Parallel simulations of texture of deformed hexagonal metals

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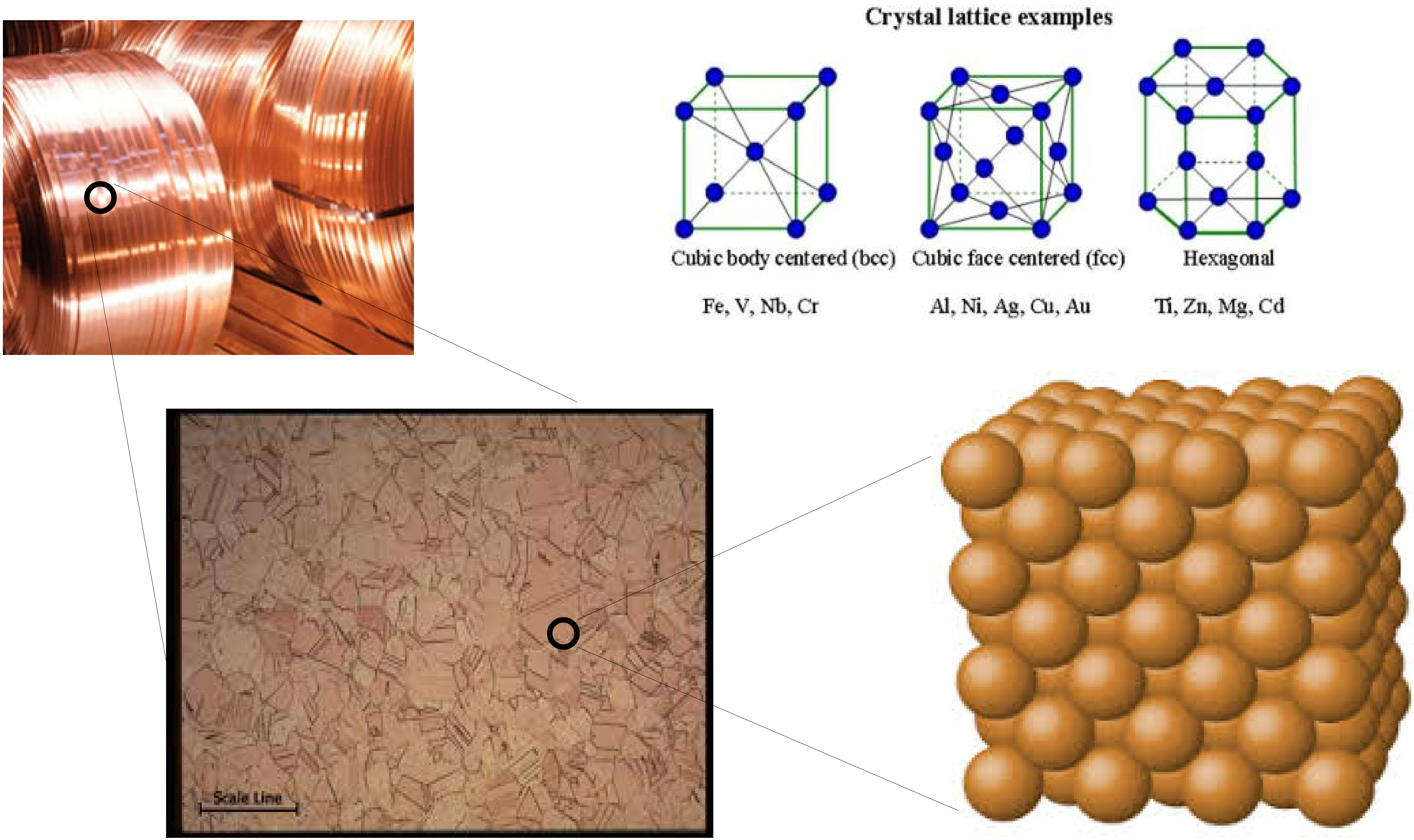
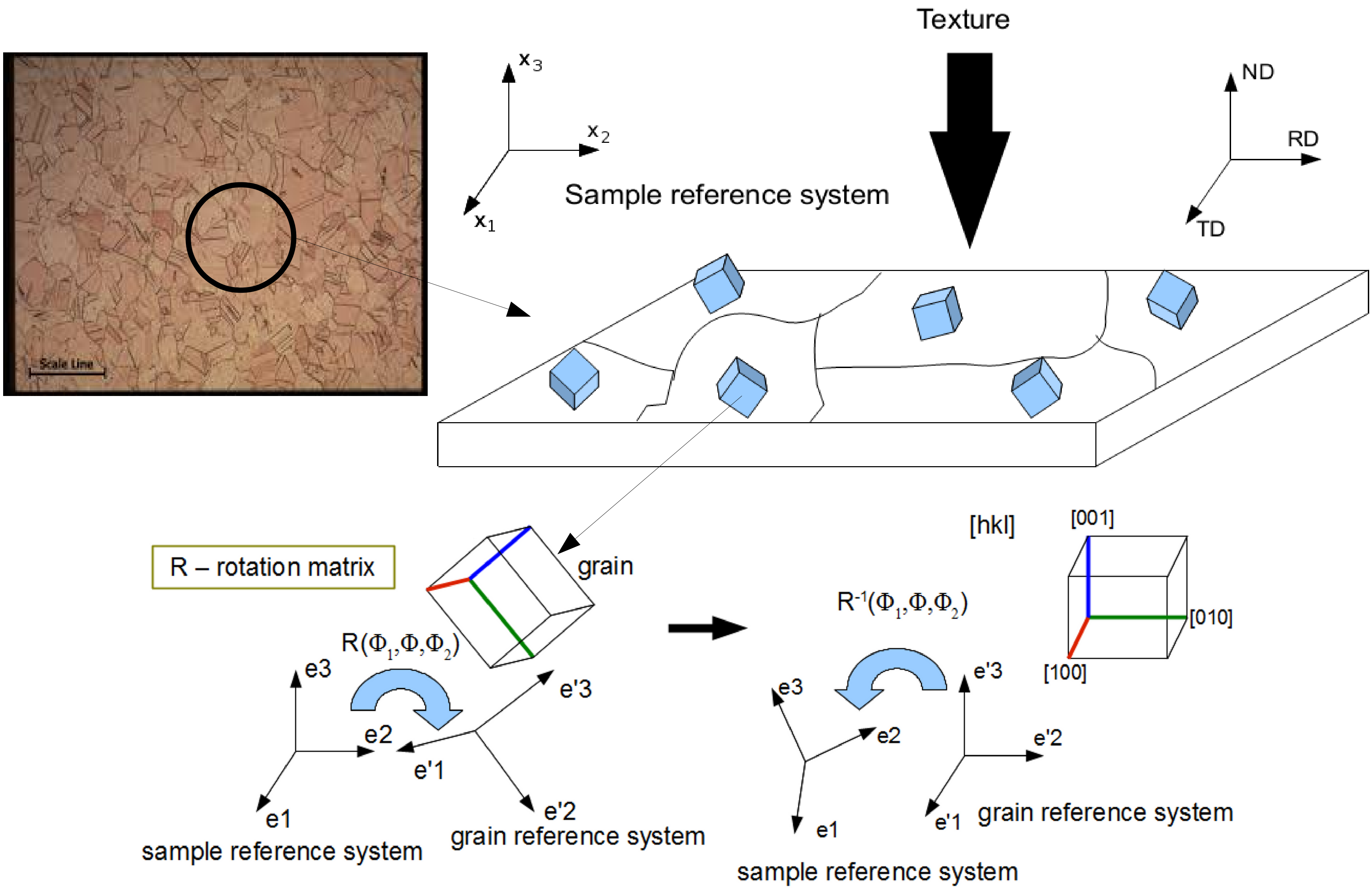
Overview

