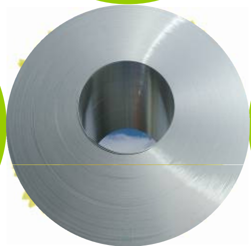
Micro-Chemistry Simulation of Al-Alloys with the ClaNG-Model



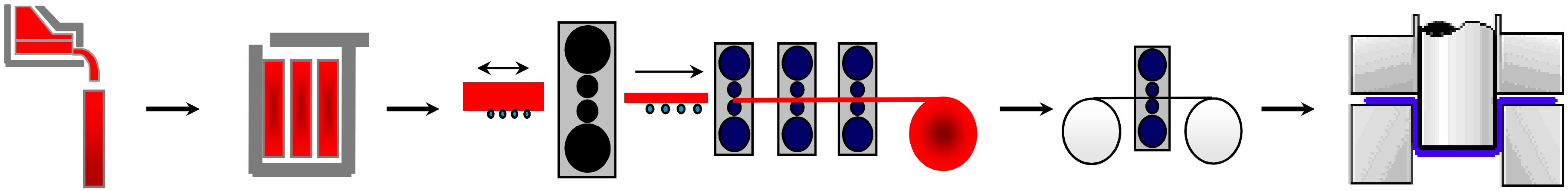
Olaf Engler, Hydro RDB

GTT Workshop, Herzogenrath, 14.09.2011

Micro-Chemistry Simulation of Al-Alloys with the ClaNG-Model

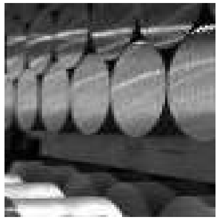
Outline

- Introduction: micro-chemistry simulation of Al-alloys
- The ClaNG-model
- Application example: homogenisation of Al alloy 8006 to improve the recrystallization behaviour



Hydro: a leading integrated aluminium and energy company

Gaining primary aluminium → **Casting and recycling** → **Fabricating aluminium**

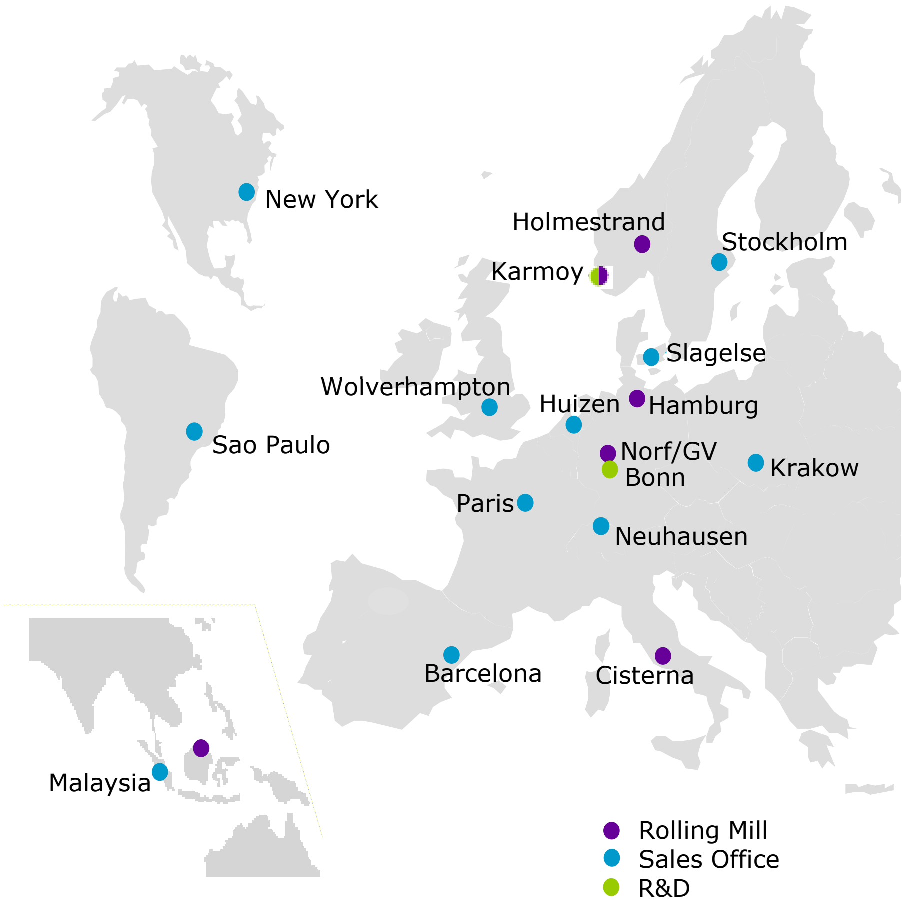
Bauxite & Alumina	Energy	Primary Metal	Metal Markets		Rolled Products	Extruded Products
						
Soon better equity in alumina	Solid long-term coverage of power 100% hydro-power in Norway Solar energy	1.4 mill. mt/year 10 metal plants in 5 countries on 3 continents **4 350 employees**	Up to 2.4 mill. mt/year Primary + cold metal + 0.5 mill. mt recycling metal Special alloys 11 remelters in 5 countries		1.0 mill. + 300,000 mt/year Operations in more than 30 countries **13 300 employees** Rolled Products with own remelting	
• Equity	• Long-term power supply	• Cost position • Technology	• Expertise in materials • Technology		• Close to customers • Service, Quality and Innovation	

Recycling

Production figures are from 2009

HYDRO

Hydro: a key player in rolled products



- We operate leading rolling assets, foremost in Europe
  - **6 plants in 4 countries**
  - + **Alunorf, the world´s largest aluminium rolling mill (50%)**
  - **2 R&D Centres**
- We employ around 4,000
- We ship up to 1 million tonnes per year
  - **77% to customers in Europe**
  - **17% market share in Europe[1]**

1 Estimate based on EAA data

HYDRO

We serve a wide range of applications

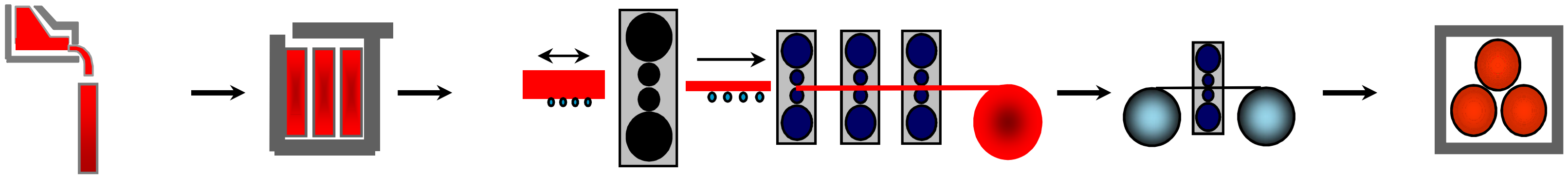
Litho
- Plain strip and sheet for offset printing plates

Packaging and building
- Plain and lacquered strip for cans and other packaging containers
- Plain and converted foil for flexible packaging and technical applications
- Plain and lacquered strip, sheet and plate for architecture: Facades, roller shutters, etc.

Automotive, heat exchanger and general engineering
- Plain, anodised and cladded strip and sheet for
  - cars, transport and heat exchanger systems
  - general engineering, solar technology and special industry

HYDRO

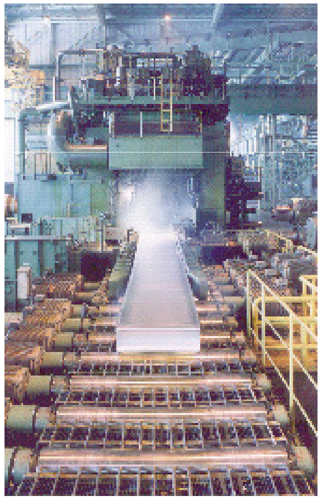
Industrial production of Al sheet process chain



DC casting → homogenisation → hot rolling → cold rolling → annealing

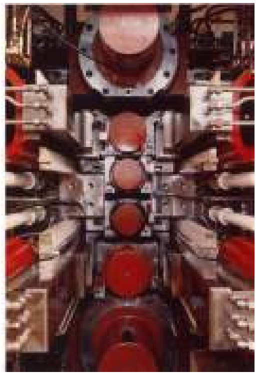
DC casting

sheet ingot



breakdown rolling mill

tandem hot rolling line



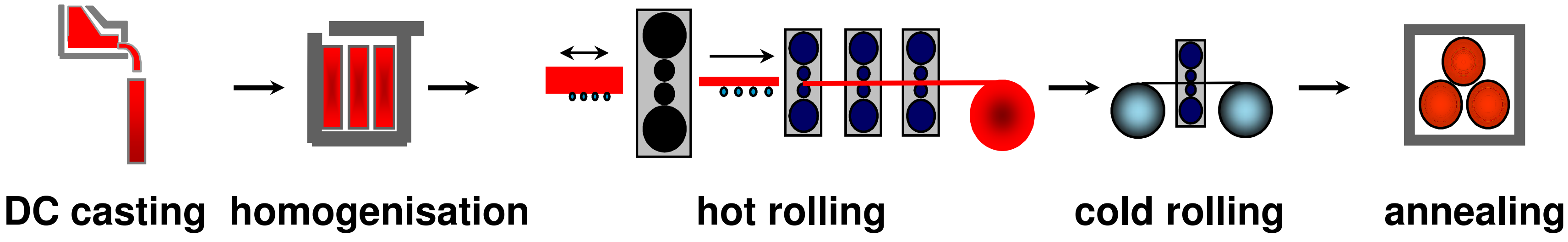
sexto cold mill

batch furnace

finished coil

HYDRO

Through-Process Modelling



Main metallurgical reactions along the process chain

- **homogenisation:** diffusion, microchemistry (solutes, phases)
- **hot rolling:** work hardening, softening, texture, microchemistry
- **cold rolling:** work hardening, texture
- **back-annealing:** softening, texture

→

- **microchemistry**
- work hardening
- softening

HYDRO

BMBF Project ClaNG Plus

Duration:

- Start: 01.01.2007
- End: 31.12.2010

Partners

- Hydro Aluminium Rolled Products GmbH, R&D Bonn (project management)
- Institut für Metallkunde und Metallphysik, RWTH Aachen
- GTT-Technologies, Herzogenrath

Workpackages:

1. Model development ClaNG (IMM, Hydro)
2. Link of ClaNG model to modern multi component thermodynamic data bases (IMM, GTT, Hydro)
3. Link of ClaNG model to property models (IMM, Hydro)
4. Evaluation of applicability to solidification (IMM, Hydro)
5. Full scale trials and characterization (Hydro, IMM)

