Modeling Texture Evolution in Metals with CA Model

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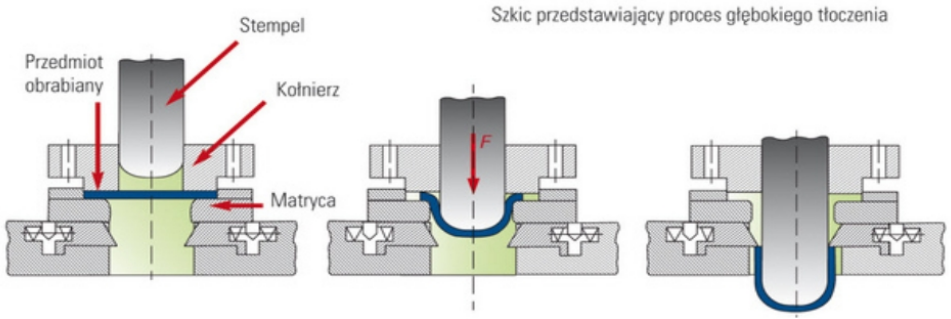
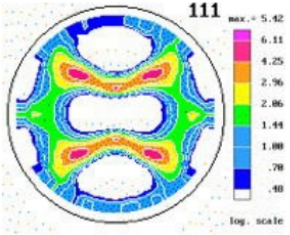
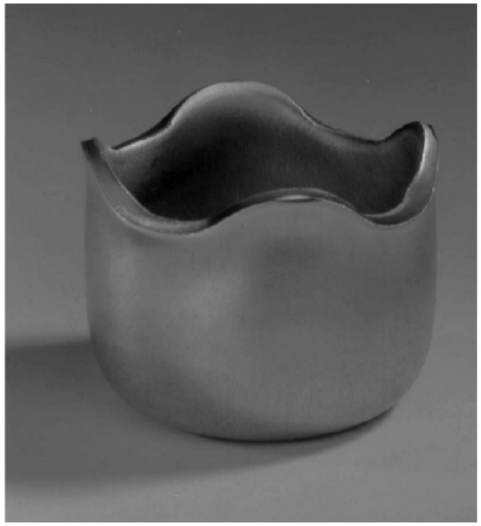
Motivation

- Increasing demand for new emerging alloys e.g: automotive and transport industry,
- New applications: **hydrogen storage, biodegradable materials**
- Anisotropy of properties
- The plastic deformation of some important alloys is rather problematic due to the strong anisotropy of hexagonal structure – formation of strong basal texture during e.g. rolling
- The ductility of the alloys can be enhanced by means of weakening texture in many different ways:
  - changing of the rolling direction
  - introducing shear component of deformation e.g. in differential speed rolling processing (DSR)
  - dynamic recrystallization (DRX)
  - DRX + massive twinning during rolling at very high strain rates (≥ 101 s-1)

Anistoropy in metals

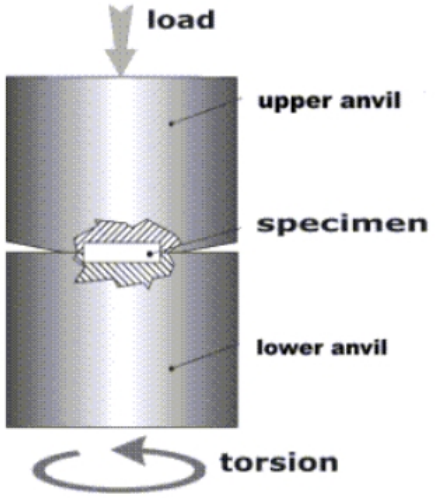




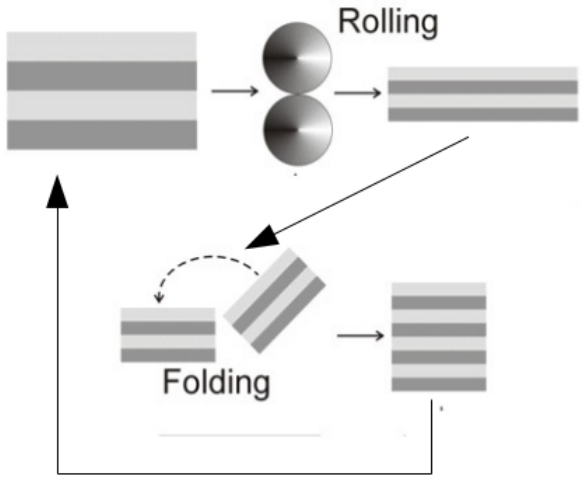


Severe plastic deformation methods

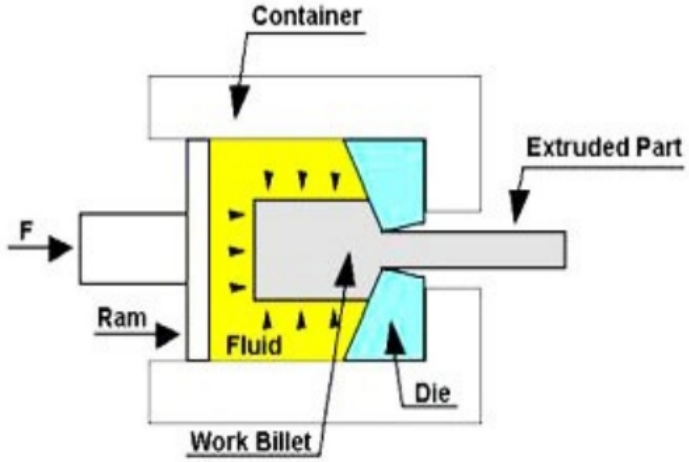
High Pressure Torsion (HPT)



