Simulation of Deformation Textures

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Acknowledgement

- The speaker wishes to thank co-workers and colleagues for help on this topic and/or for many valuable discussions:

Saiyi Li
Marc Seefeldt
Laurent Delannay
Olaf Engler
Misha Crumbach
Gunther Gottstein
Pete Bate

The research teams of Hydro and Corus during the VIRFORM project

The research team of OCAS

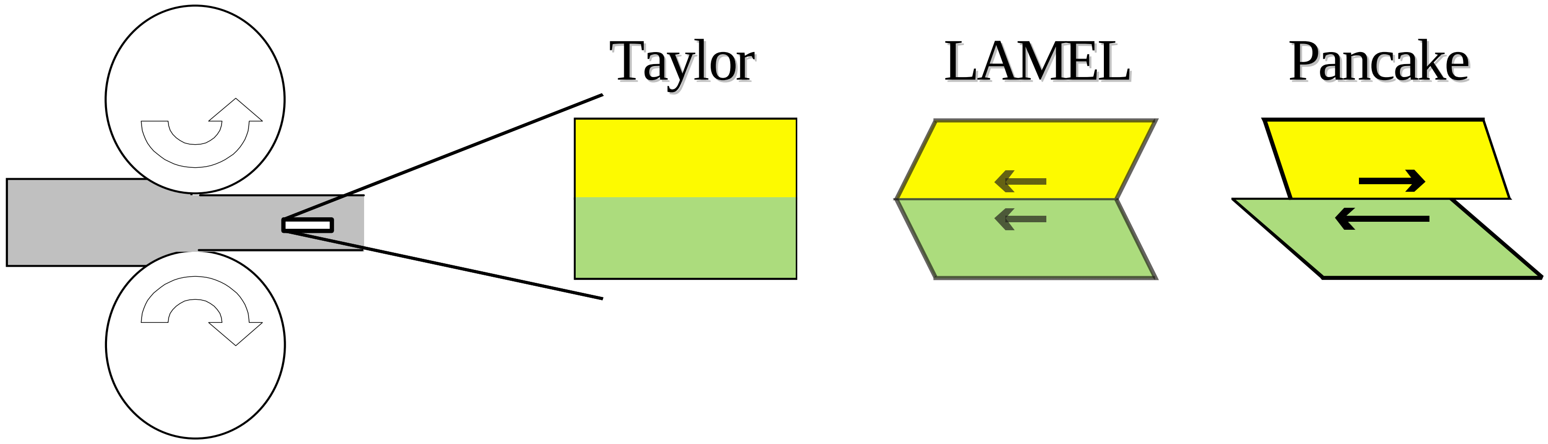
Overview

- Introduction
- Models for deformation texture prediction
- Validation for: aluminium alloys, IF steel, rolling
- Discussion and Conclusions

- **Goal: the development of a model for the prediction of deformation textures which**
  - **predicts quantitatively correct ODFs**
  - **works for all single-phase materials, especially Al alloys**
  - **works for all strain modes**
  - **is fast enough to be incorporated in FE simulations of forming processes or for models which predict formability**

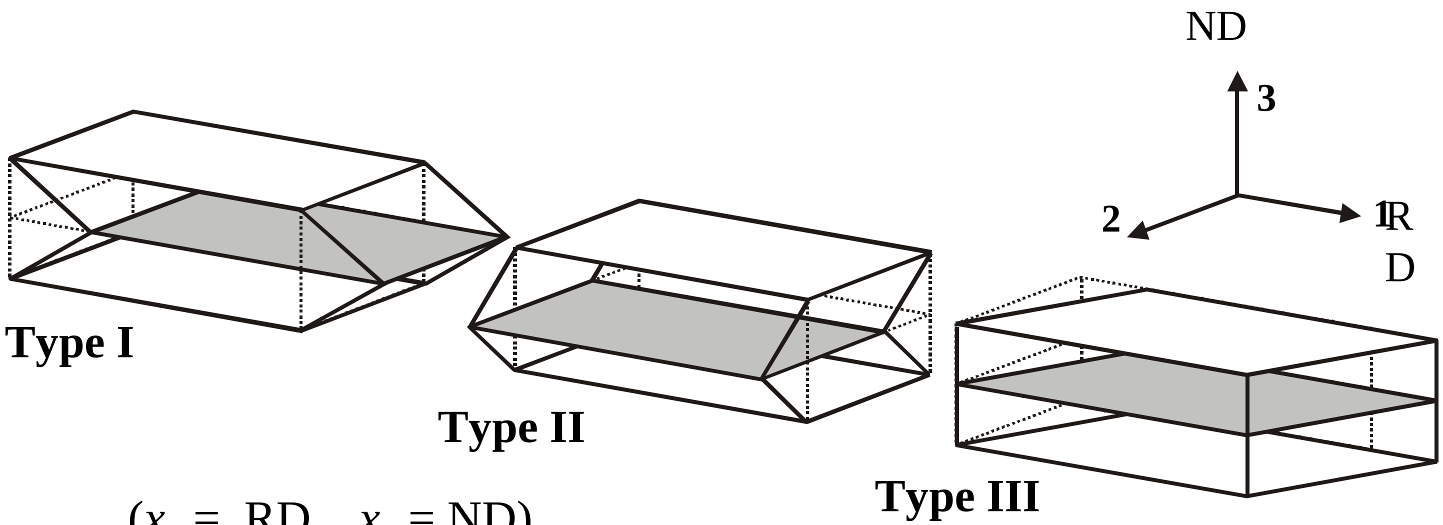
- **Validations are presented for:**
  - **rolling of:**
    - **AA 1200, AA 5182**
      {111}<110> slip systems
    - IF steel
      {110}{112}<111> slip systems