- Introduction to texture of metals
- Effect of texture on metals properties
- Example of textures
- Modeling of texture
- Simulations of texture
- Parallelize of simulations
- Conclusions

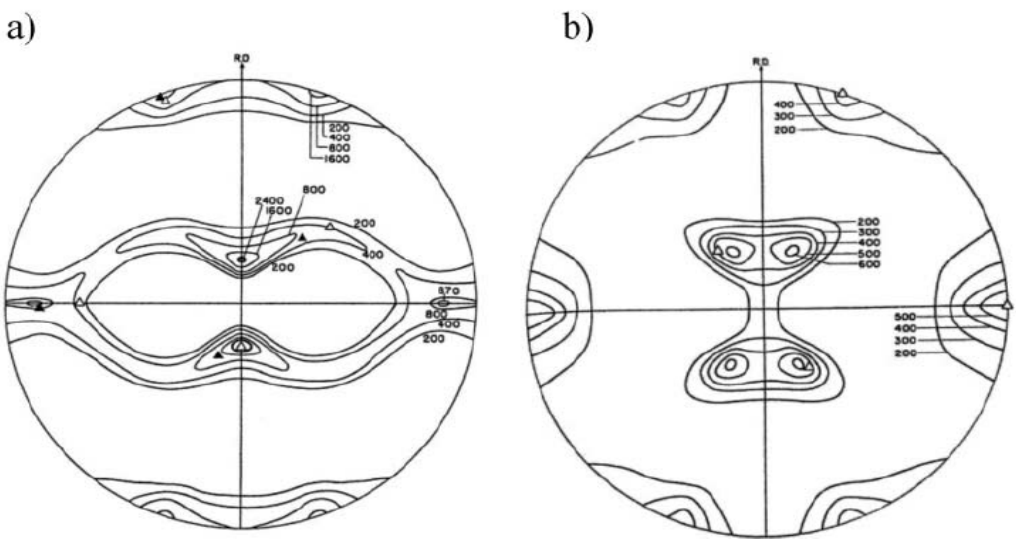
The structure of metals



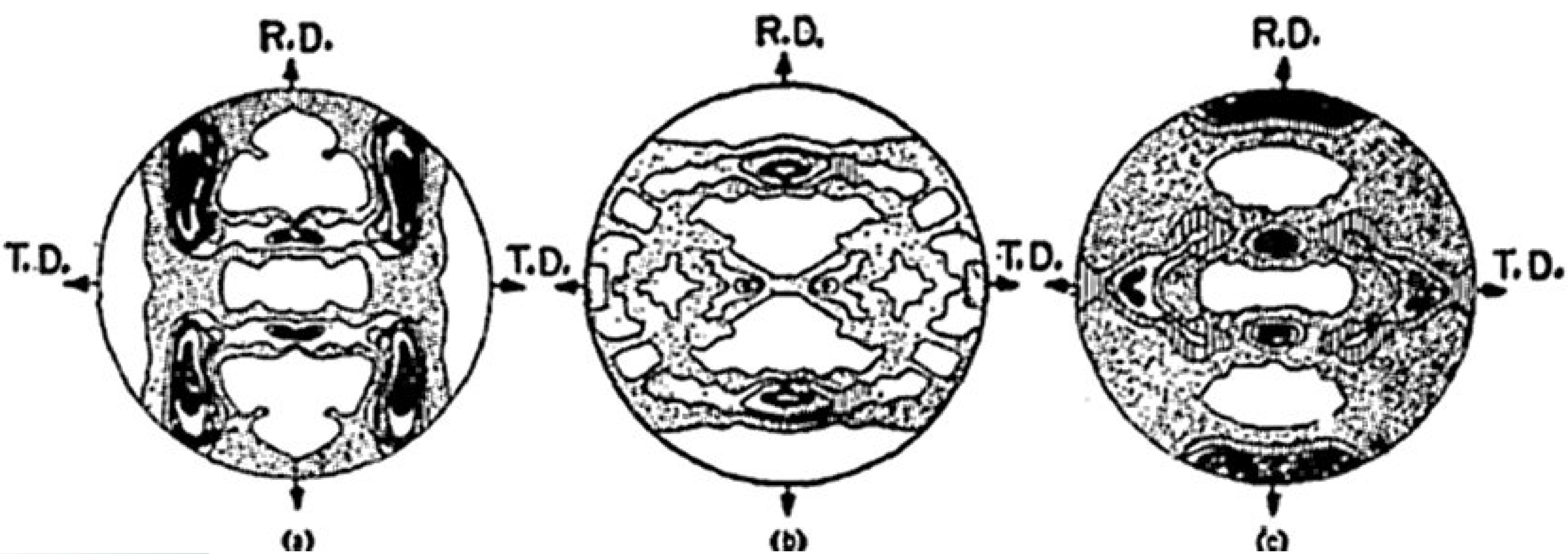
What is texture in metals?