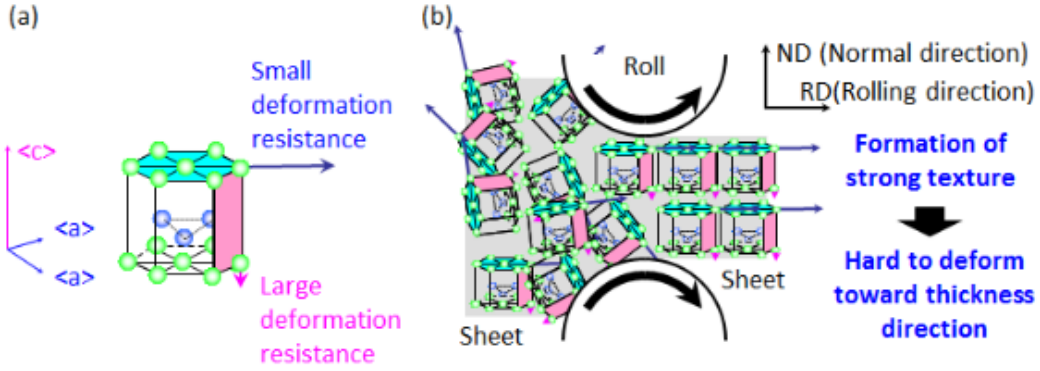
Cold Rolling and Folding (CR&F)

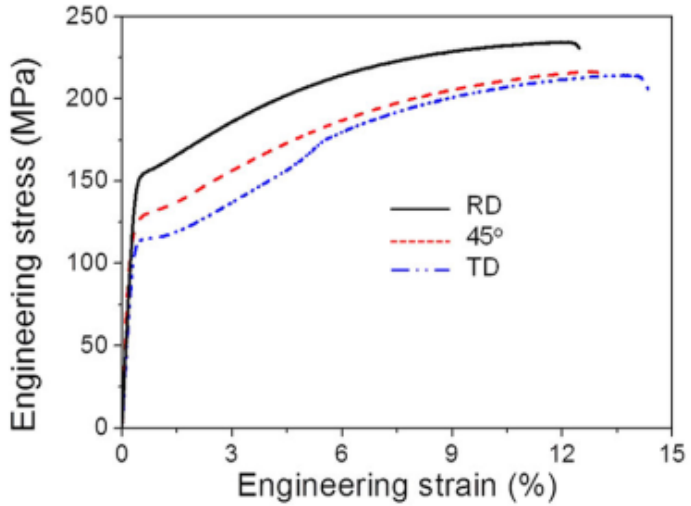


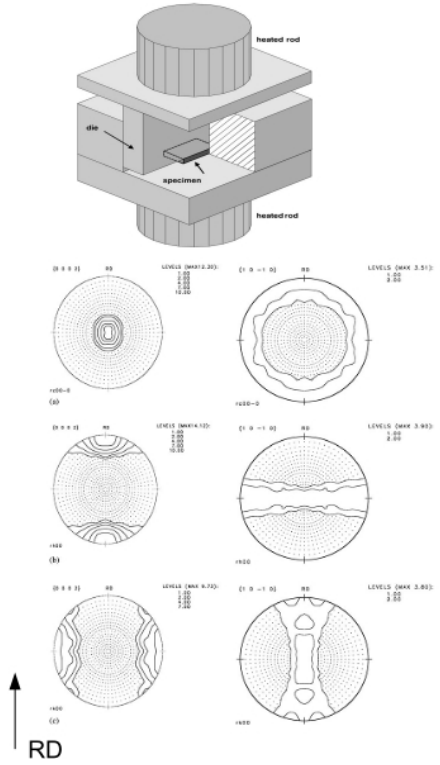
Hydrostatic Extrusion (HE)