ClaNG Modell "*Cla*ssical *N*ucleation and *G*rowth" model overview

Goal: determine the precipitation kinetics

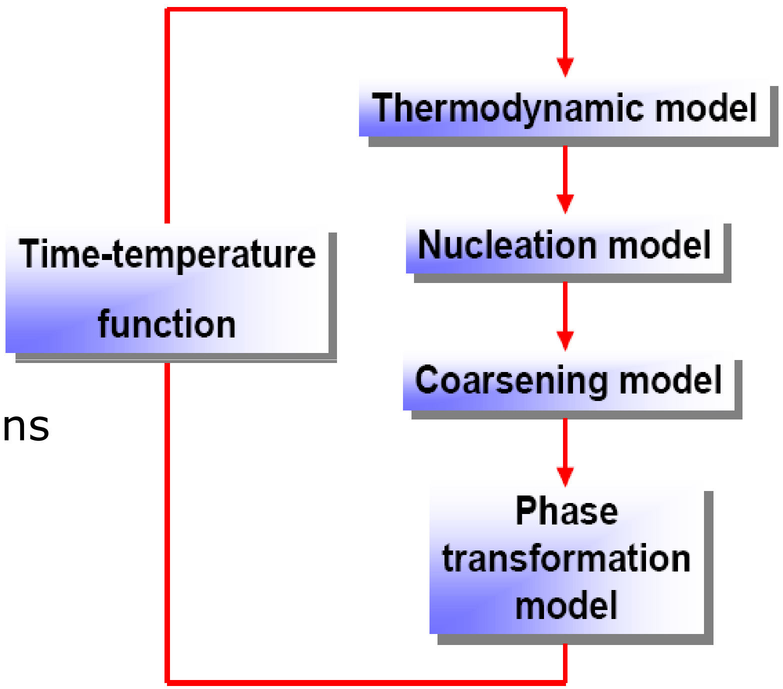
classical theories:

- Nucleation: *Becker and Döring*
- Growth: *Zener*
- Evolution of precipitate size distributions: continuity equation (*Kampmann and Wagner*)

Decision based on thermodynamic calculations using ChemApp (*GTT Technologies*)

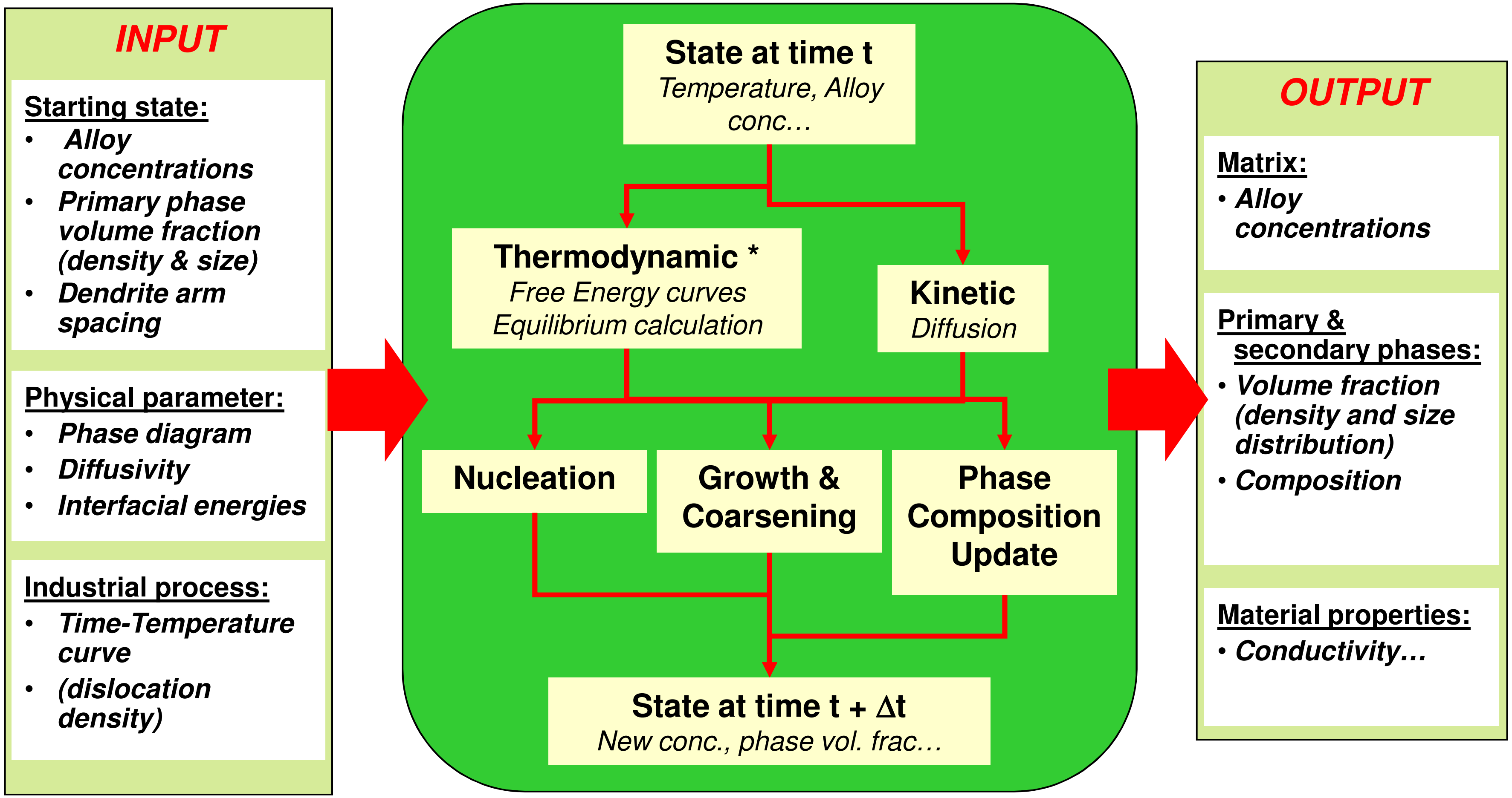
- Data base: *Thermotech AlTT* (8 elements: Al-Cr-Cu-Fe-Mg-Mn-Si-Ti)

developed by L. Löchte (RDB), G. Gottstein (IMM) and M. Schneider (Diss. IMM, 2006), advanced by E. Jannot (Diss. IMM, 2008) and Z.S. Liu (Diss. 2011)



HYDRO

ClaNG Modell "*<u>Cla</u>*ssical *<u>N</u>*ucleation and *<u>G</u>*rowth" model overview



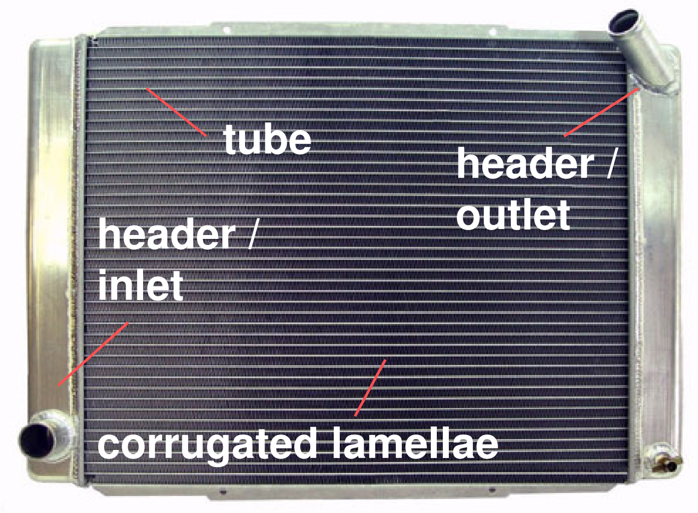
* : performed using *ChemApp* (GTT)

Al alloy AA 8006 (AlFe1.5Mn)

Medium strength foil alloy (semi-ridgid packaging applications, menue trays, candle lights, …)

Fin stock

Alloy Designations		Si	Fe	Cu	Mn	Mg	Cr	Ni	Zn
AA	EN [1] (alphanumeric)	min max	min max	min max	min max	min max	min max	min max	min max
AA 8006	AL FE 1,5 MN	0,40	1,2 2,0	0,30	0,30 1,0	0,10			0,10