Example of textures



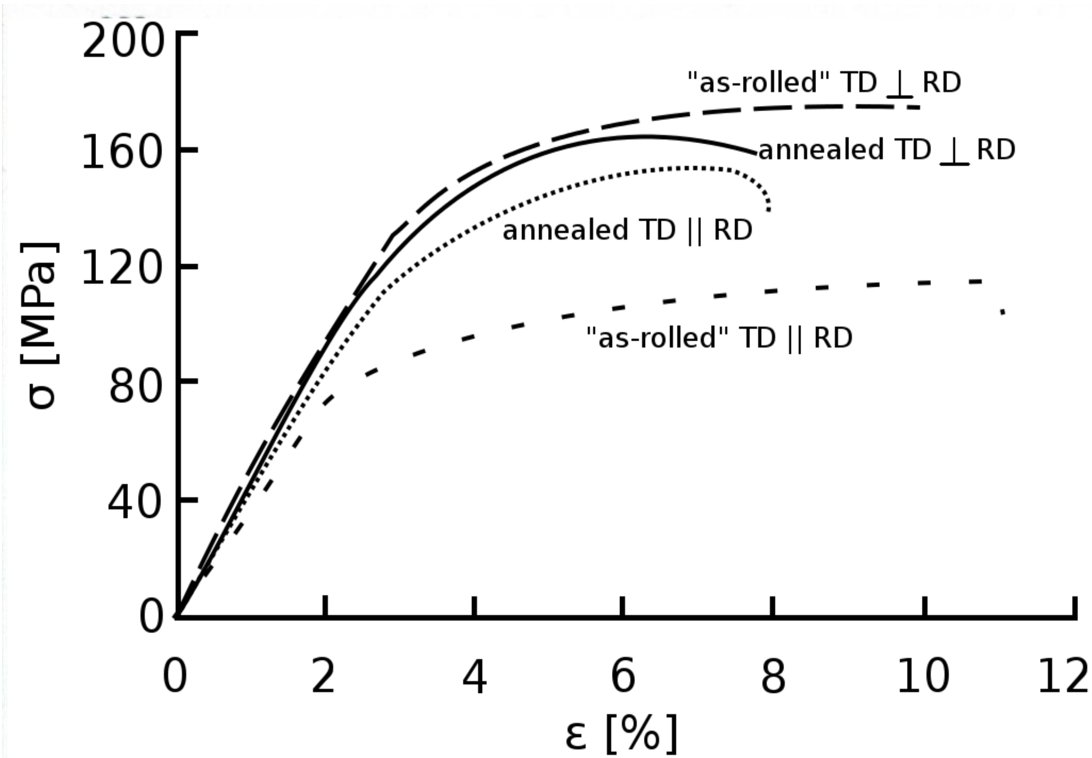
Copper type texture after rolling of Cu

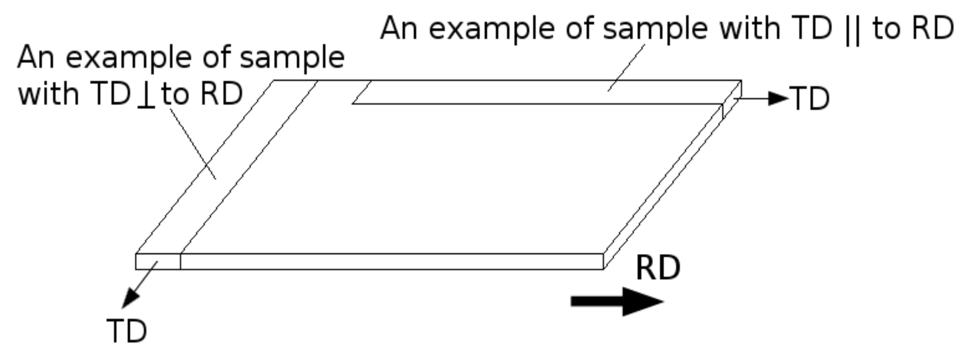


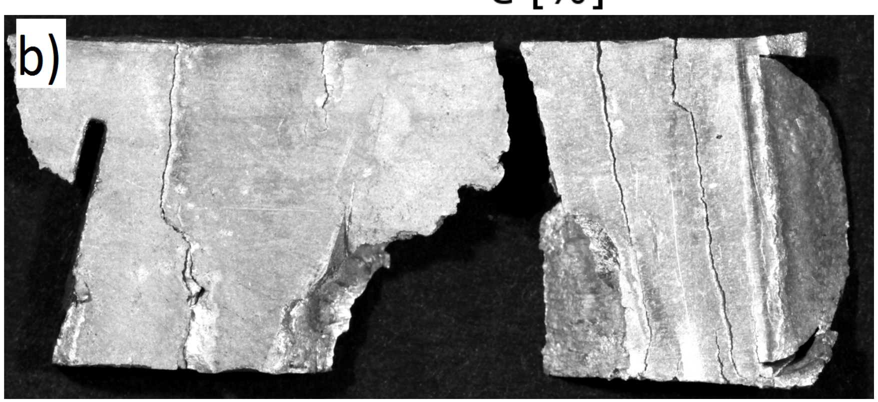
Brass type texture after rolling

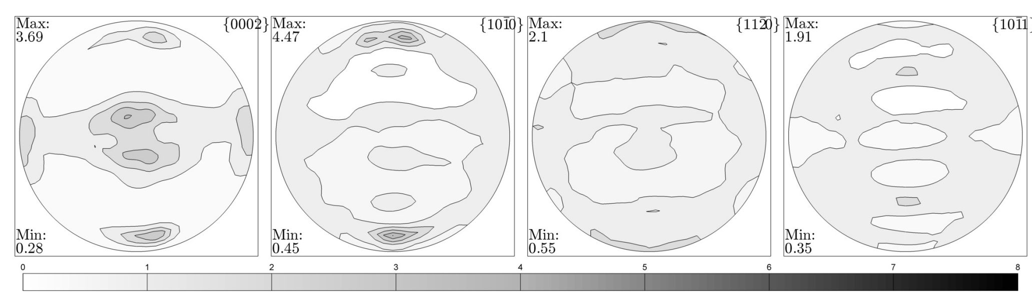
Effect of texture on mechanical properties of metals

Hot-rolled AZ61 magnesium alloy









Failure of AZ61 magnesium sample during rolling

Sachs versus ***Taylor***

- Diagrams illustrate the difference between the Sachs iso-stress assumption of single slip in each grain (a, c and e) versus the Taylor assumption of iso-strain with multiple slip in each grain (b, d).