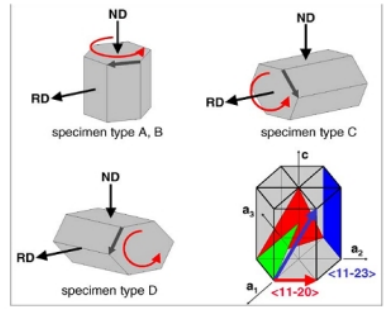


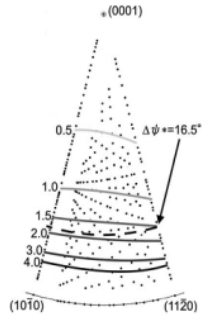
Mechanical anisotropy of HCP metals





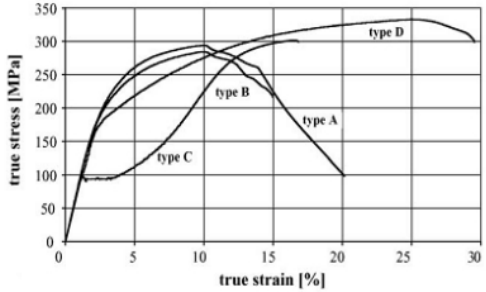






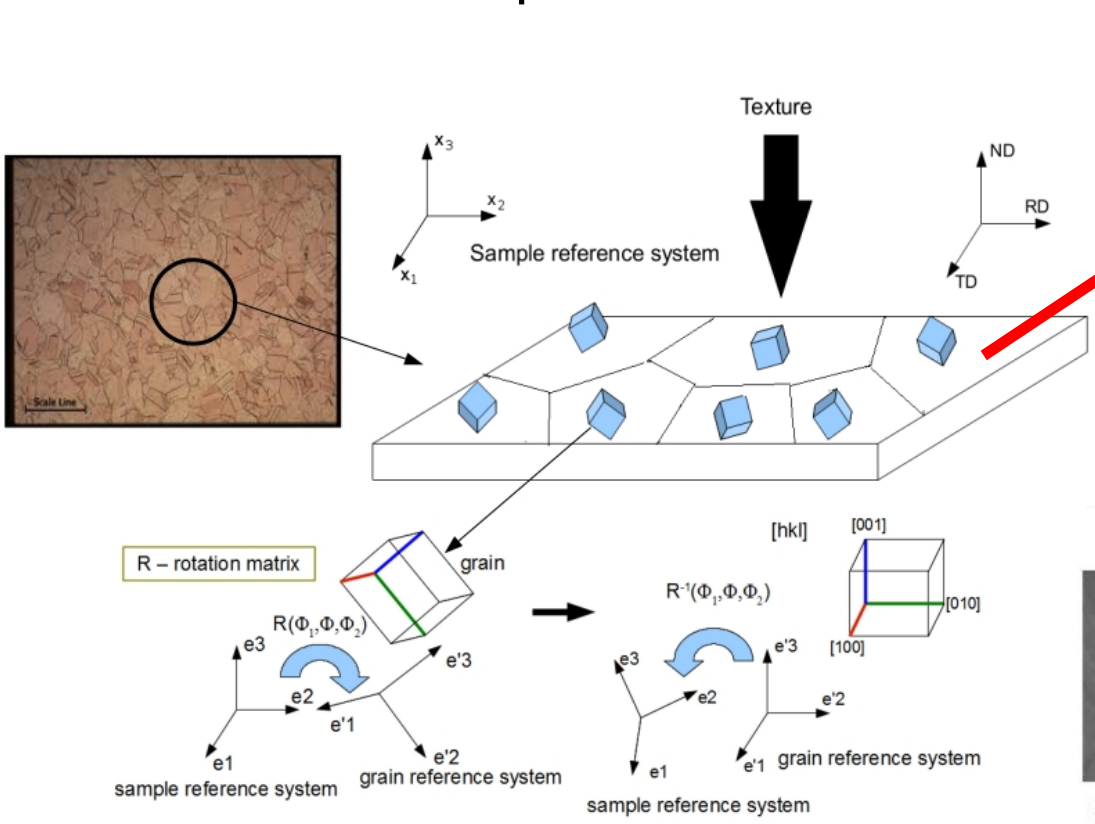
Acta Materialia 53 (2005) 1963–1972
J. Koike, R. Ohyama