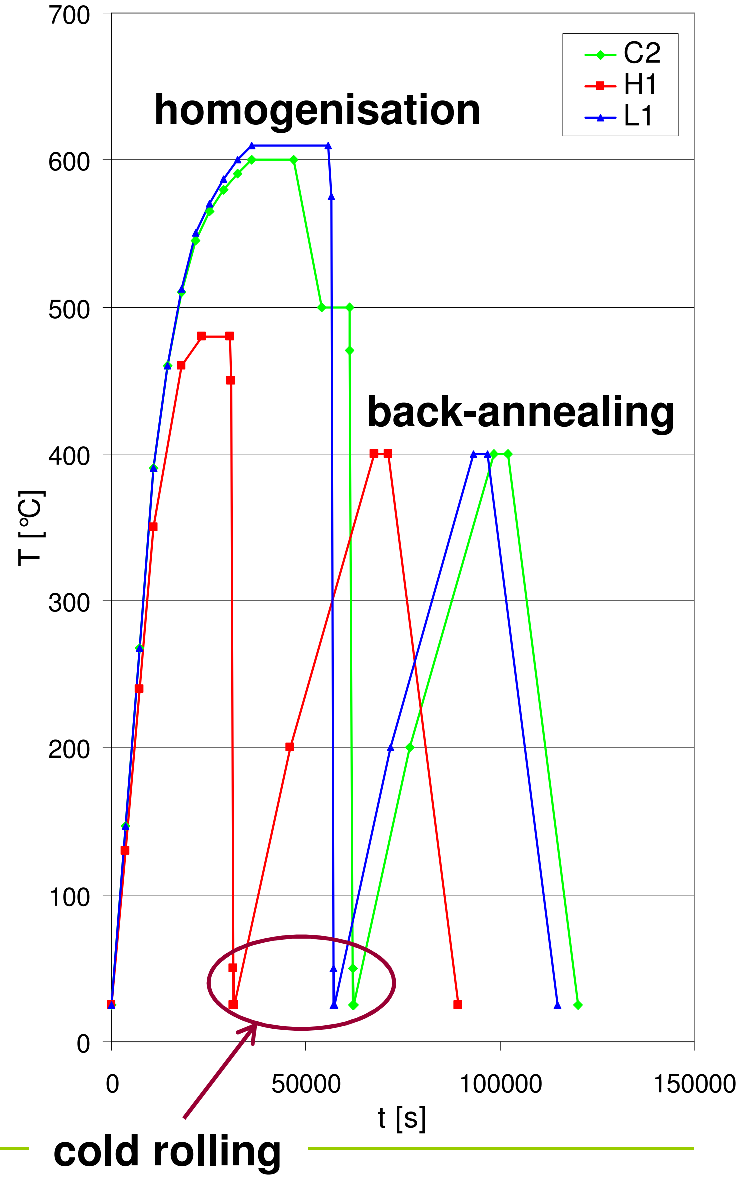


HYDRO

Recrystallization of AA 8006 Experiments

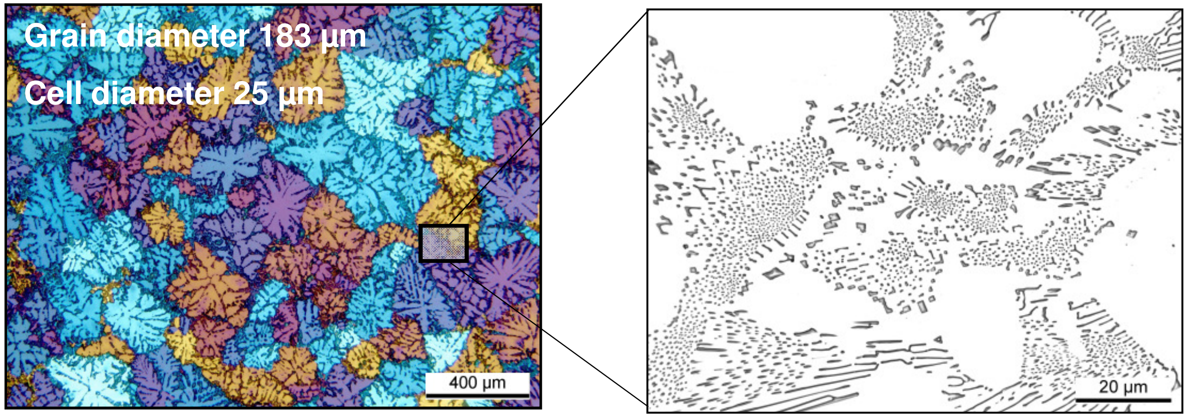
Experiments

- **Alloy: AA 8006 (AlFe1.5Mn0.5)**
- **as-cast material (DC-cast)**
- **homogenisation trials**
  - L1 (600°C)
  - H1 (480°C)
  - C2 (600°C/500°C)
- **water quenching**
- **cold rolling to 2.0mm (90%)**
- **back-annealing 200 … 400°C**

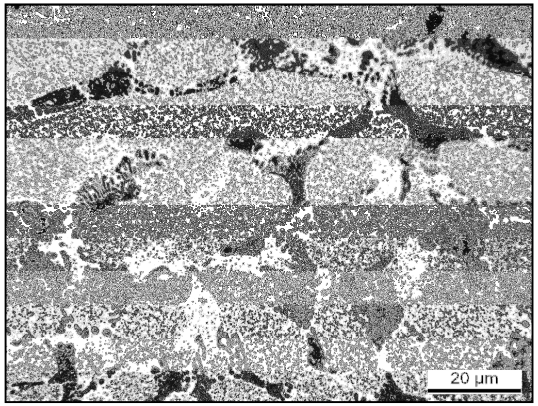


Recrystallization of AA 8006
Metallography as-cast / homogenised

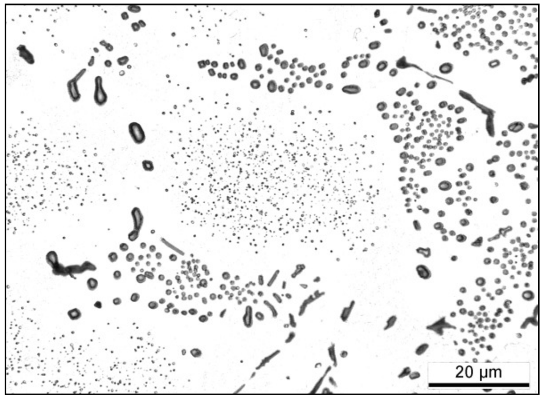
as-cast



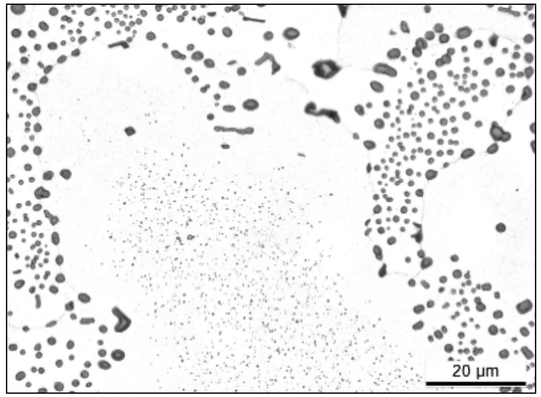
homogenised



H1 (480°C)



C2 (600°C/500°C)

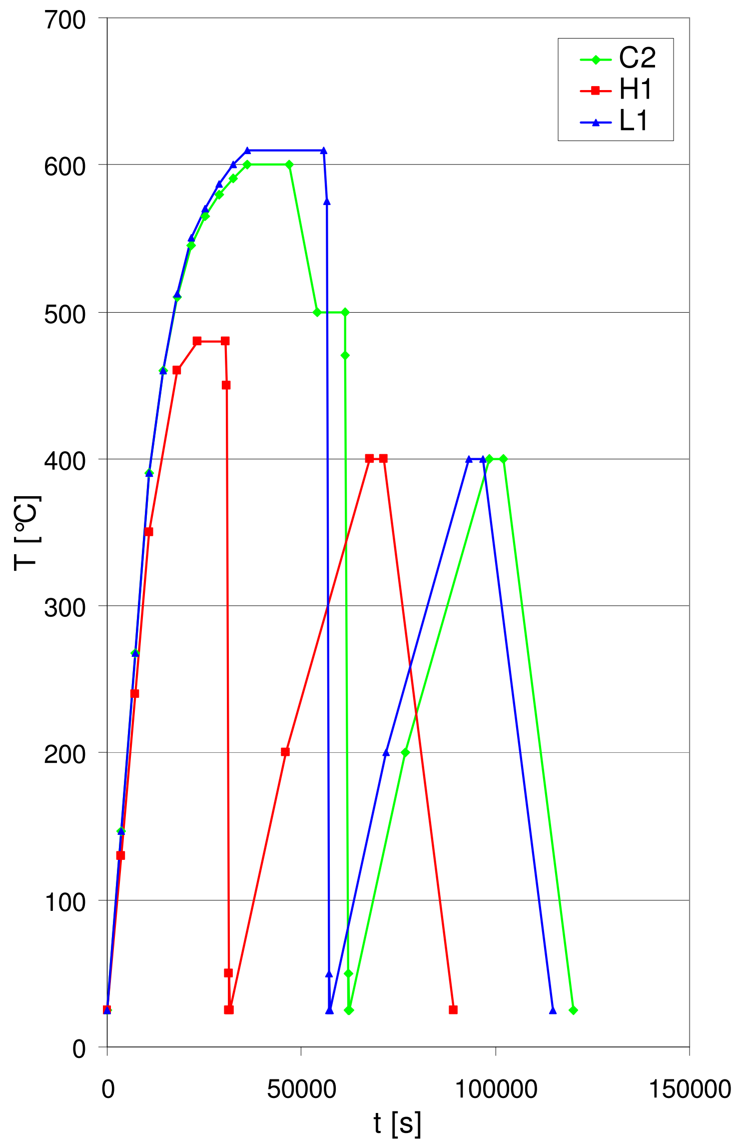


L1 (600°C)

Recrystallization of AA 8006 Metallography

el. conductivity / resistivity

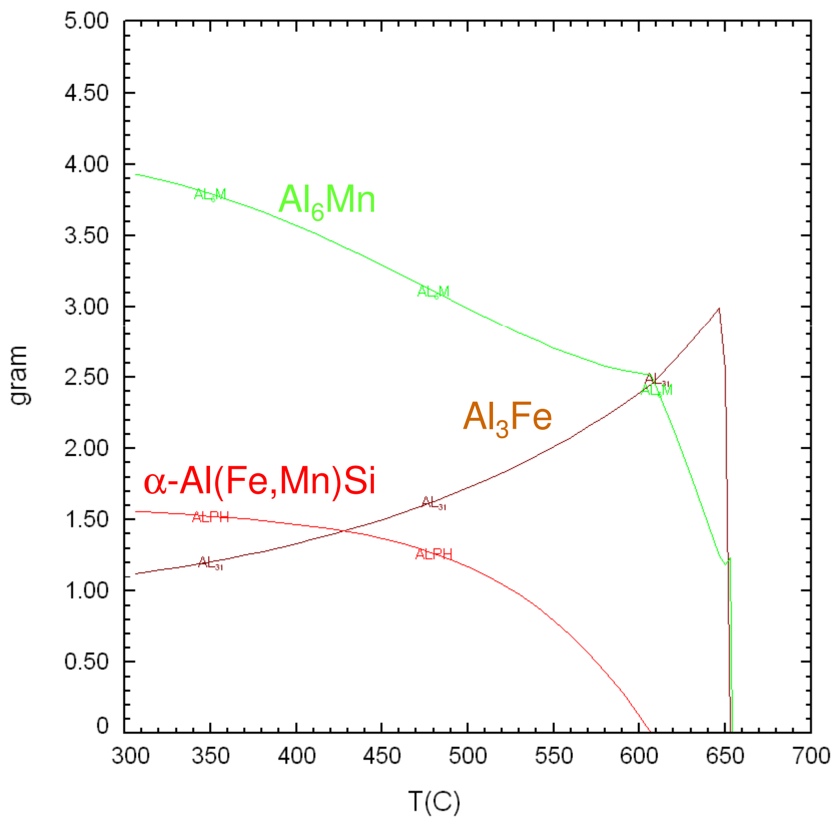
Probe	el.Leitf. bei 4,2K $\left[\frac{m}{\Omega\, mm^2}\right]$	RW bei 4,2K $[\mu\Omega.cm]$	el.Leitf. bei 293K $\left[\frac{m}{\Omega\, mm^2}\right]$	RW bei 293K $[\mu\Omega.cm]$
Guss	**77.92**	**1.2833**	**23.36**	**4.2805**
H1	**162.74**	**0.6145**	**27.20**	**3.6767**
C2	**144.38**	**0.6926**	**27.28**	**3.6655**
L1	**106.34**	**0.9404**	**25.90**	**3.8614**