- 2-Grain **Interaction** Model: LAMEL:
  - The interaction of each grain with 1 neighbour is taken into account by forbidding grain boundary sliding (boundary parallel to rolling plane)



  - The plastic work is minimised at once for two grains.
  - The crystallite orientation of each of the 2 grains is chosen at random from the ODF of the sample
    (The ODF is defined as one with triclinic sample symmetry)

- Types of relaxations:



(x_1 = RD x_3 = ND)

- Original Lamel model: Type I (l_{13}) + Type II (l_{23})
- New variant: also Type III (l_{12})

- Relation microscopic-macroscopic deformation for the Lamel model:
  - Grain 1 Grain 2

$$\mathbf{l}^1 = \mathbf{L} - \sum_{r=1}^{R} \tilde{\mathbf{K}}^r \dot{\gamma}_r^{\mathrm{RLX}} \qquad \mathbf{l}^2 = \mathbf{L} + \sum_{r=1}^{R} \tilde{\mathbf{K}}^r \dot{\gamma}_r^{\mathrm{RLX}}$$

R = 2 or 3

Prescribed velocity gradient

Extra unknown variable, to be found

= *R relaxations!*

Meaning of $\tilde{\mathbf{K}}^r$:
(macroscopic frame)

$$\left[\tilde{K}_{ij}^1\right] = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \left[\tilde{K}_{ij}^2\right] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \quad \left[\tilde{K}_{ij}^3\right] = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- Relation is established between **local velocity gradient l** and the slip rates on all slip systems (Taylor equation) *for any given grain*:

$$\mathbf{l} = \mathbf{W}^{\mathrm{L}} + \sum_{s=1}^{N} \hat{\mathbf{b}}^{s} \otimes \mathbf{m}^{s} \dot{\gamma}_{s}$$

Slip rate on slip system *s*

Lattice spin

Unit vector in slip direction

normal to slip plane

This tensor equation is valid in any frame which **does not rotate** with respect to the reference frame of the polycrystal = *macroscopic frame*
The equation can be expressed in scalar notation, using either:
- the macroscopic frame
- the *crystal frame*= a frame which:
at the instant considered is parallel with an orthogonal frame fixed to the principal axes of the crystal,
does not rotate with respect to the macroscopic frame!

- Taylor equations *for the two grains of the Lamel model*:

Grain 1

$$\mathbf{L} = \mathbf{W}^{1\mathrm{L}} + \sum_{s=1}^{N} \hat{\mathbf{b}}^{1s} \otimes \mathbf{m}^{1s} \dot{\gamma}_s^1 + \sum_{r=1}^{R} \tilde{\mathbf{K}}^r \dot{\gamma}_r^{\mathrm{RLX}}$$

Grain 2

$$\mathbf{L} = \mathbf{W}^{2\mathrm{L}} + \sum_{s=1}^{N} \hat{\mathbf{b}}^{2s} \otimes \mathbf{m}^{2s} \dot{\gamma}_s^2 - \sum_{r=1}^{R} \tilde{\mathbf{K}}^r \dot{\gamma}_r^{\mathrm{RLX}}$$

Symmetric parts:

$$\mathbf{D} = \sum_{s=1}^{N} \mathbf{M}^{1s} \dot{\gamma}_s^1 + \sum_{r=1}^{R} \mathbf{D}^r \dot{\gamma}_r^{\mathrm{RLX}}$$

$$\mathbf{D} = \sum_{s=1}^{N} \mathbf{M}^{2s} \dot{\gamma}_s^2 - \sum_{r=1}^{R} \mathbf{D}^r \dot{\gamma}_r^{\mathrm{RLX}}$$

Minimisation of rate of plastic work: 1 equation for both grains together:

$$P^* = \sum_{I=1}^{2} \sum_{s=1}^{N} \tau_s^{cI} \left| \dot{\gamma}_s^I \right| + \sum_{r=1}^{R} \tau_r^{\mathrm{RLX}} \dot{\gamma}_r^{\mathrm{RLX}} \quad = \ \mathrm{Min}$$

To be solved for: $\dot{\gamma}_s^1, \dot{\gamma}_s^2, \dot{\gamma}_r^{\mathrm{RLX}}$

- Stress:
  - Relaxations of Type I and Type II:

    It can be proved that $\sigma'^{1}_{13} = \sigma'^{2}_{13}$ and $\sigma'^{1}_{23} = \sigma'^{2}_{23}$

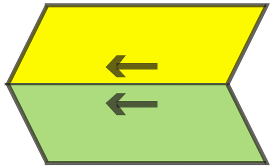
  - Relaxation of Type III:

    As in conventional relaxed constraints model: $\sigma'^{1}_{12} = 0$ and $\sigma'^{2}_{12} = 0$

  - Activated slip systems:
    - Type I + Type II only:
      4 in each grain,
      or 3 in one grain and 5 in the other
    - Type I + Type II + Type III:
      3 in each grain,
      or 4 in one grain and 2 in the other,
      or 5 in one grain and 1 in the other