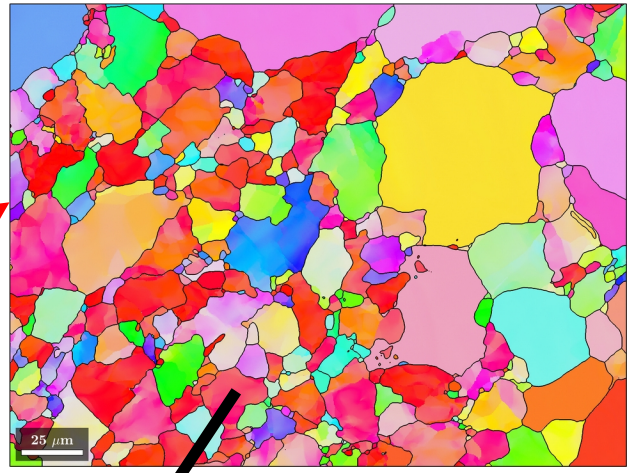
AZ31 at 100 ℃

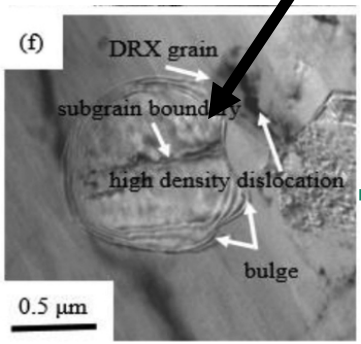


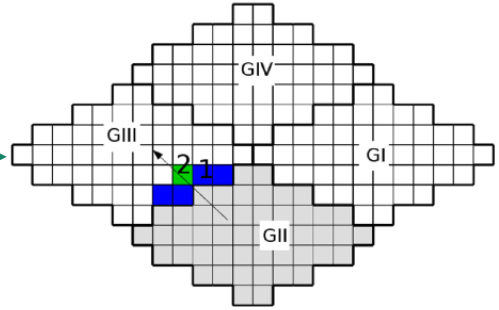
Materials Science and Engineering A 395 (2005) 338–34
R. Gehrmann, MM. Frommert, G. Gottstein

Substructure in hcp metals





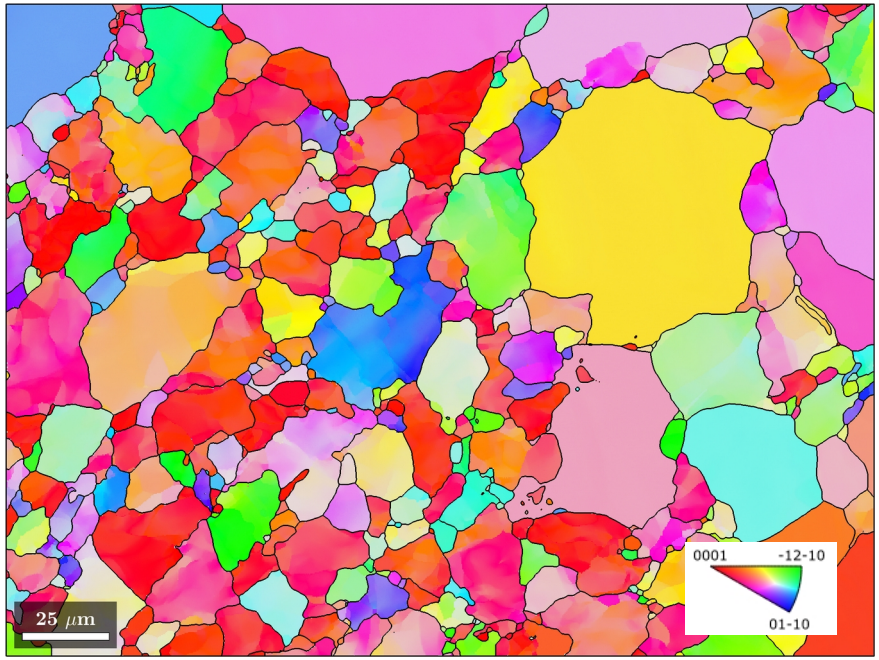


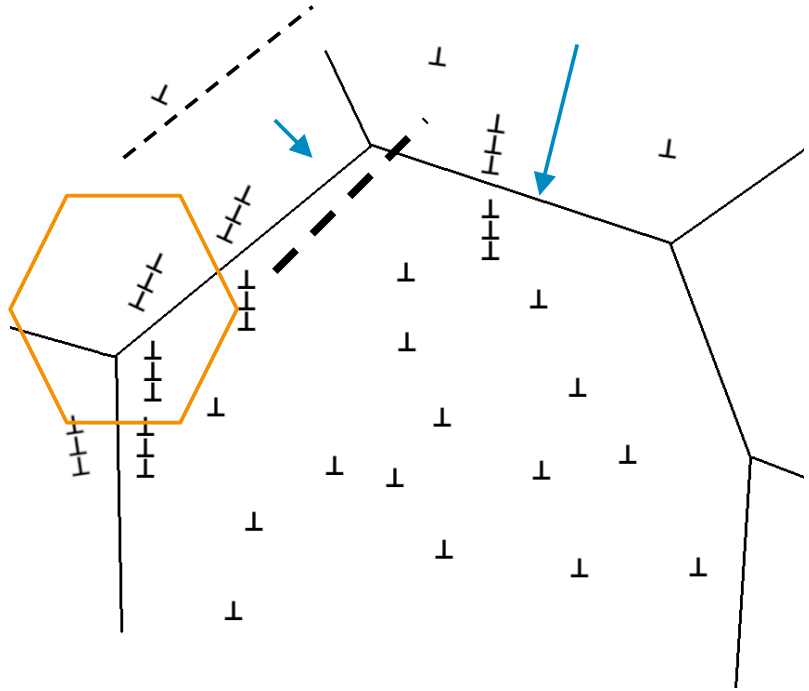


d≈20-30μm ⟶ in 1 cm^3 is about 10^7 grains

Meijuan Hao et al.,
Texture evolution induced by twinning and dynamic recrystallization in dilute Mg-1Sn-1Zn-1Al alloy during hot compression,
10.1016/j.jma.2019.10.002, Journal of Magnesium and Alloys, 2020