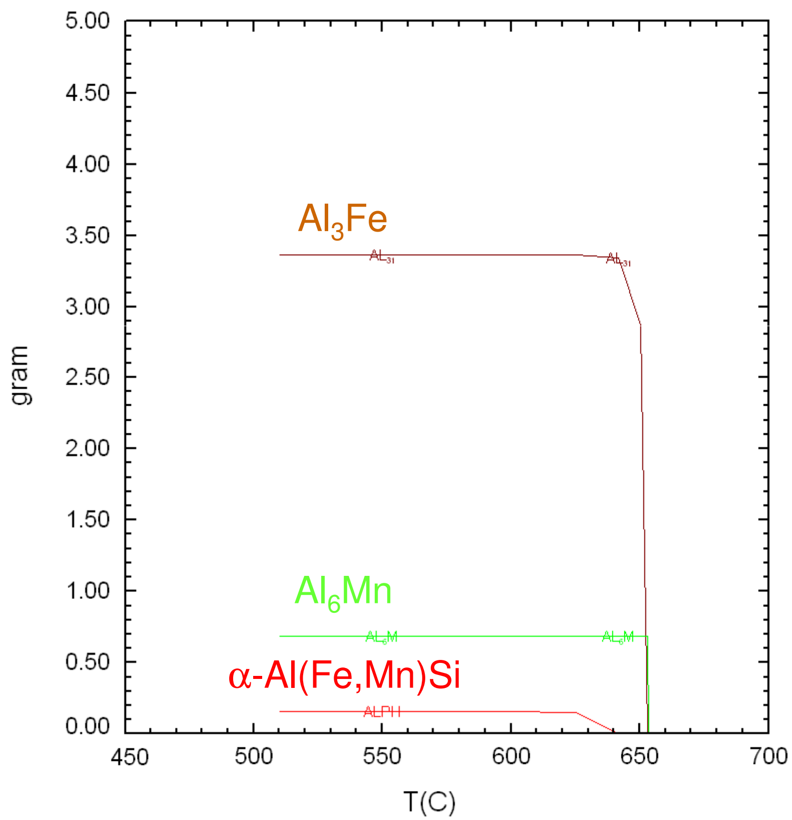
HYDRO

Recrystallization of AA 8006
Thermodynamic simulation

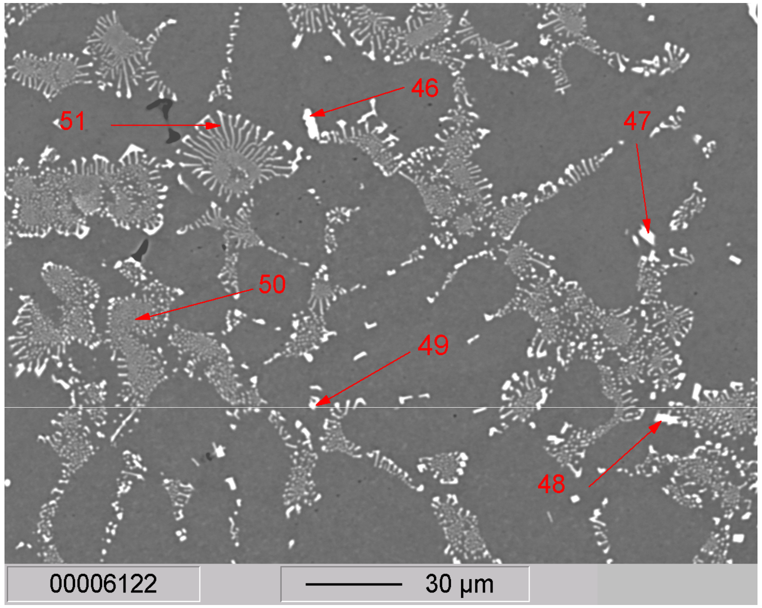
equilibrium



Scheil



Recrystallization of AA 8006
microprobe analysis



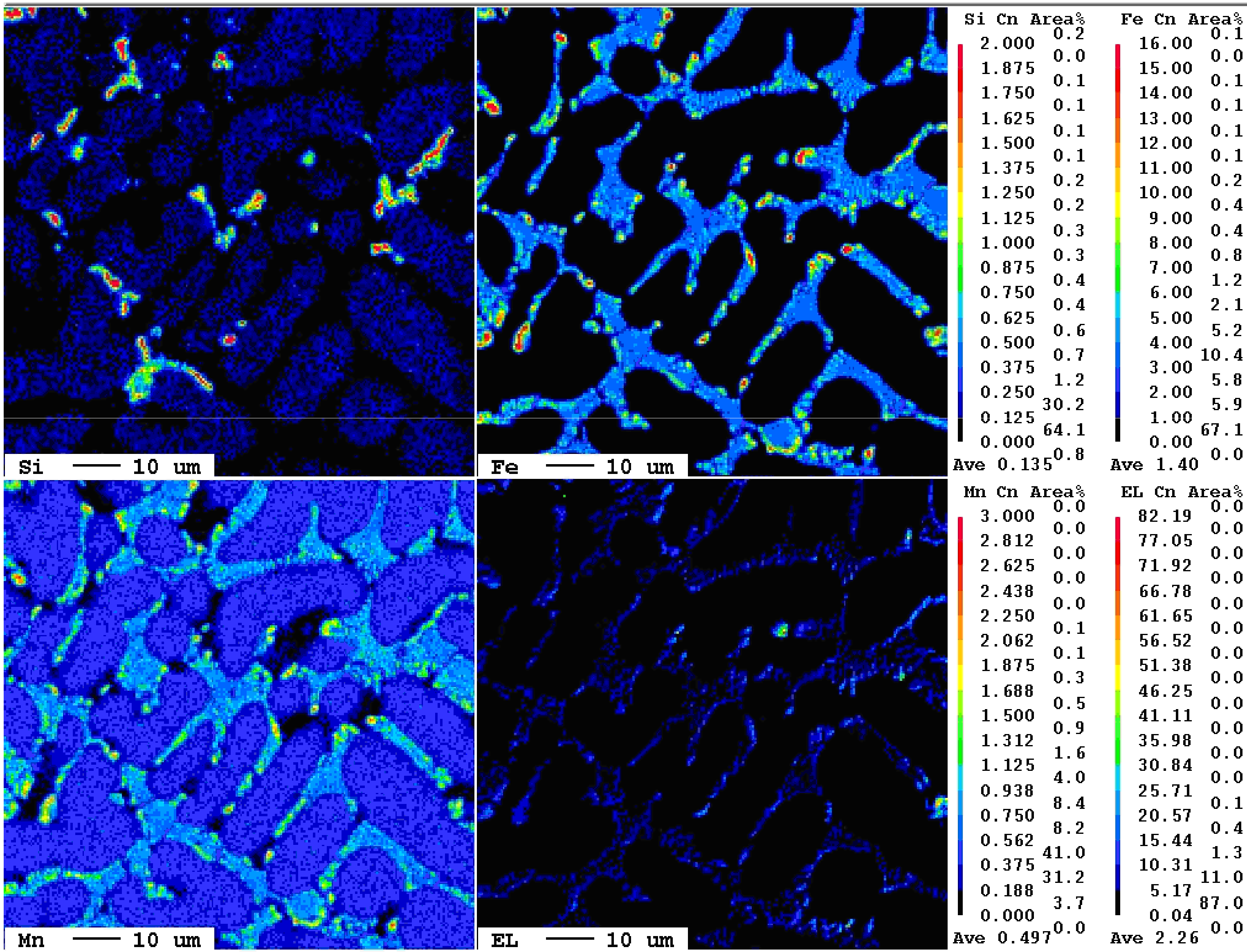
Pos.	Mg	Si	Mn	Fe
46	--	6,6	1,0	26,1
47	--	0,1	2,0	21,8
48	--	0,1	2,5	20,8
49	--	0,1	2,7	19,8
50				
51				
52	--	0,1	2,4	21,4
53	--	0,1	2,1	21,8
54	--	9,5	1,3	24,7
55	--	0,2	1,6	17,1
56	0,1	0,1	0,4	--

Summary

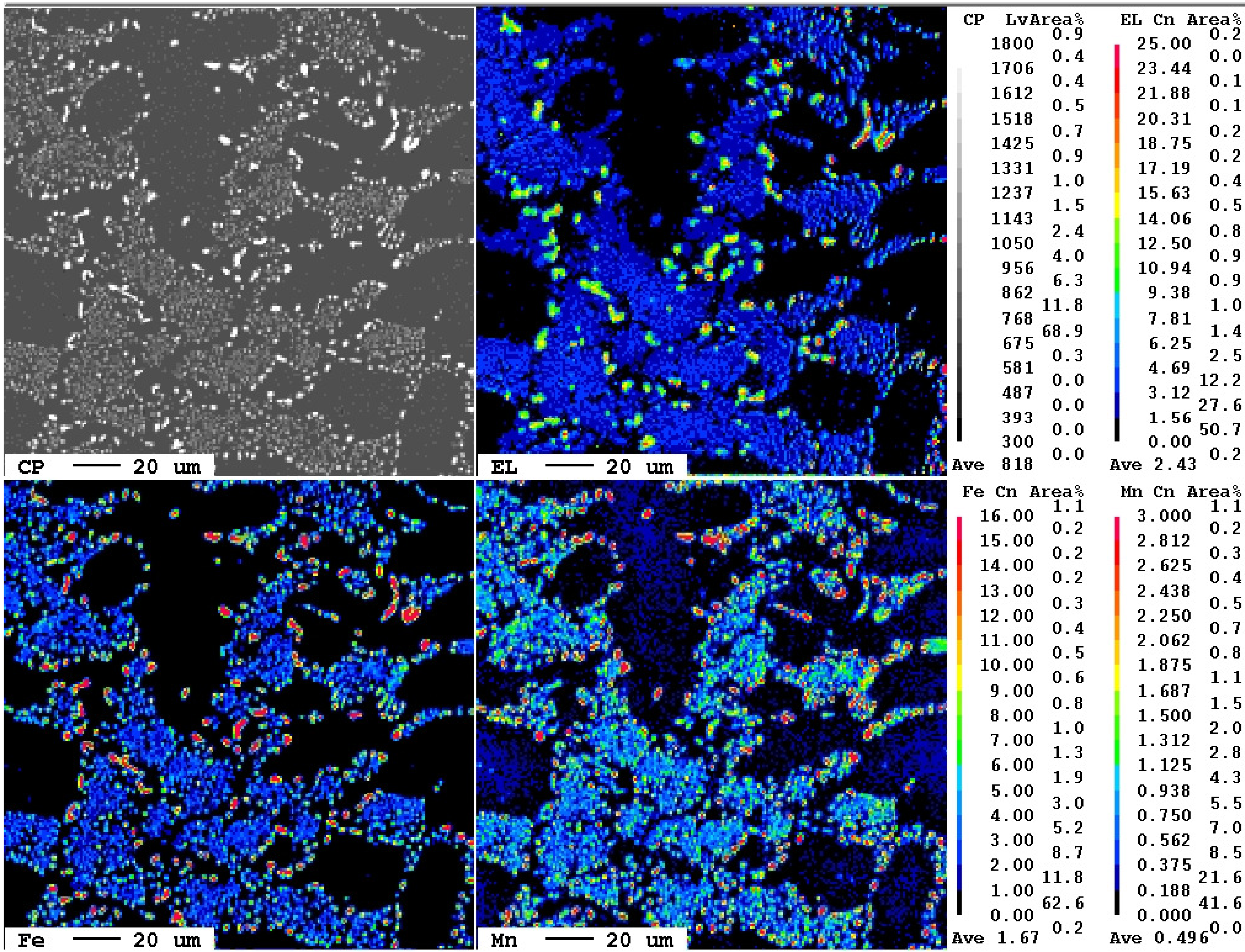
- **$Al_3(Fe,Mn)$: 0.9% Fe/Mn >10:1**
- **$Al_6(Mn,Fe)$: 4.5% Fe/Mn 4~5:1**
- **α-Al(Fe,Mn)Si**