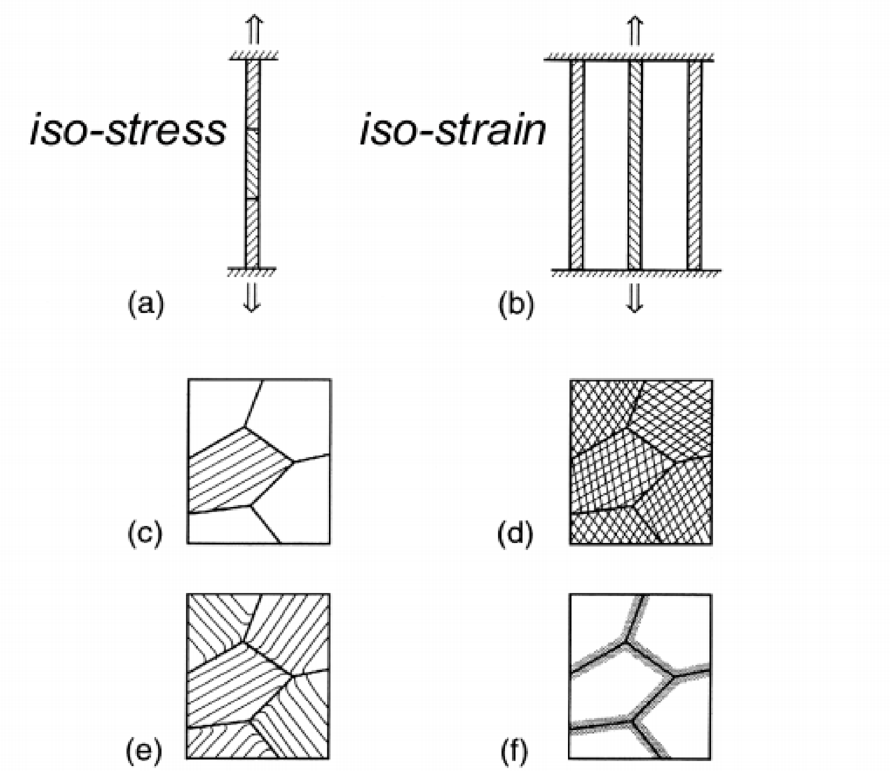


Fig. 23. Schematic description of various polycrystal plasticity models: (a) a true lowe bound for a linear serial polycrystal; (b) the Sachs model (independent parallel grains) (c) a true lower bound for a 3-D polycrystal (only one grain deforms at any instant); (d a true upper bound (also the Taylor model); (e) the Kochendörfer model (single sli plus bending); (f) the Ashby model (polyslip plus 'geometrically necessar dislocations').

Modeling of texture by Taylor model

- Finding independent five active slip systems

Given :

- **Slip system -** c_3; $\dot{\gamma}_{c3}$
- **Unit vector in the slip direction –** $n = \frac{1}{\sqrt{3}}(-1,1,1)$
- **Unit normal vector to the slip plane –** $b = \frac{1}{\sqrt{2}}(1,1,0)$

The contribution of the c_3 system is given by

$$\frac{1}{2}(bn+nb)\dot{\gamma}_{c3} = \frac{\dot{\gamma}_{c3}}{2\sqrt{6}}\begin{bmatrix} -2 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

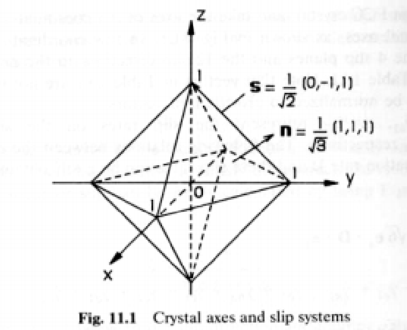
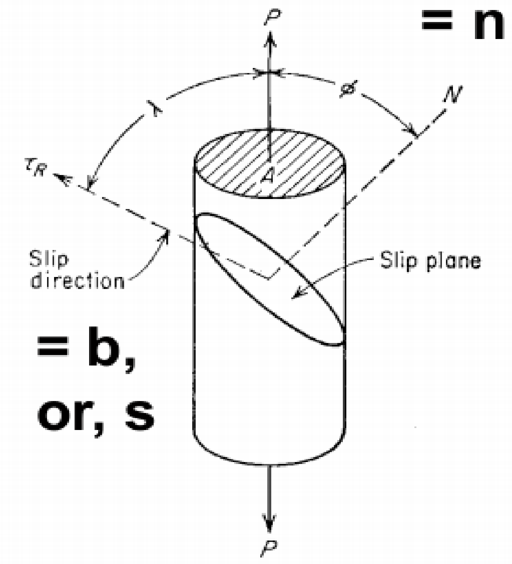