Dislocation structure in the grains

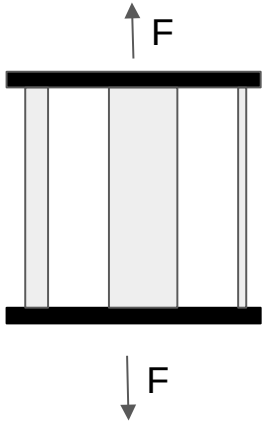




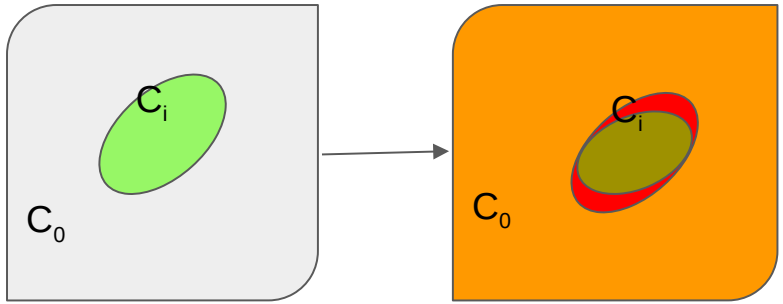
Models for texture evolution in deformed metals

Model Sachsa

Model Taylora



Model vpsc



$$\dot{\gamma}_s = \dot{\gamma}_0 (|\frac{\tau_c^s}{\tau_0^s}|)^{\frac{1}{m}} sign(\tau_c^s)$$

$$\tau_c^s = \tau_0^s + (\tau_1^s + \theta_1^s)(1 - exp(\frac{(-\theta_0^s)}{(\tau_1^s)}))$$

- P. Van Houtte, A Comprehensive Mathematical Formulation of an Extended Taylor-Bishop-Hill Model Featuring Relaxed Constraints, the Renouard-Wintenberger Theory and a Strain Rate Sensitivity Model, Textures and Microstructures, 8-9 (1988), 313-350
- P. Van Houtte, S. Li, M. Seefeldt, L. Delannay, Deformation texture prediction: from the Taylor model to the advanced Lamel model, International Journal of Plasticity 21 (2005), 589–624
- S. Graff, Micromechanical Modeling of the Deformation of HCP Metals, GKSS-Forschungszentrum Geesthacht GmbH, Geesthacht, (2008)
- H.R. Piehler, Crystal-Plasticity Fundamentals, ASM Handbook Volume 22A: Fundamentals of Modeling for Metals Processing (2009)
- H. Wang, P.D. Wu, J. Wang, C.N. Tomé, A crystal plasticity model for hexagonal close packed (HCP) crystals including twinning and de-twinning mechanisms, International Journal of Plasticity 49 (2013), 36–52

Model for texture evolution in hot deformed metals

1	7	7	5	5	6
1	1	5	5	5	5
1	1	5	5	5	5
1	2	2	2	5	4
3	2	2	2	4	4
3	3	2	2	4	4

- D. Raabe, Introductiori of a scalable three-dimensional cellular automaton,with a probabilistic switching rule for the discrete mesoscale simulation of recrystalization pbenomena, Philosophical Magazine A, 79 (1999), 2339-2358
- D. Raabe, L. Hantcherli, 2D cellular automaton simulation of the recrystallization texture of an IF sheet steel under consideration of Zener pinning, Computational Materials Science 34 (2005), 299–313
- L. Wang, G. Fanga, L. Qian, Modeling of dynamic recrystallization of magnesium alloy using cellular automata considering initial topology of grains, Materials Science and Engineering A 711 (2018), 268–283

$$\dot{x} = n\mathfrak{m}p = n\mathfrak{m}_0 \exp\left(\frac{-Q_{GB}}{k_B T}\right) p$$

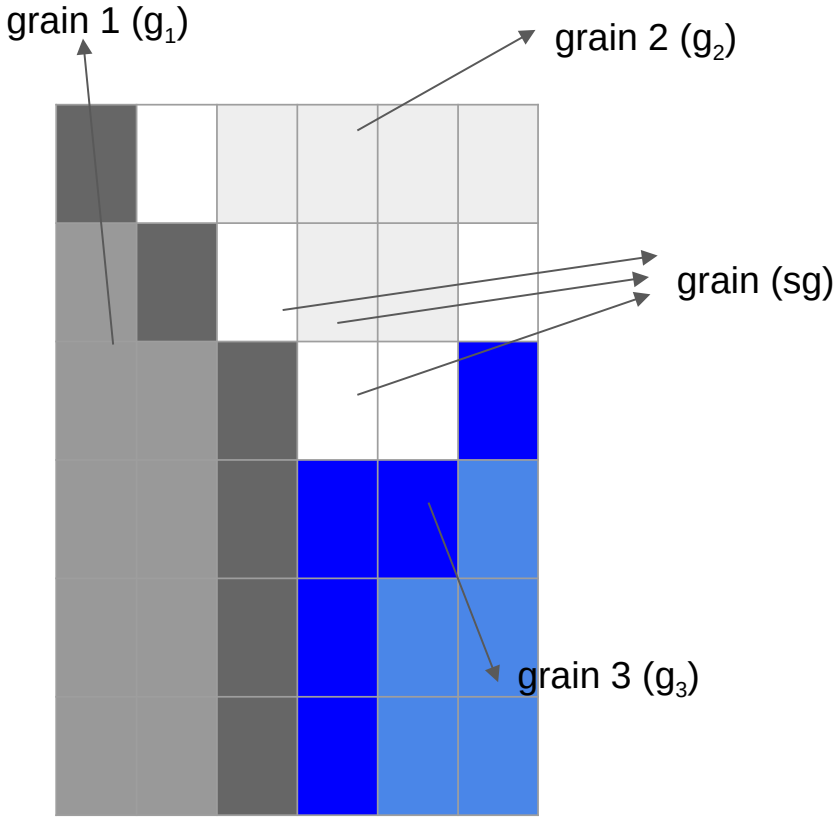
$\dot{x}$ – prędkość przemieszczania się granicy ziarna,
n – normalna do płaszczyzny granicy ziarna,
$\mathfrak{m}$, $\mathfrak{m}_0$ – parametry opisujące ruchliwość granicy ziarna,
Q_{GB} – energia aktywacji przemieszczania się granicy ziarna,
k_B – stała Boltzmanna,
T – temperatura bezwzględna,
p – parametr opisujący sumaryczne naprężenie pędne działające na granicę ziarna.