HYDRO

AA 8006 microprobe / element-maps (H1, 480°C)



AA 8006 microprobe / element-maps (L1, 600°C)

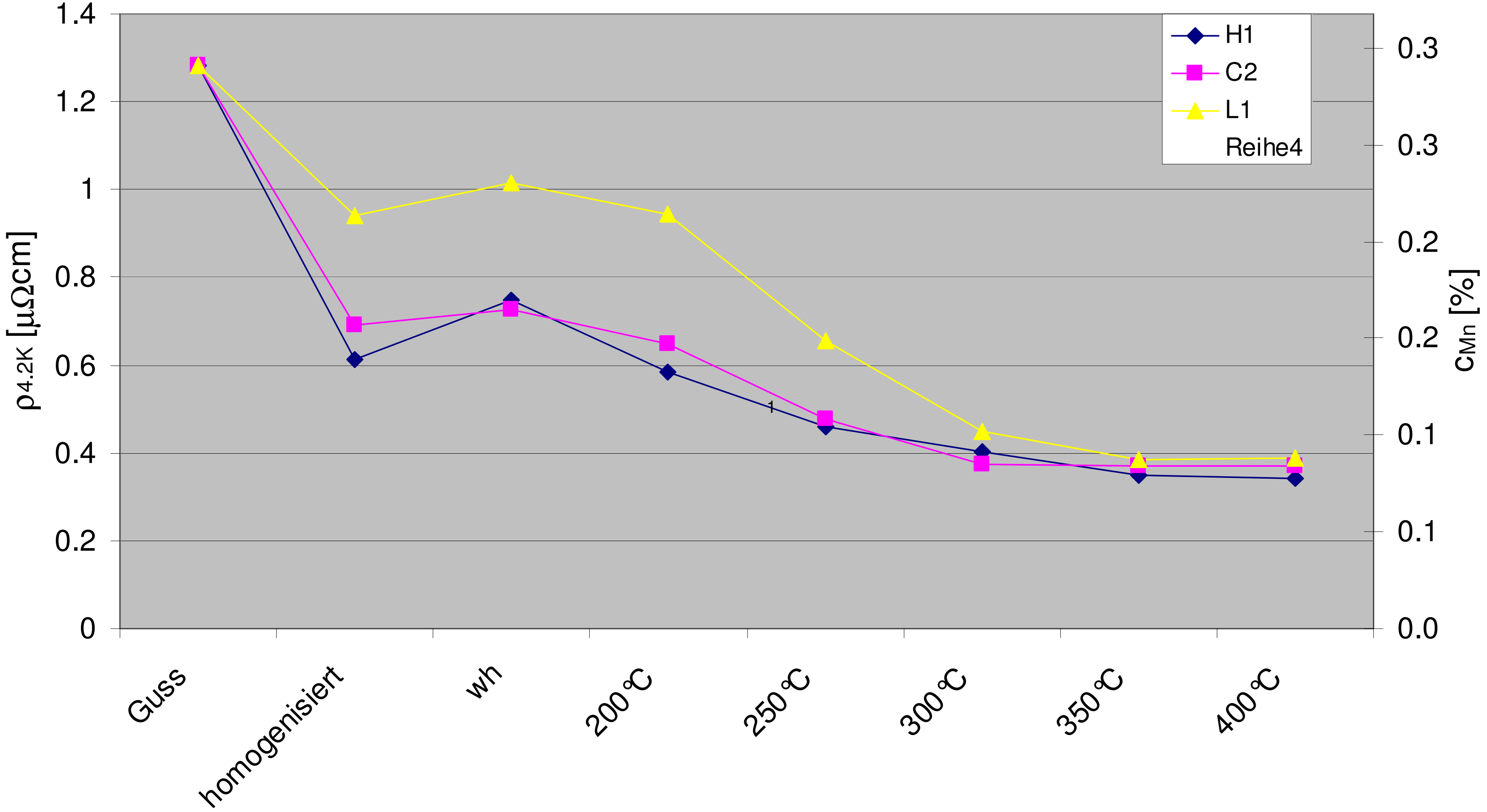


HYDRO

Recrystallization of AA 8006 electrical resistivity

$$\rho_{4.2K} \approx \alpha_{Mn} \cdot c_{Mn}$$

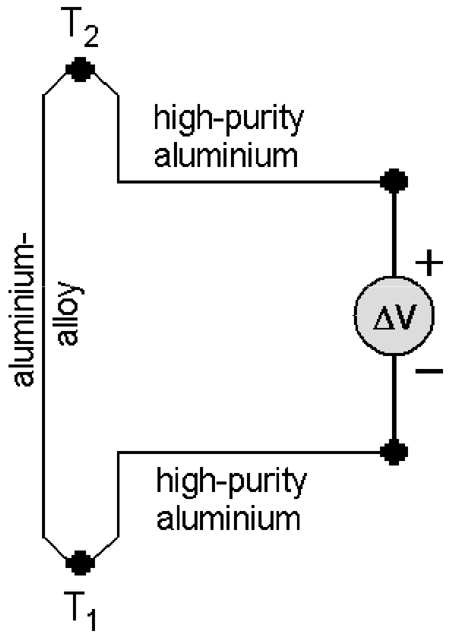
$$\alpha_{Mn}^{4.2K} = 3.7775 \quad \mu\Omega \cdot cm / wt\%$$



Recrystallization of AA 8006

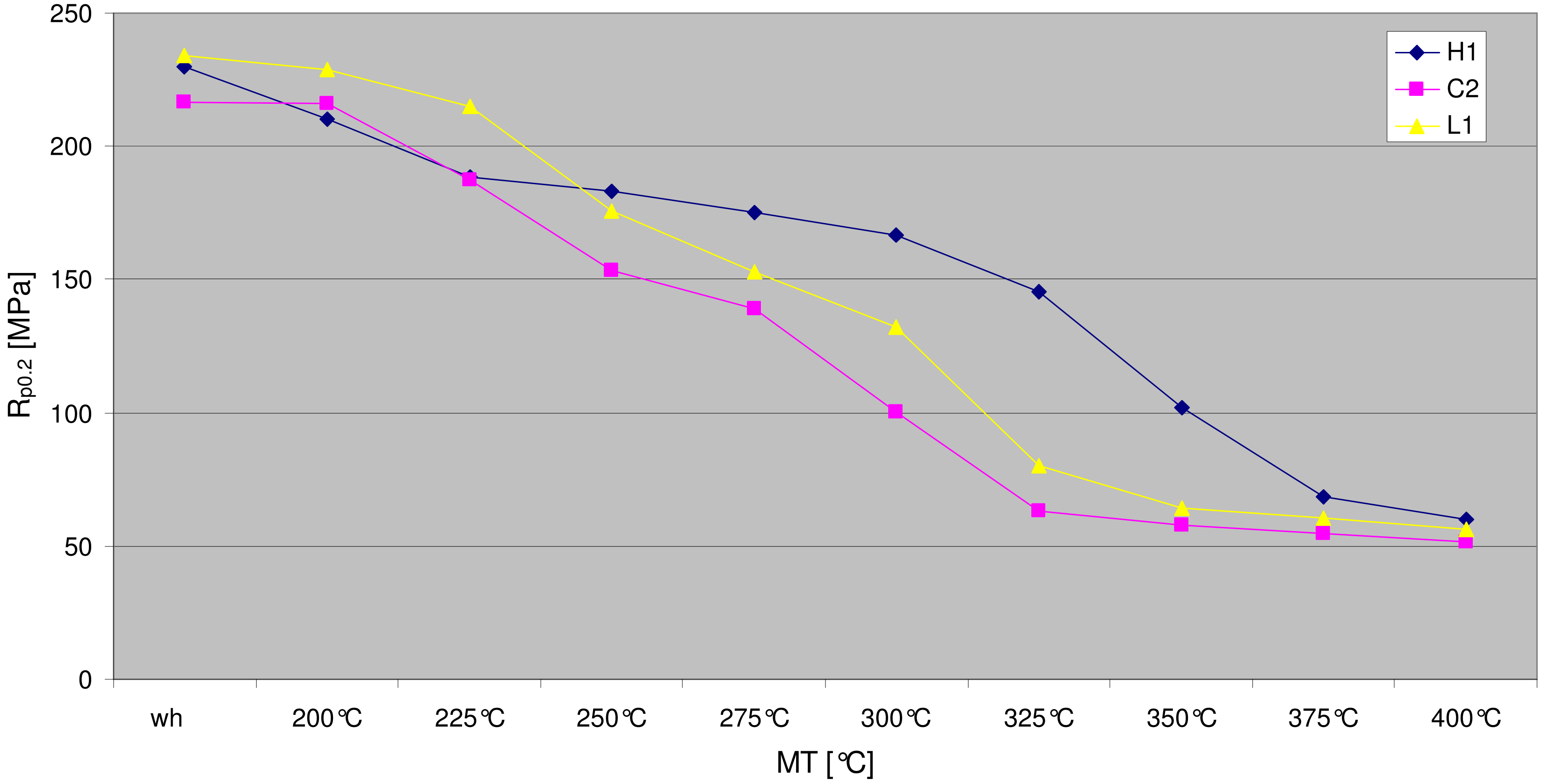
Thermo-Electric Power (TEP)

	as-cast		homogenised			RX 400°C	
	1048	746	747	748	764	765	766
Si	**0.106**	**0.009**	**0.056**	**0.107**	**0.003**	**0.003**	**0.003**
Fe	**0.048**	**0.048**	**0.048**	**0.044**	**0.002**	**0.002**	**0.010**
Cu	0.052	0.057	0.046	0.058	0.002	0.002	0.002
Mn	**0.214**	**0.066**	**0.080**	**0.135**	**0.041**	**0.054**	**0.054**
Mg	0.033	0.004	0.005	0.033	0.002	0.002	0.002
Cr	0.002	0.002	0.002	0.002	0.002	0.002	0.002
Zn	0.003	0.003	0.003	0.003	0.003	0.003	0.003
Ti	0.004	0.004	0.004	0.004	0.004	0.004	0.004
	as-cast	H1	C2	L1	H1	C2	L1