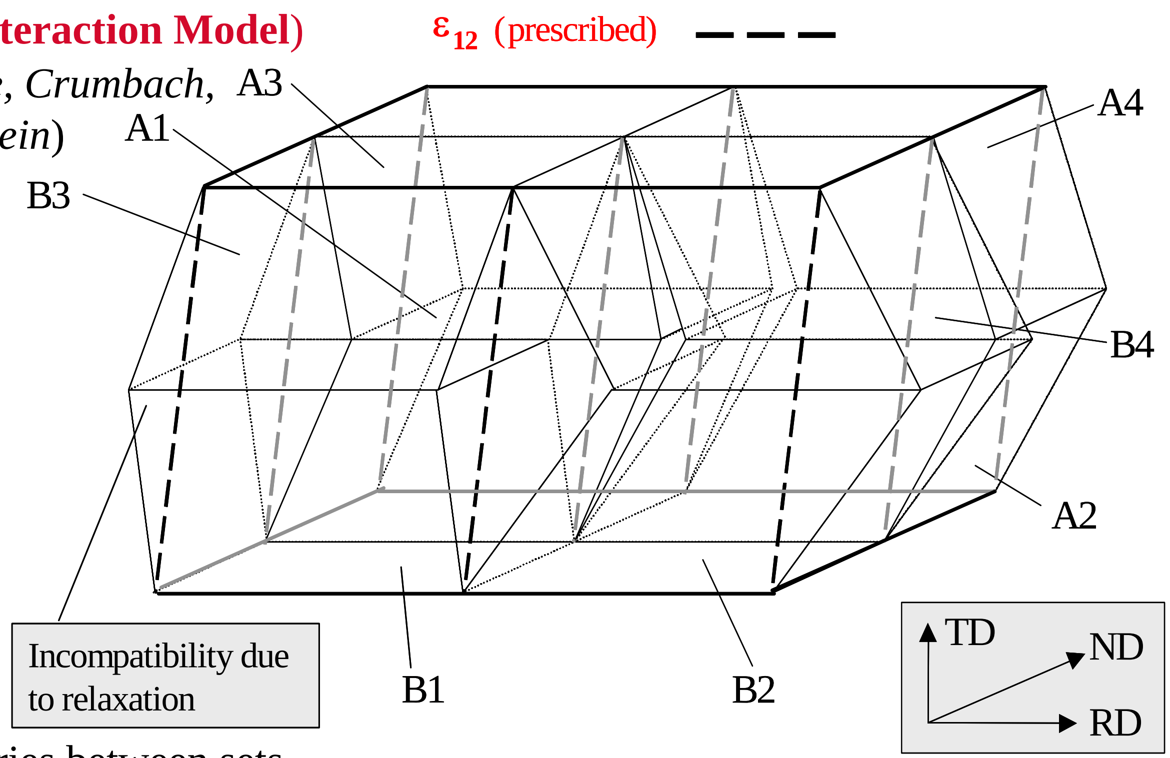
Assessment of LAMEL model:

- Taylor ambiguity does normally NOT occur
- For ROLLING and for ELONGATED grains only
- most opportunities for co-operative slip are recognised and taken into account
- Stress equilibrium: only achieved along interface boundary between Grain 1 and Grain 2 (parallel with rolling plane)



Co-operative slip

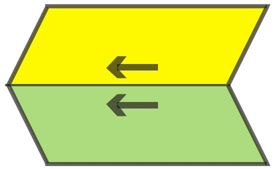
- 8-Grain Interaction Model:
  GIA (Grain **Interaction Model**)
  (*Wagner, Lücke, Crumbach, Pomana, Gottstein*)



- 12 boundaries between sets of 2 grains exist within such cluster.
- Along these boundaries: shears of Type I and Type II (as in the Lamel model) are relaxed.

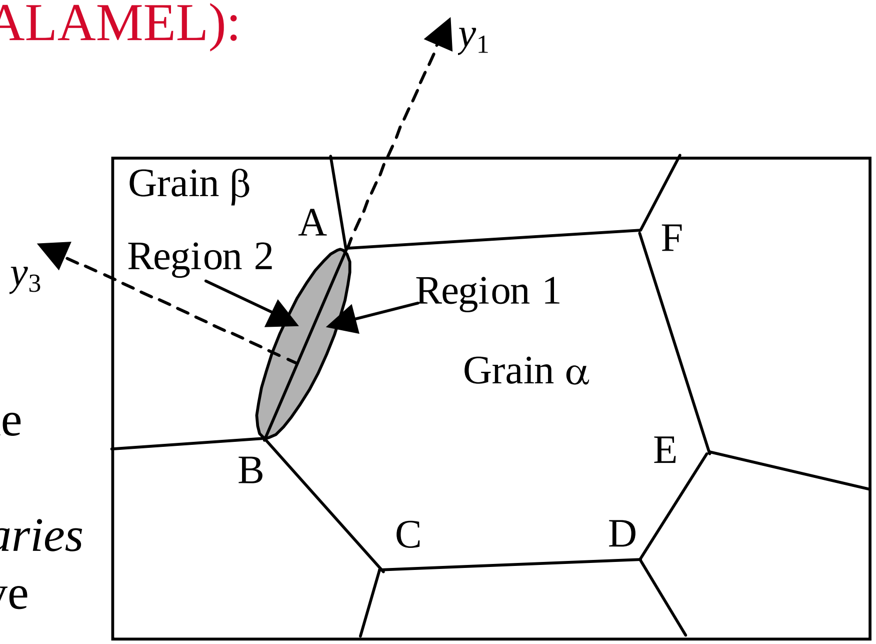
- Taylor equations are written for the 8 grains, taking the relaxations into account (as in the Lamel model)
- The plastic work needed for the deformation of the 8 grains must be minimised.
- The relaxations are restricted by a penalty term in the work equation, derived from the energy needed to accommodate the misfits at internal and external interfaces. The misfit accommodation is supposed to be achieved by geometrically necessary dislocations.

- **Assessment of GIA model:**
  - In principle generally applicable
  - In case of rolling: most opportunities for co-operative slip are taken into account.



