low angle grain boundaries on the texture evolution during recrystallization.

- Further simulations are needed in order to get data which can be compared with experimental results.

The Düsseldorf Max-Planck Team