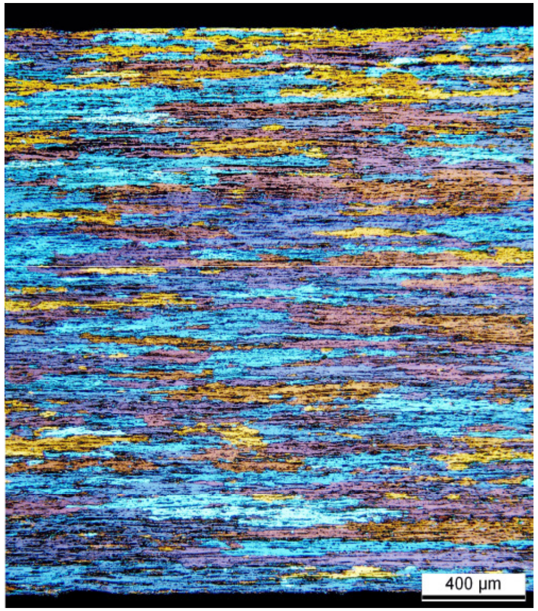
HYDRO

Recrystallization of AA 8006 mechanical properties

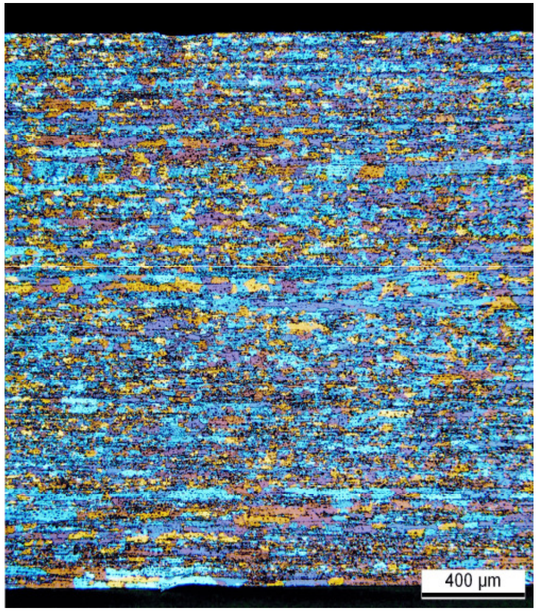


Recrystallization of AA 8006
Metallography

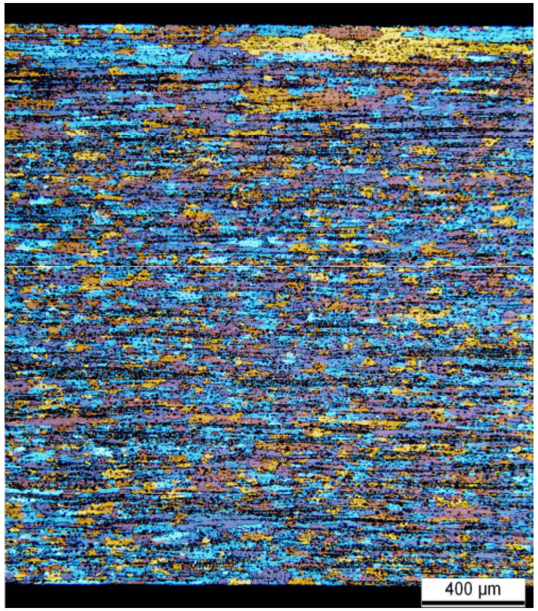
cold rolled, back annealed at 400°C (anodised, longitudinal section, 50:1)



H1 (480°C)

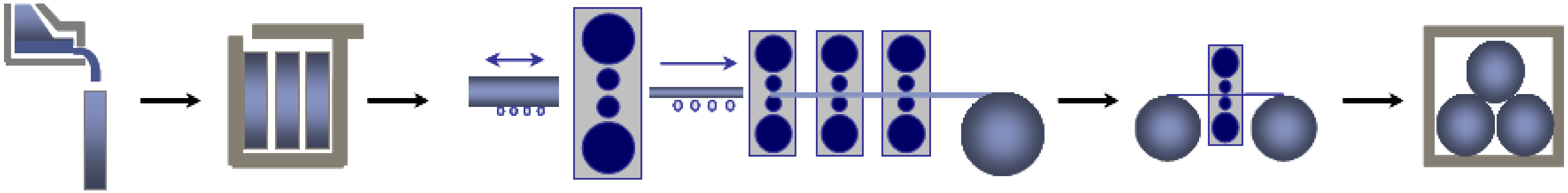


C2 (600°C/500°C)



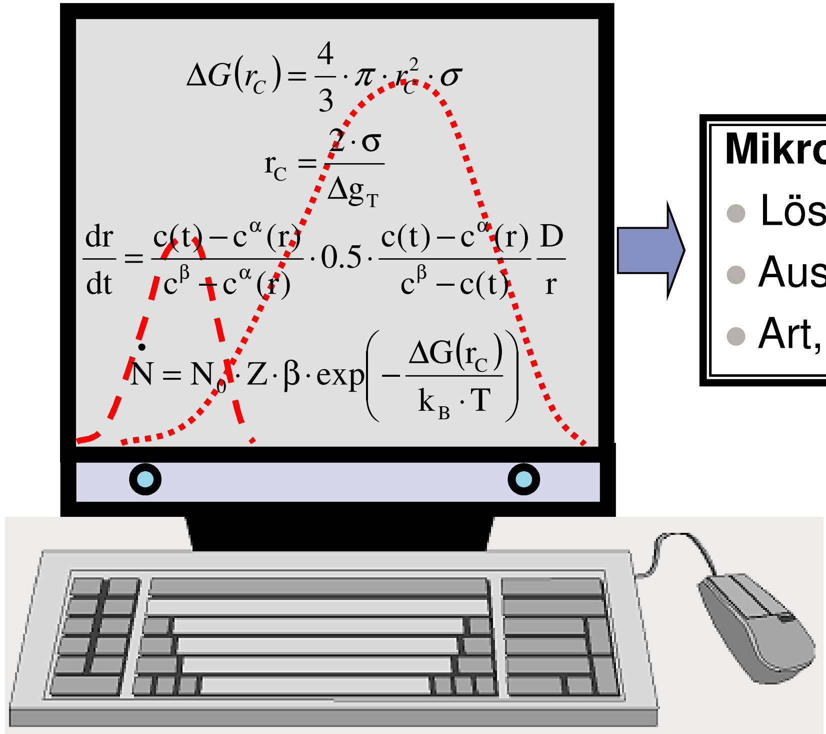
L1 (600°C)

Einleitung: ClaNG Modell
"*Cla*ssical *N*ucleation and *G*rowth"



Prozess-Parameter
- Zeit
- Temperatur
- Versetzungsdichten

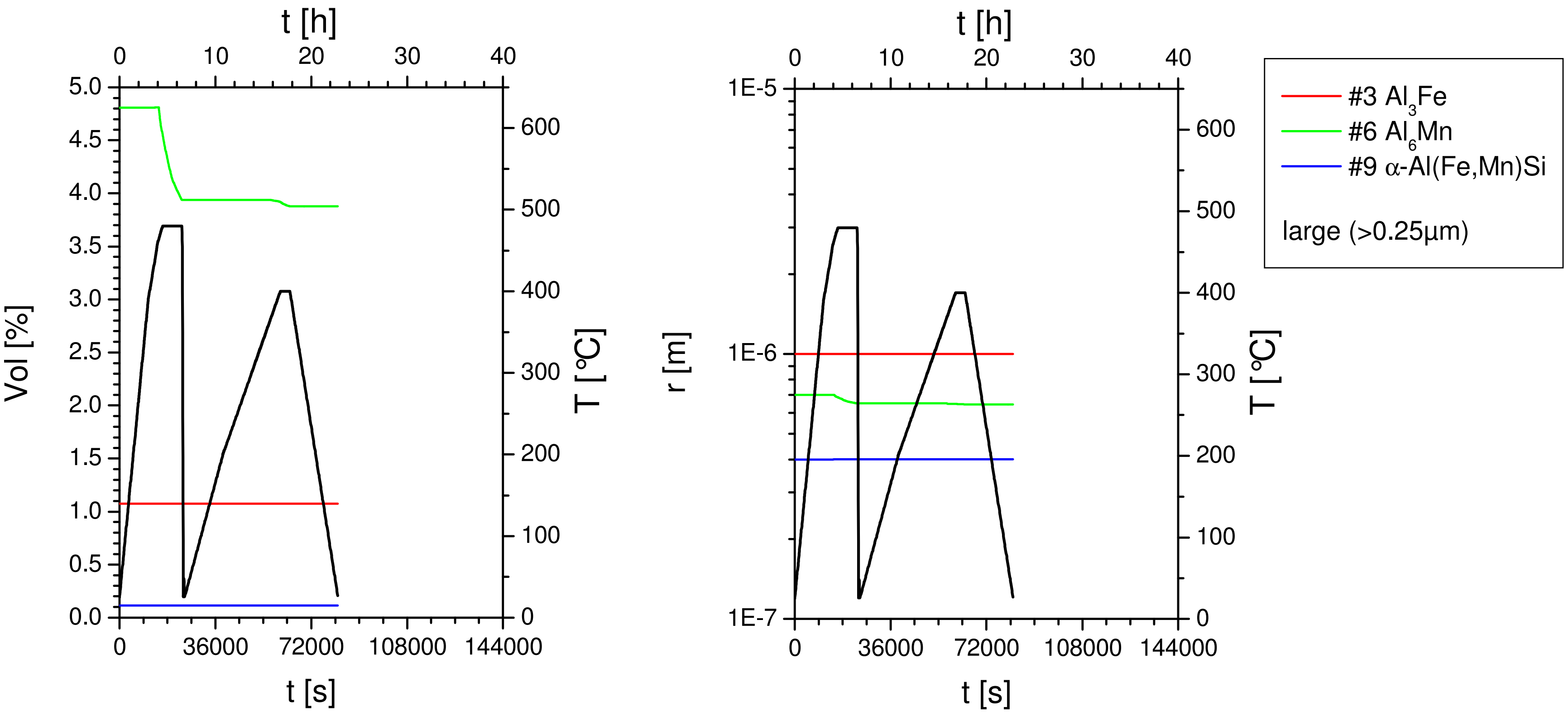
Thermodynamische Daten
- Legierung
- Zustandsdiagramm
- Diffusionskoeffizienten
- Grenzflächenenergie