Co-operative slip

- Advanced Lamel Model (ALAMEL):
  Interaction Model



- schematic representation of microstructure:
- Not the orientations in the *centres* of the grains, but those at the *grain boundaries* are taken as representative for the texture of the poly-crystal
- It is assumed that at the grain boundaries (in Region 1 and Region 2), the slips activities are
  - different in both regions (*different lattice orientations!*)
  - stress equilibrium is achieved at the boundary
  - geometrical compatibility exists at the boundary

Models for Deformation Prediction: ALAMEL

- slip activity must be different along different grain boundaries, since the neighbouring crystallites all have different lattice orientations
  - a gradient in slip activity / plastic strain rate is assumed to exist along a line going from one grain boundary to the next across a grain
  - as a result, a gradient in crystallite orientation is assumed to develop as strain goes on

- Region 1 + 2 are treated as a pair of grains in the Lamel Model.

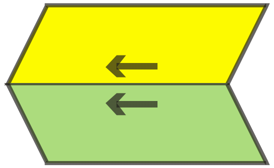
- The evolution of the lattice orientation of ‘Region 1’ and ‘Region 2’ for a set of grain boundaries randomly chosen from the textured polycrystal

- In this, the current microstructure is taken into account

- This requires an additional model (using basic continuum mechanics) to simulate the evolution of the microstructure.

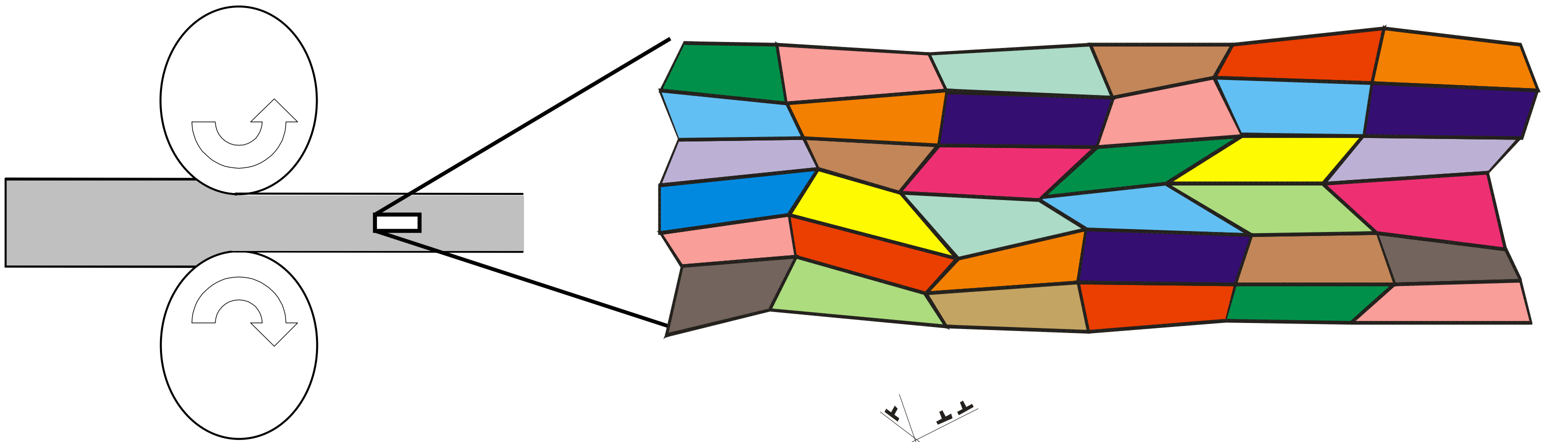
Assessment of ADVANCED LAMEL model:

- Taylor ambiguity does normally NOT occur
- Physical justification possible for ALL microstructures and ALL strain modes
- In principle generally applicable
- All cases of co-operative slip should be recognised and taken into account

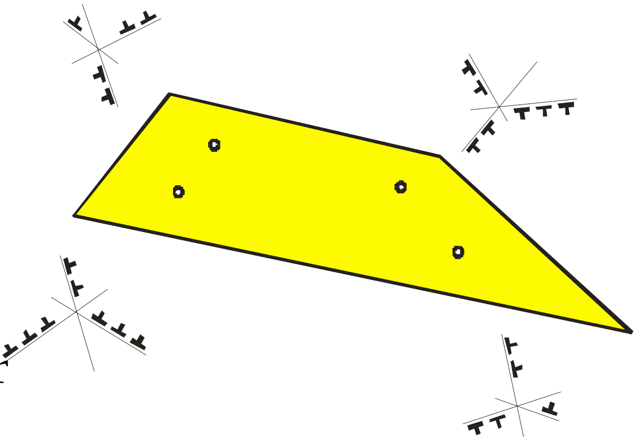


Co-operative slip

- CPFEM (Crystal Plasticity Finite Element Model)