$$w^{ij} = \zeta\left(\frac{\mathfrak{m}_0^{ij} p^{ij}}{\mathfrak{m}_0^{\max} p^{\max}}\right)\exp\left(\frac{Q^{ij}}{k_B T}\right)$$

w^{ij} – prawdopodobieństwo zmiany stanu komórki c_i na stan komórki c_j,
ζ – maksymalna dozwolona wariancja,
$\mathfrak{m}_0^{ij}$ – mobilność granicy ziarna pomiędzy komórkami c_i i c_j,
p^{ij} – naprężenia działające na granicę ziarna między komórkami c_i i c_j,
$\mathfrak{m}_0^{\max}$ – maksymalna mobilność granicy ziarna,
$p^{\max}$ – maksymalne naprężenie działające na granicę ziarna,
Q^{ij} – energia aktywacji przemieszczania się granicy ziarna pomiędzy komórkami c_i i c_j.

Description of the new *vpsc+CA*

B. Sulkowski, R. Chulist, Modeling of dynamic recrystallization texture in hot extruded Mg, Materials Characterization 201 (2023) 112968



1. $\forall g \forall s : \dot{\gamma}_s = \dot{\gamma}_0 (|\frac{\tau_c^s}{\tau_0^s}|)^{\frac{1}{m}} sign(\tau_c^s)$

$$\tau_c^s = \tau_0^s + (\tau_1^s + \theta_1^s)(1 - exp(\frac{(-\theta_0^s)}{(\tau_1^s)}))$$

$$\forall g : \frac{d\rho_\epsilon}{d\epsilon} = K_1 \sqrt{\rho} - K_2 \rho$$

$$\dot{\omega}_{ij} = \sum_{s=1}^{n} \frac{1}{2}(m_{ij}^s - m_{ji}^s)\dot{\gamma}^s$$

2. $\forall sg : \bar{\rho}_{GNDS} = \frac{2\theta_{nm}}{n\lambda|b_d|}, n \neq m$

$$\bar{\rho} = \rho_\epsilon + \bar{\rho}_{GNDS}$$

grain boundaries movement

$$w^{nm} = \sigma(\frac{m_0^{nm} p^{nm}}{m_0^{max} p^{max}}) exp \frac{-Q_{nm}^{local} + Q_{nm}^{min}}{k_B T}$$