Mikrochemie
- Lösungszustände c_i
- Ausscheidungen $V_i(r)$
- Art, Größe, Volumen

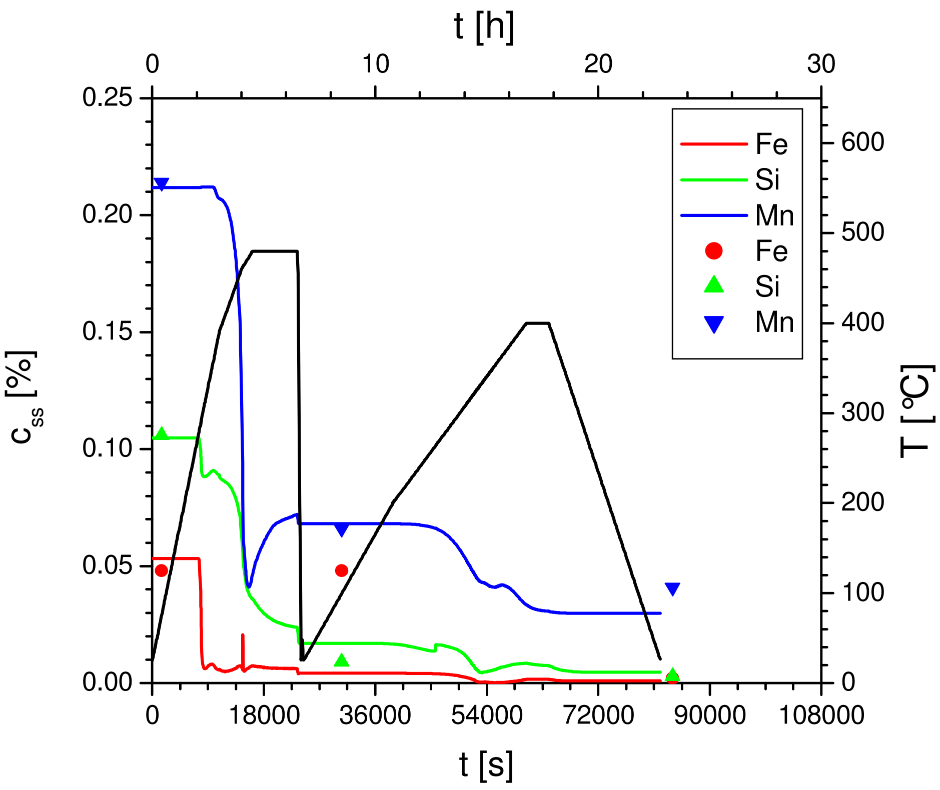
Input → ClaNG-Modell → Output

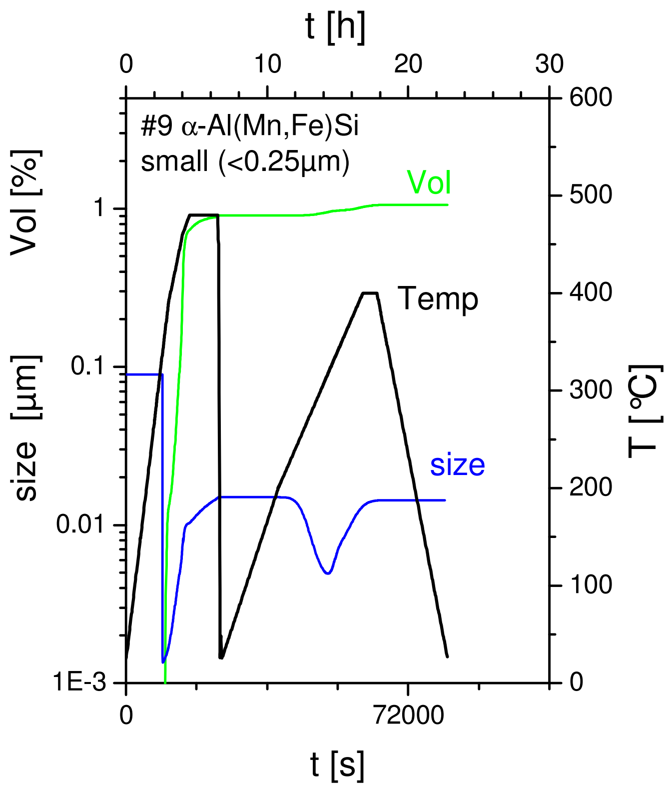
Recrystallization of AA 8006
ClaNG simulation constituents (H1)



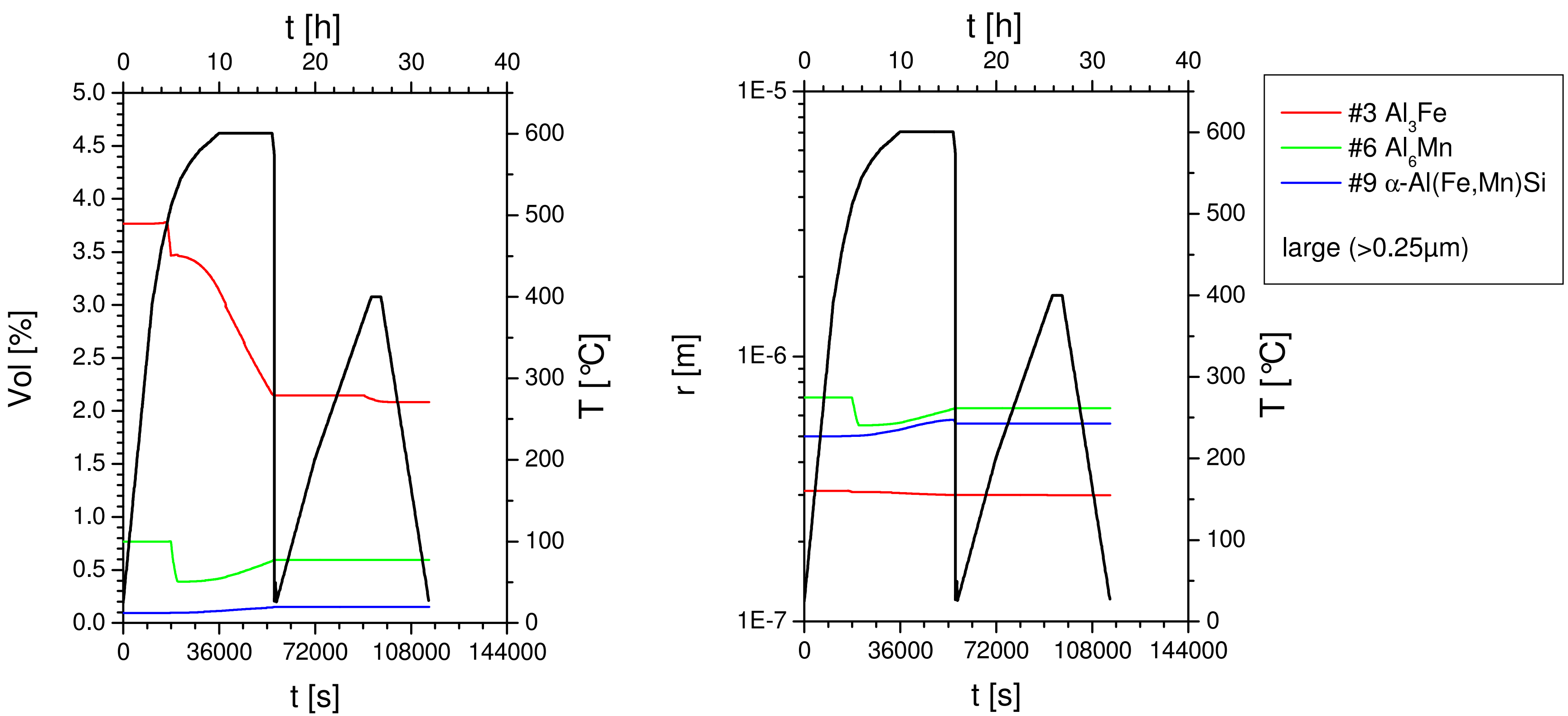
HYDRO

Recrystallization of AA 8006
ClaNG simulation solids & dispersoids (H1)