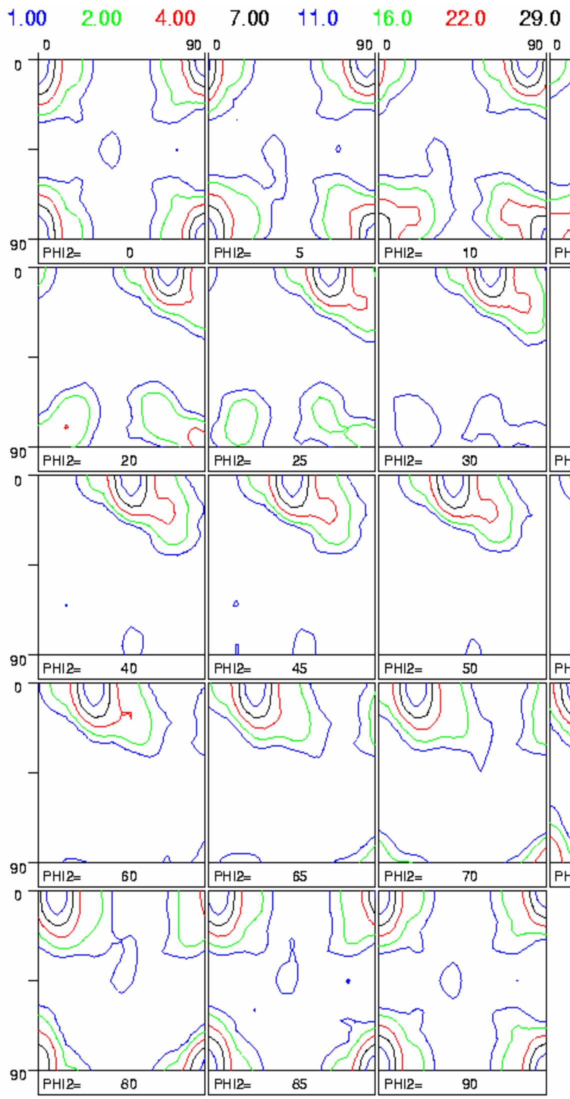


- Takes interactions between grains into account
- Heterogeneous deformation among and within the grains
- Requires huge computation power

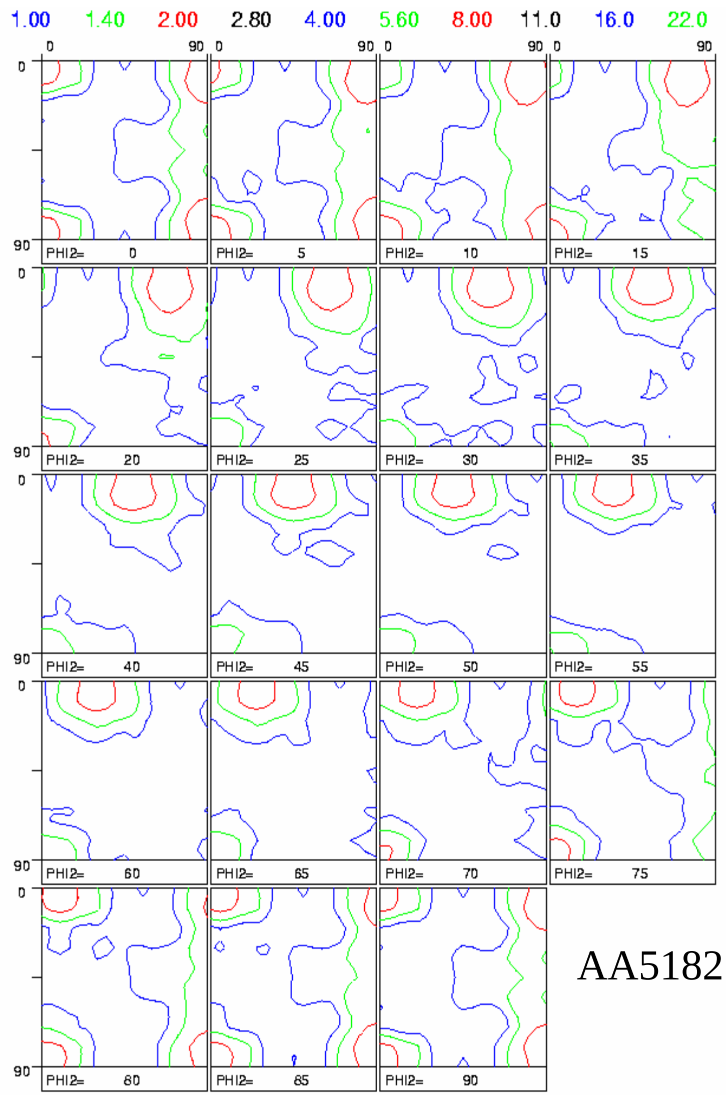


- **VPSC (Visco Plastic Self Consistent Model)::**
  - Self Consistent Model:
  - Each grain is treated in turn as an ellipsoid-shaped inclusion
  - Surrounded by the “Matrix”, i.e. a homogenous medium with average properties of the polycrystalline material. *(Tomé et al. , Los Alamos)*
  - Interaction between “inclusion” and “Matrix” is calculated
- **Assessment:**
  - Co-operative slip between neighbouring crystallites with favourable orientations is NOT recognised