$akceptuj\ jeśli\ r \leq w^{nm}$

$odrzuć\ jeśli\ r > w^{nm}$

nucleation

$$\rho_c = (\frac{20\gamma\dot{\epsilon}}{3blM|\tau^2}))^{1/3}$$

Experimetns and simulations

Mg, AZ31, AM50, AZ61

rolling, extrusion
180°C, 280°C, 380°C

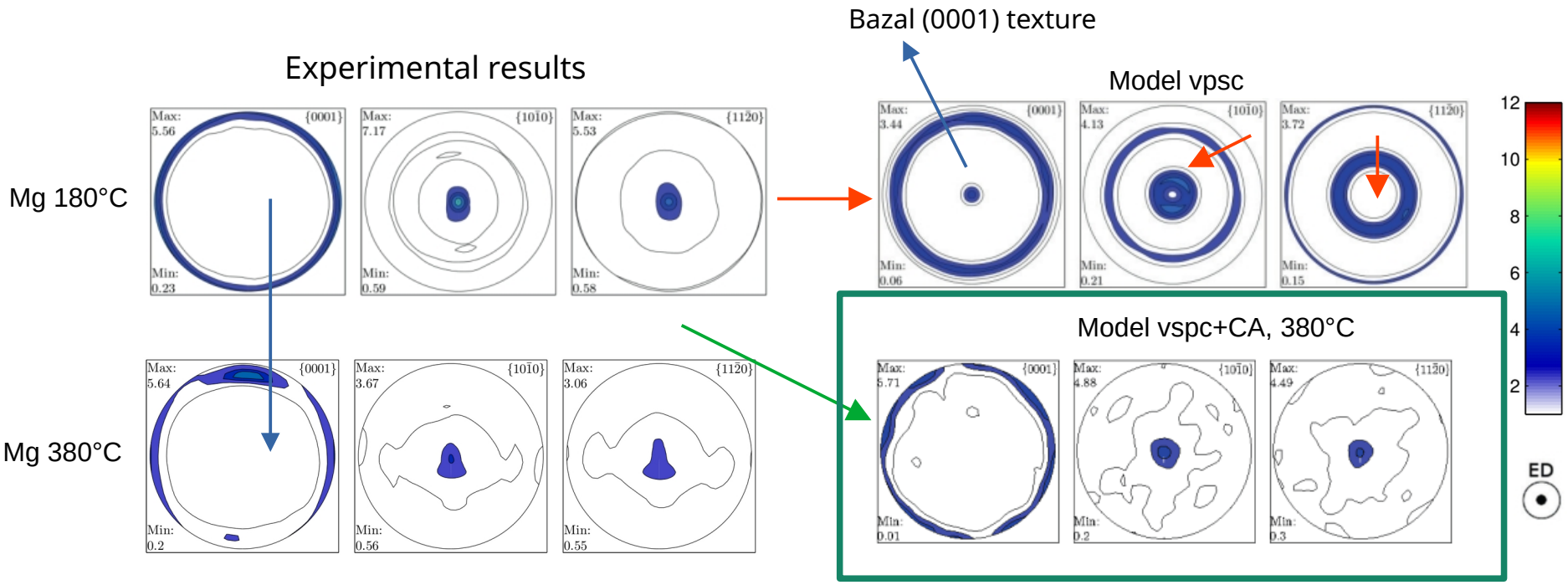
structural investigations, EBSD, texture

simulations
- vpsc
- vpsc+CA

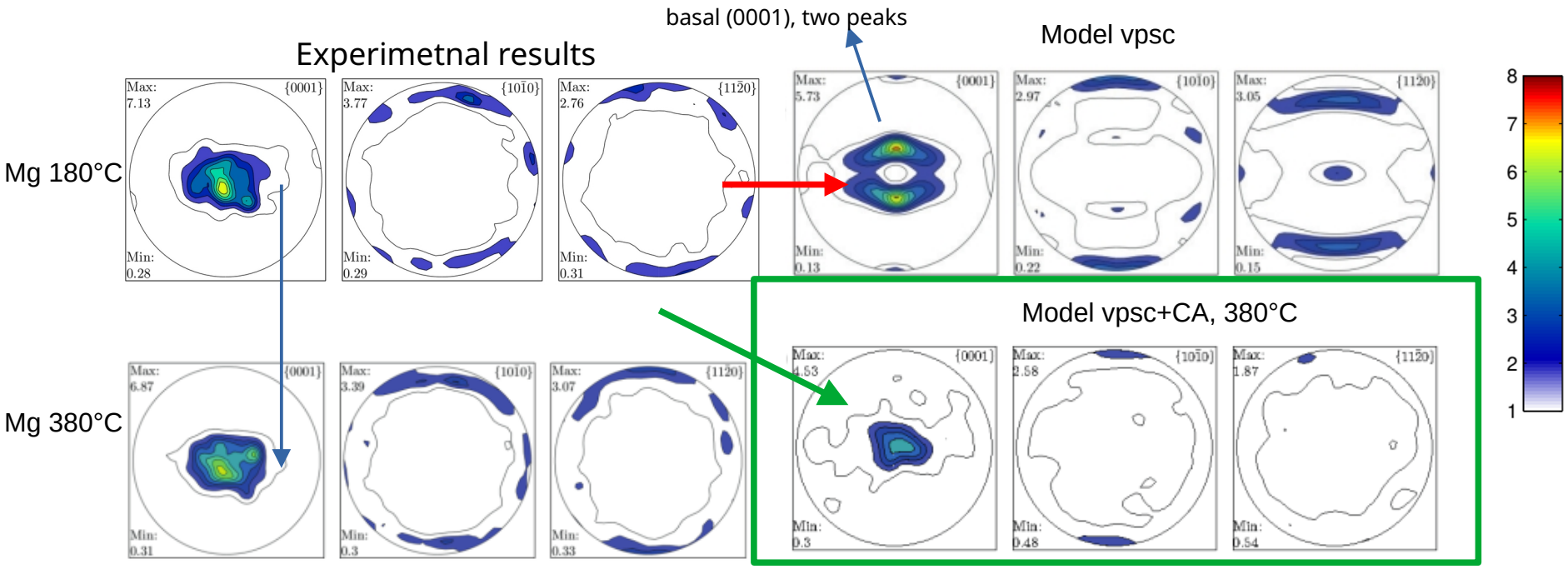
Stop (ASTM)	PN-EN 1753:2001	Al (% wag.)	Zn (% wag.)	Mn (% wag.)	Mg (% wag.)
Mg	EN-MCMg99,8	-	-	-	99,8
AZ31	EN-MCMgAl3Zn1	2,5-3,5	0,6-1,4	-	reszta
AM50	EN-MCMgAl1Mn0	4,4-5,4	0,22	0,26-0,6	reszta
AZ61	EN-MCMgAl6Zn1	5,8-7,2	0,4-1,5	-	reszta