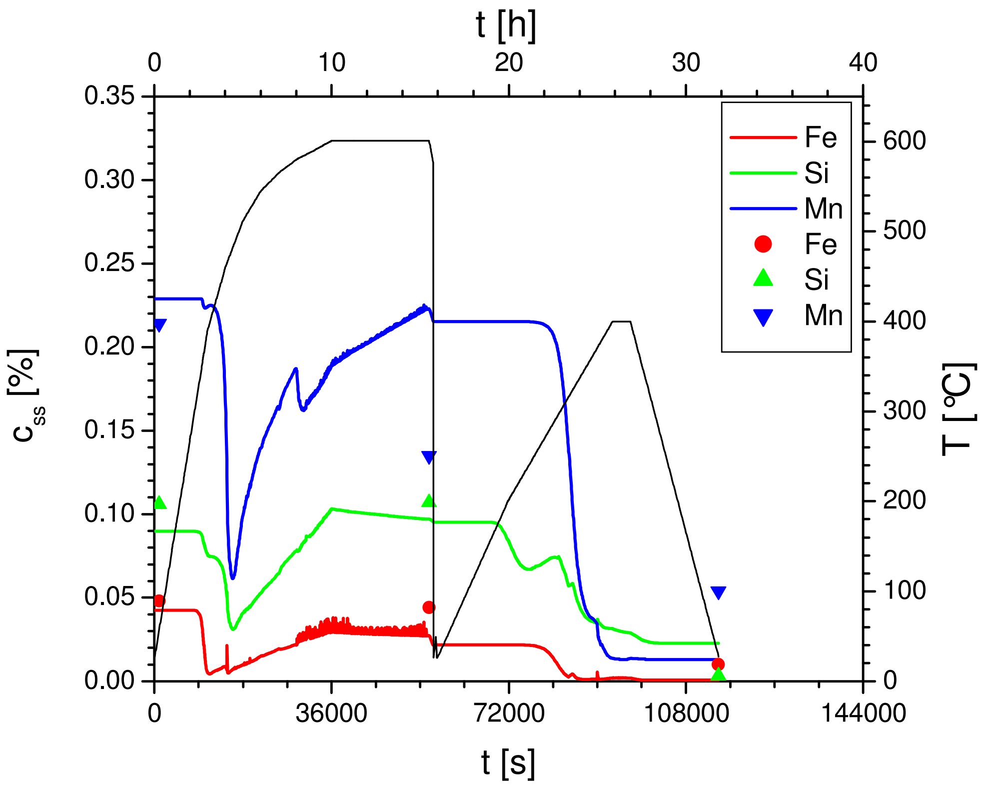


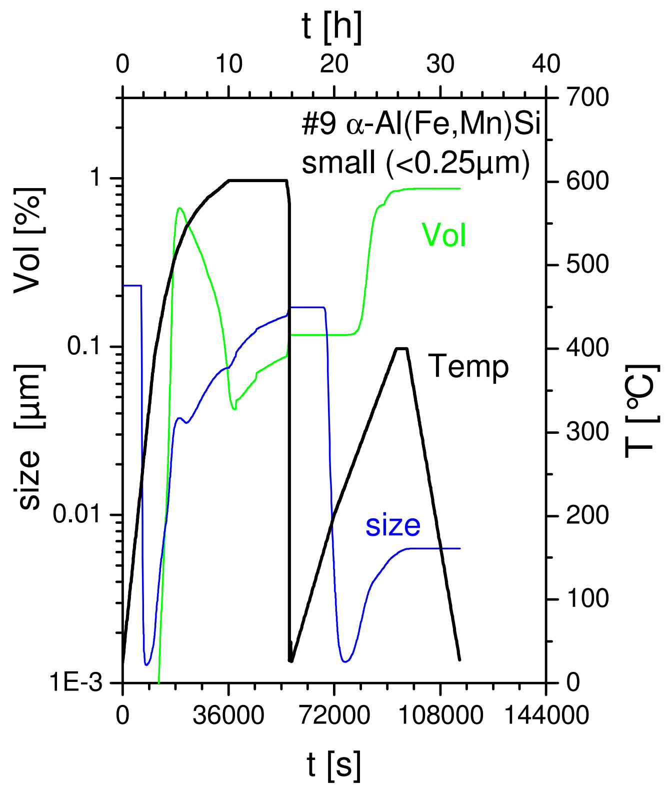
Recrystallization of AA 8006
ClaNG simulation constituents (L1)



HYDRO

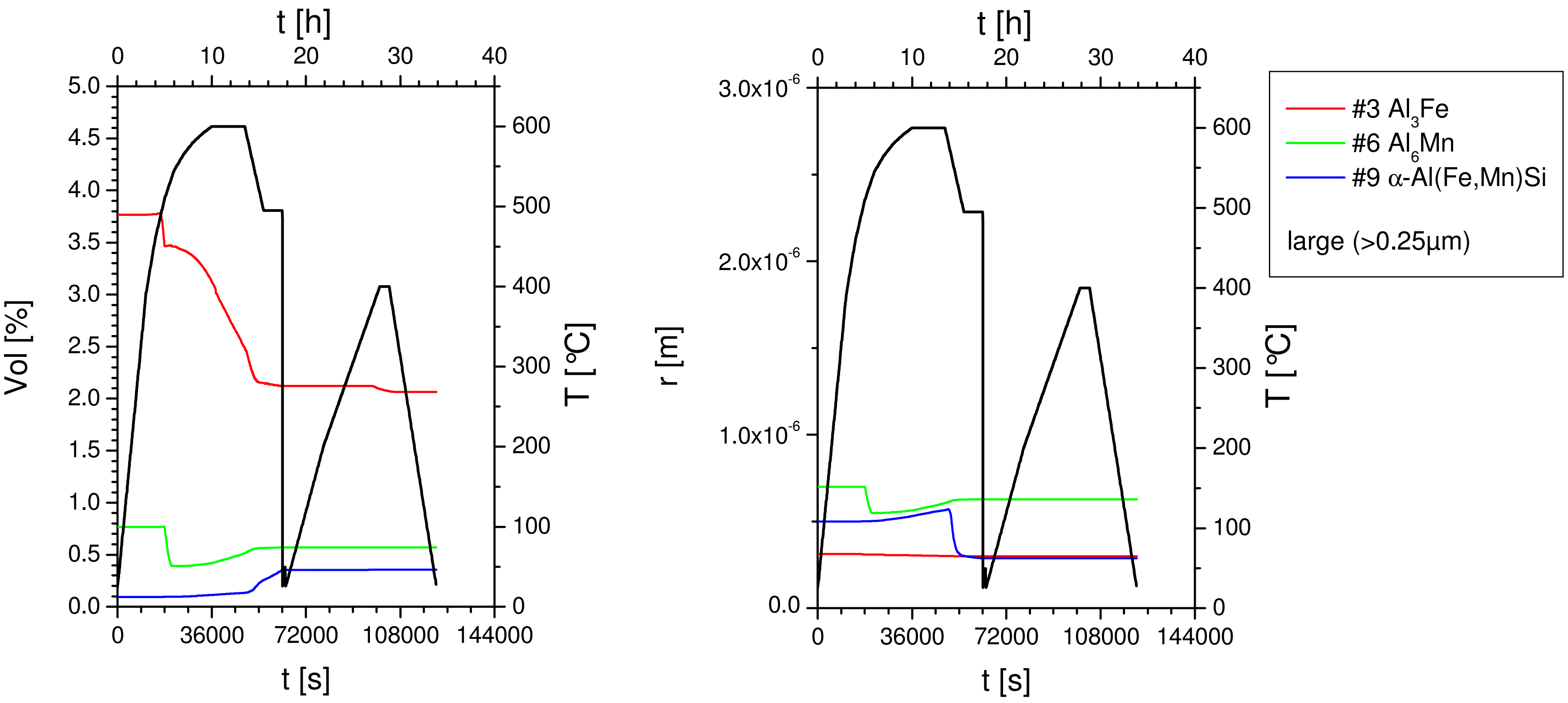
Recrystallization of AA 8006
ClaNG simulation solids & dispersoids (L1)





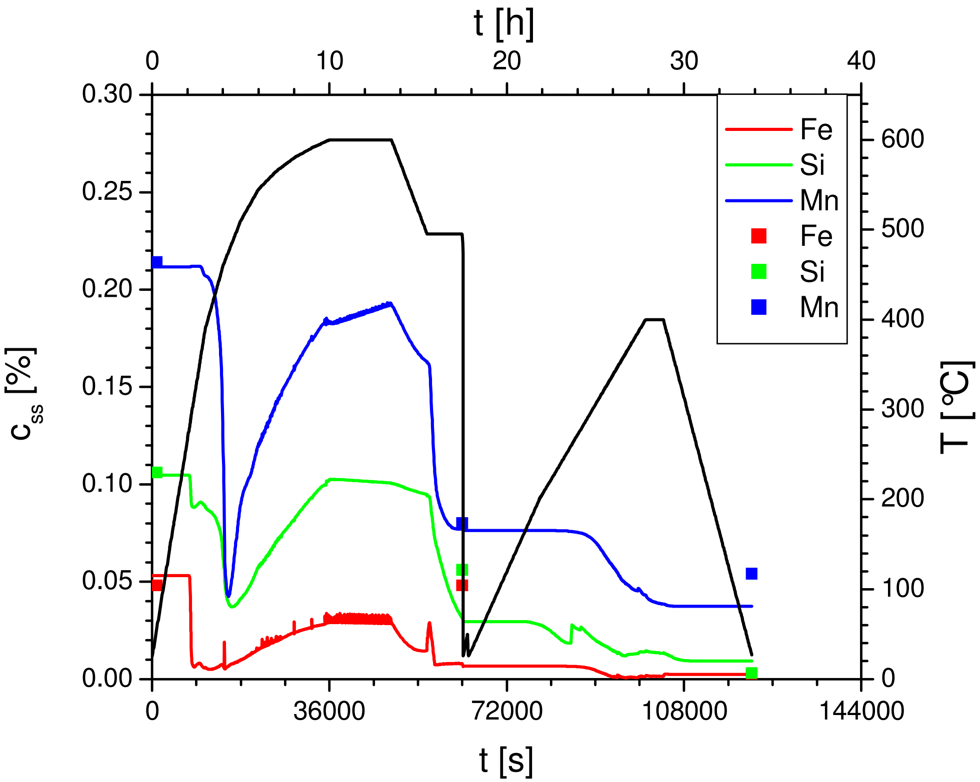
HYDRO

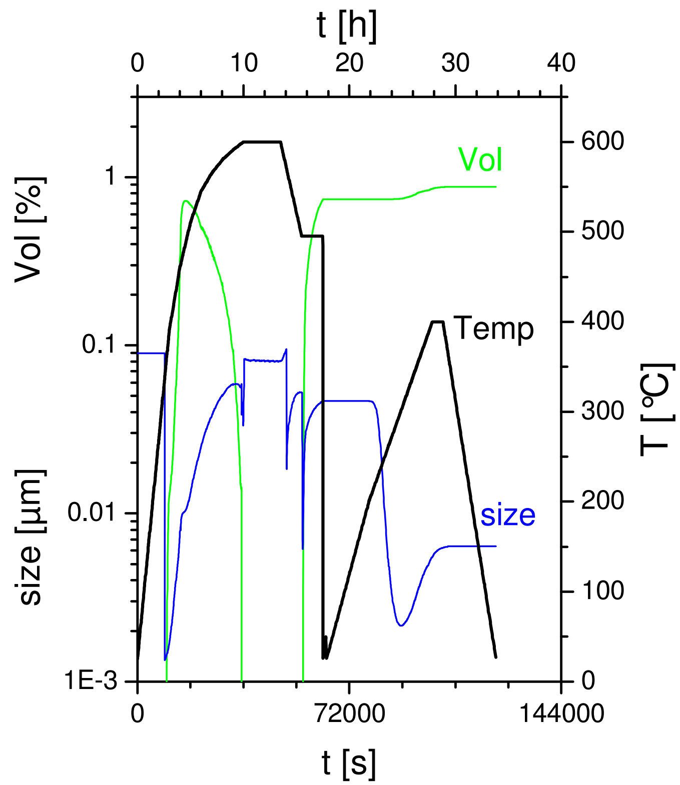
Recrystallization of AA 8006
ClaNG simulation constituents (C2)



HYDRO

Recrystallization of AA 8006
ClaNG simulation solids & dispersoids (C2)





Recrystallization of AA 8006
Summary and Conclusions

- **Homogenisation**
  - H1 (480°C): massive precipitation of Mn-bearing secondary phases
  - C2 (600/500°C): (i) precipitation and re-dissolution of Mn-bearing secondary phases, (ii) precipitation of coarse Mn-bearing dispersoids and/or growth of constituents
  - L1 (600°C): precipitation and re-dissolution of Mn-bearing secondary phases

- **Rolling + recrystallisation**
  - H1: high density of fine secondary phases → strong inhibition of ReX
  - C2: coarse dispersoids → minimum inhibition of ReX
  - L1: strong supersaturation but „concurrent precipitation" → medium inhibition of ReX
- **the ClaNG model allows analysing the evolution of micro-chemistry (solutes, particles) along the process chain of Al-alloys**

www.hydro.com

HYDRO