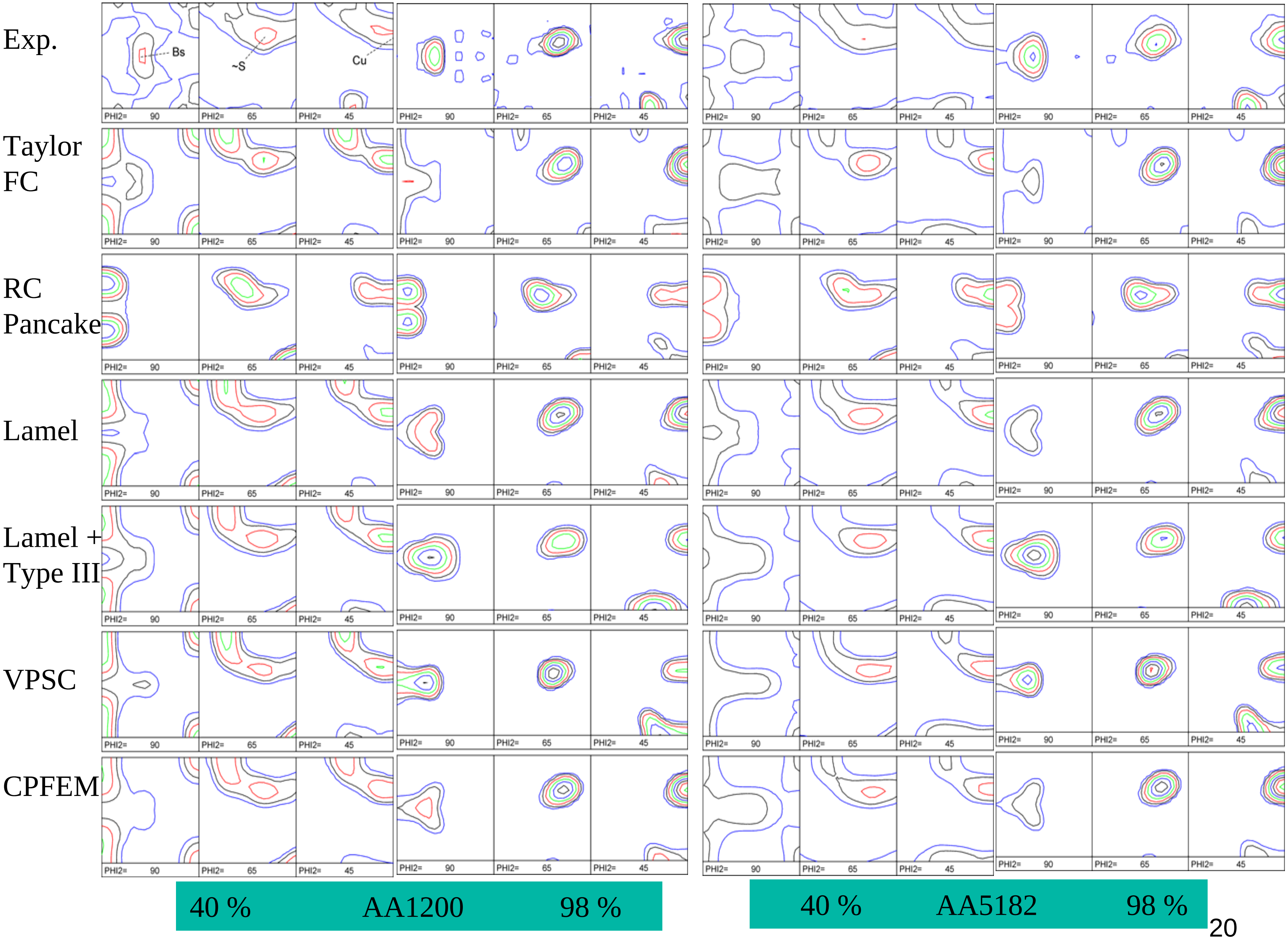
Results for some aluminium alloys: Hot rolling textures:



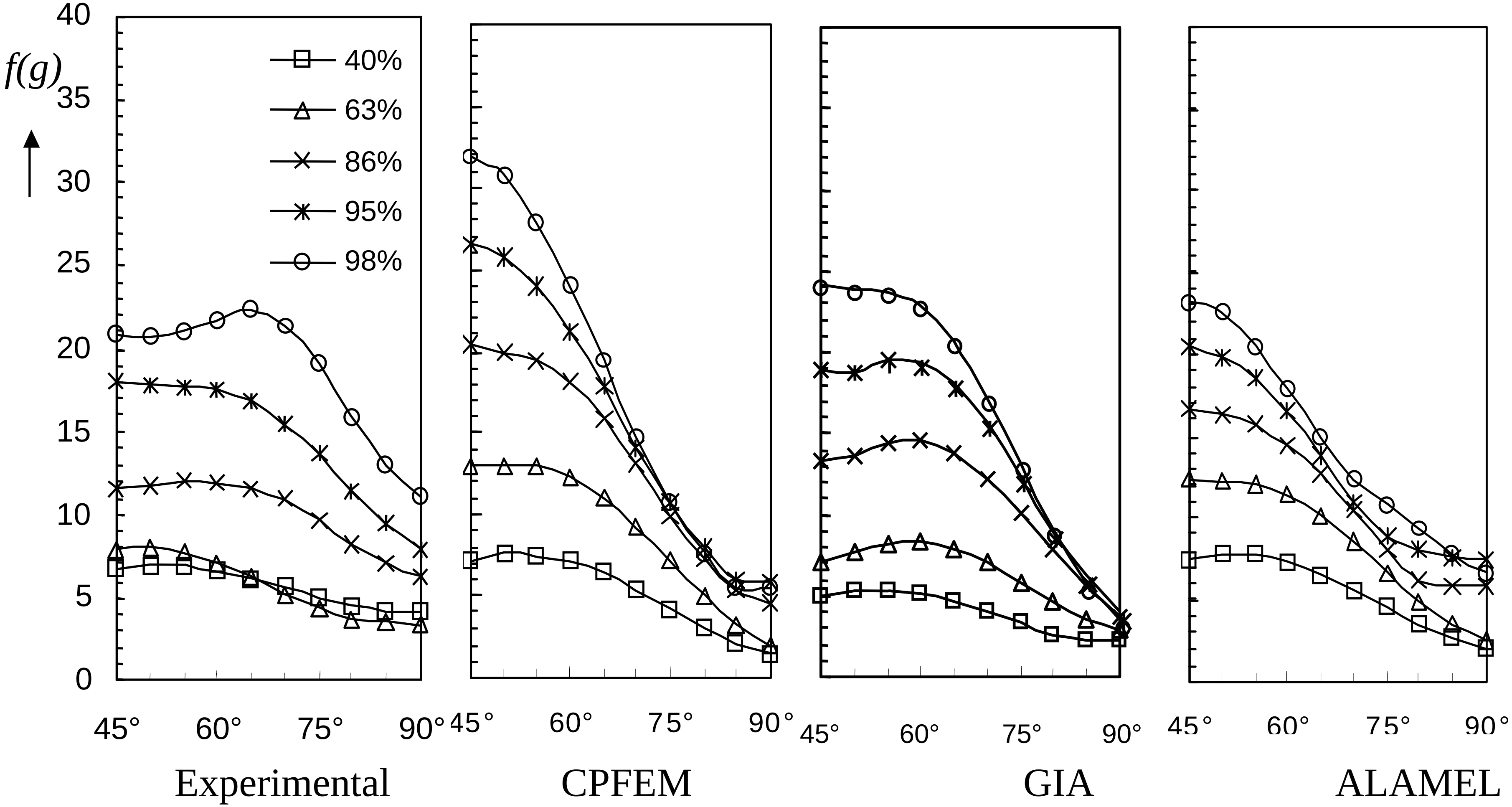
AA1200



AA5182

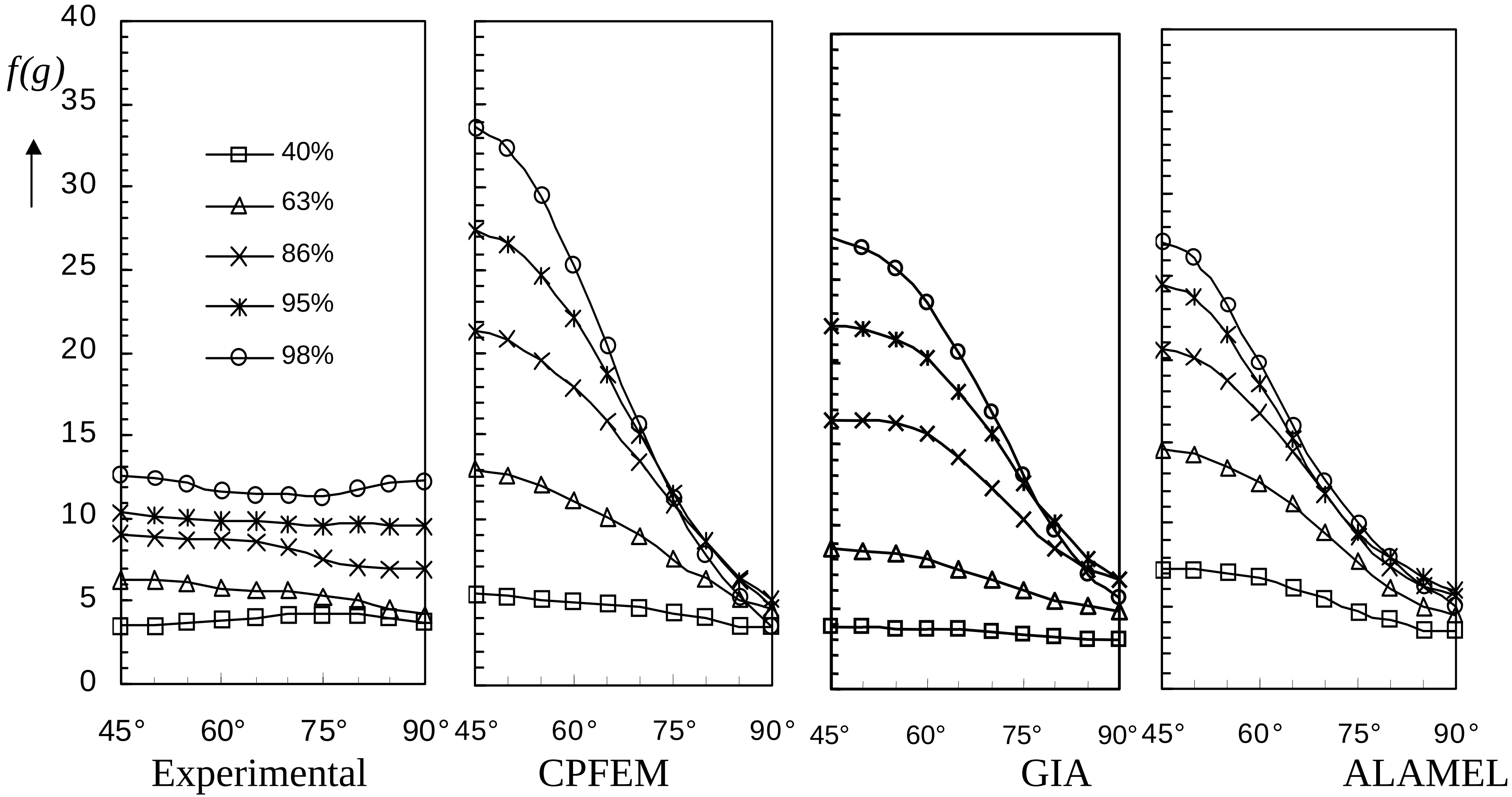

Exp.
Taylor FC
RC Pancake
Lamel
Lamel + Type III
VPSC
CPFEM
Bs
~S
Cu
PHI2= 90
PHI2= 65
PHI2= 45
40 %
AA1200
98 %
40 %
AA5182
98 %