- Number of grains 10^3 – 10^5
- Number of subgrains for each grain 36 – 64
- MPI libraries
- Ares Supecomputer
- 1 node x 1 cpu – 4 nodes x 48 cpus

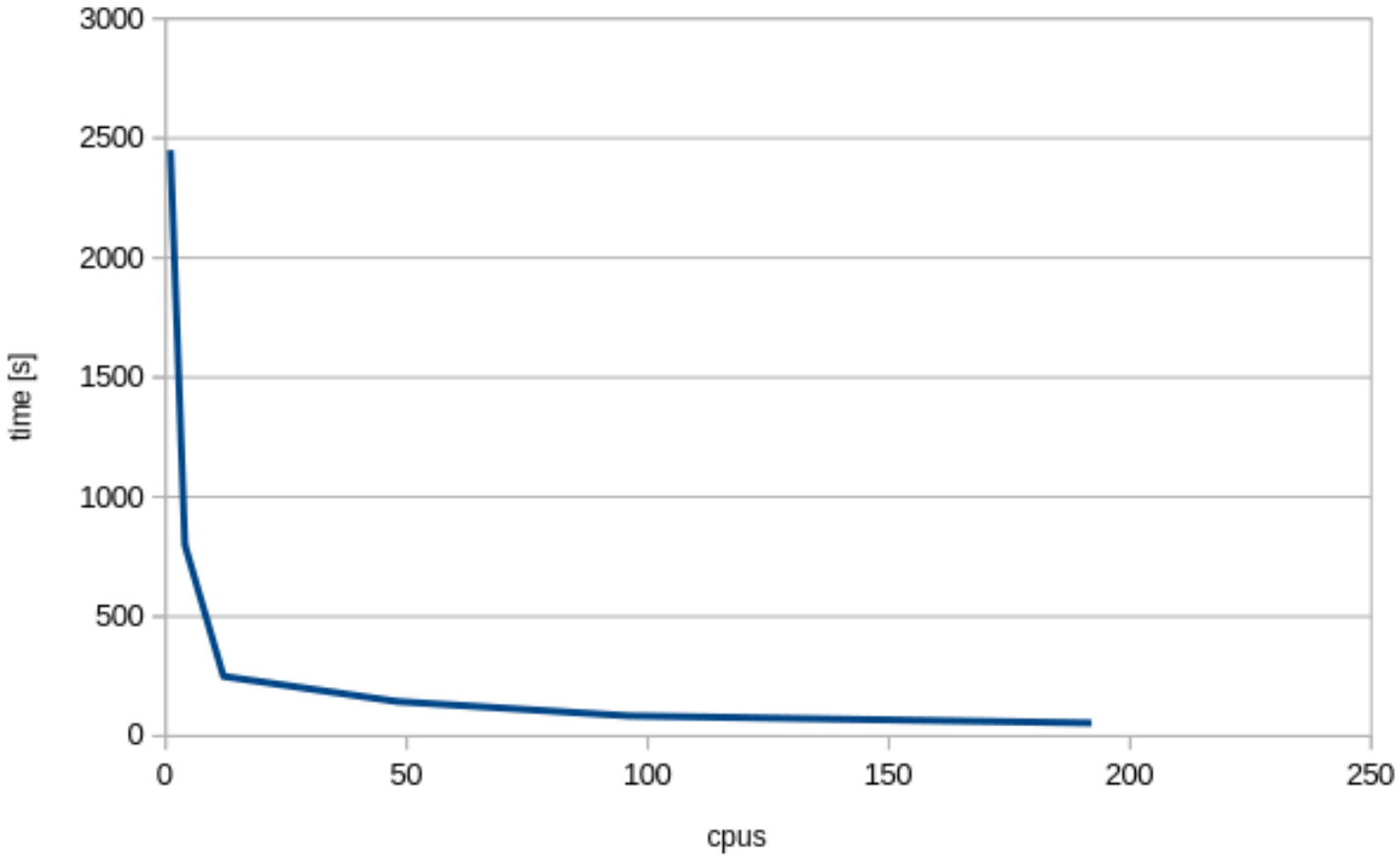
Results for extrusion



Results for rolling



Calculation time



Summary

- Main texture component during rolling is basala
- Main texture componetn during extrusion is {10-10} fibre and {11-20} fibre
- During hot deformation texture is weakened
- VSCP model cant predict hot deformed texture
- VSCP+CA predictions of texture are comparable with experimetns
- Due to the complexity of vpsc+CA model parallel calculations on supercomputer have to be performed

Thank you for your attention