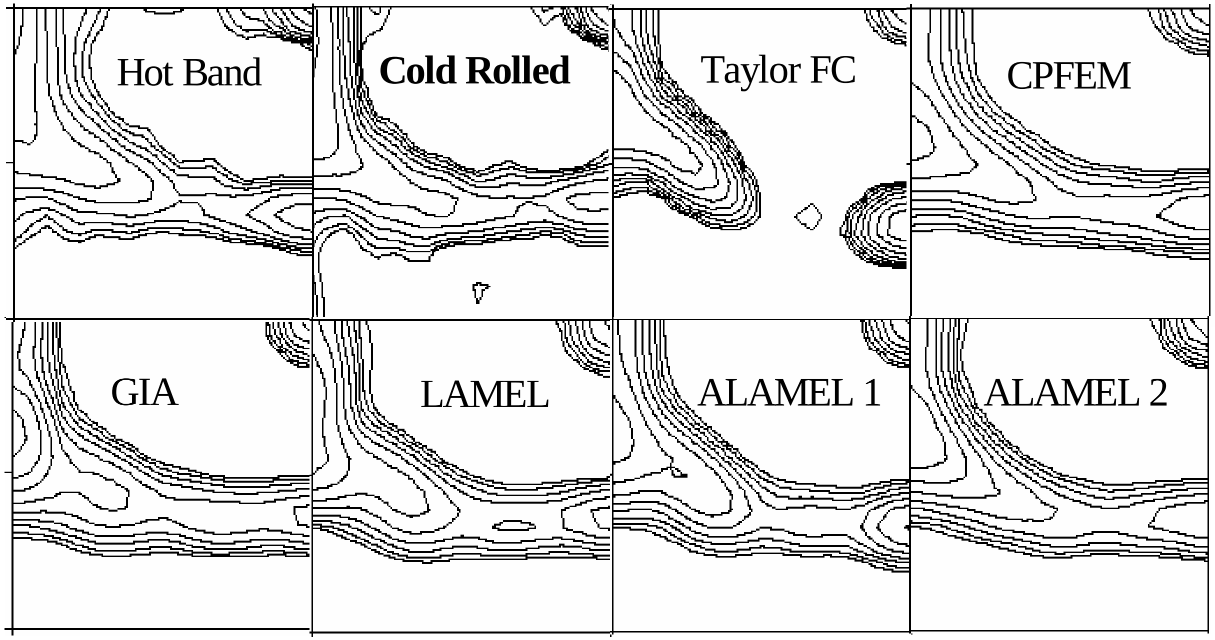
AA1200 β-fibre: from Cu over S to Bs → φ_2



Results: Rolling of Al alloys (VIRFORM)

AA5182 β-fibre: from Cu over S to Bs → φ_2





Levels:
1; 1.4; 2;
2.8; 4; 5.6;
8; 11; 16;
22

φ_2=45° sections of the ODF of: hot band texture; texture after 70% cold rolling reduction; simulated textures according to 6 models:
CPFEM by Bate (1999).
ALAMEL 1: starting from equiaxed grains;
ALAMEL 2: starting from elongated grains (as if the grains of the hot rolled microstructure already had 40% rolling reduction) and using additional {123}<111> slip systems.

Results: Quantitative Validation

- Based on the ENTIRE ODF (Large + small components)
- Texture Index of Difference ODF:

$$I(\Delta f) = \oint \left[f^{\text{exp}}(g) - f^{\text{model}}(g) \right]^2 \mathrm{d}g$$

Results: Quantitative Validation (Aluminium alloys)

Material	AA1200				
Reduction	*40%*	*63%*	*86%*	*95%*	*98%*
FC	0.54	1.43	2.87	1.87	3.58
RCP	4.25	4.03	4.60	6.69	9.57
CPFEM	0.42	0.92	1.62	1.48	2.52
VPSC	1.11	2.02	2.26	2.81	4.29
GIA	0.57	0.87	1.16	1.35	2.34
Lamel	0.89	1.60	1.56	1.26	1.81
Lamel+TypeIII	0.49	0.99	1.45	2.25	3.35
ALamel	0.49	1.06	1.38	1.07	1.58

Results: Quantitative Validation (Aluminium alloys)

Material	AA5182				
Reduction	*40%*	*63%*	*86%*	*95%*	*98%*
FC	0.29	1.43	2.58	2.84	4.53
RCP	1.89	0.84	2.60	3.37	3.89
CPFEM	0.16	0.76	1.41	2.51	3.72
VPSC	0.57	1.33	1.92	2.18	2.68
GIA	0.12	0.35	0.90	1.67	2.51
Lamel	0.46	1.15	1.66	2.41	2.83
Lamel+TypeIII	0.32	0.81	0.96	1.19	1.49
ALamel	0.27	1.09	1.29	1.70	2.08

Results: Quantitative Validation (IF Steel)

CPFEM	FC	GIA	LAMEL[1]	ALAMEL[1]	ALAMEL[2]
0.182	0.6945	0.113	0.088	0.161	0.097

CPFEM: developed by Bate (1999); FC= FC Taylor theory;
GIA: developed by Crumbach et al. (2001);
LAMEL: standard LAMEL model;
ALAMEL1: Advanced LAMEL Model, starting from equiaxed grains;
ALAMEL2: starting from elongated grains (as if the grains of the hot rolled microstructure already had 40% rolling reduction) and using additional {123}<111> slip systems

Discussion

- No model was found which was "the best" for all cases studied
- Only grain interaction models perform well
- Agreement between predictions and measurements is more satisfactory for IF steel and AA1200 than for AA5182
- Lamel+Type III sometimes performs well for the wrong reason: it artificially overestimates the Brass component beyon 40%
- *AA5182 seems to have an a-typical behaviour. It has a weak initial texture and has 2nd phase particles!*
- *Note that more attention must be given to the description of work hardening in CPFEM, ALAMEL and GIA!*
- Validation tests have to be repeated for other deformation modes
- Taylor FC, GIA and ALAMEL can be used to predict plastic anisotropy and implement it in FE or FLD codes.

Paul Van Houtte and Leo Kestens cordially invite you!

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