Fig. 11.1 Crystal axes and slip systems



P is a *unit vector* in the loading direction

Minimal internal or maximum external work criterion

(Taylor or Taylor-Bishop method)

$$m_{ij}^{(\alpha)} = b_i^{(\alpha)} n_j^{(\alpha)}$$

$$\sum_{\alpha=1}^{n} \tau_c \dot{\gamma}_\alpha \le \sum_{\alpha=1}^{n} \tau_\alpha^* \dot{\gamma}_\alpha^*$$

Modeling of texture by Taylor model

- Construct deformation matrix from active slip systems

$$D = D^p = \sum_{\alpha=1}^{n} m_\alpha \dot{\gamma}_\alpha$$

- Anti-Symmetric part of deformation matrix gives information about change in orientation
- Update actual orientation of grain
- Repeat until last step of deformation

Results of simulations

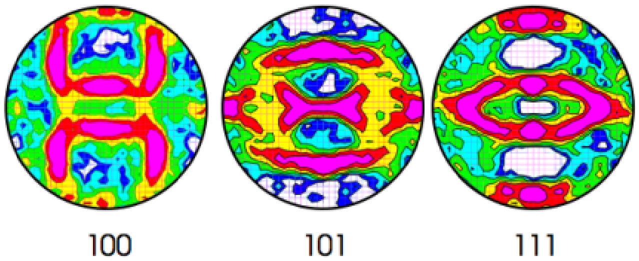
- Modeling of textures for: magnesium and copper
- Strain tensor: rolling
- Deformation: 80%
- Deformaton step: 0.025
- Initail sample size: 1000, 10 000, 100 000 elements
- Multi slip, Taylor model
- CPU: Intel Core i7 3630QM @ 2,4 GHz
- Supercoumpter Zeus:

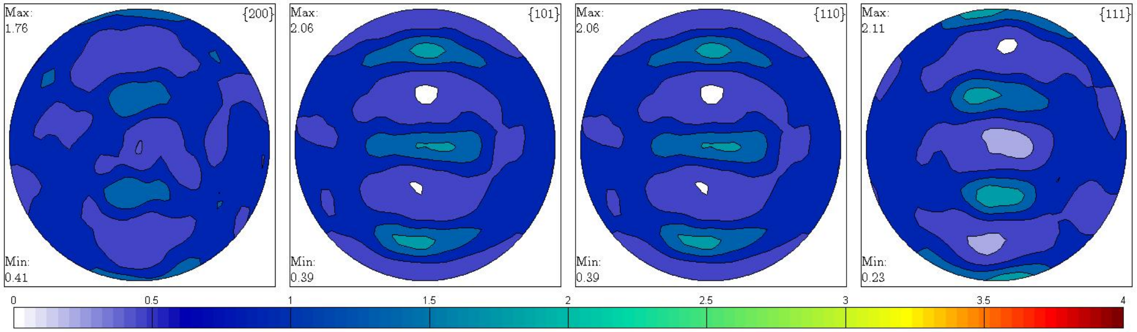
  Intel(R) Xeon(R) CPU X5650 2.67GHZ

  AMD Opteron(TM) Processor 6276
- Supercomputer Prometheus:

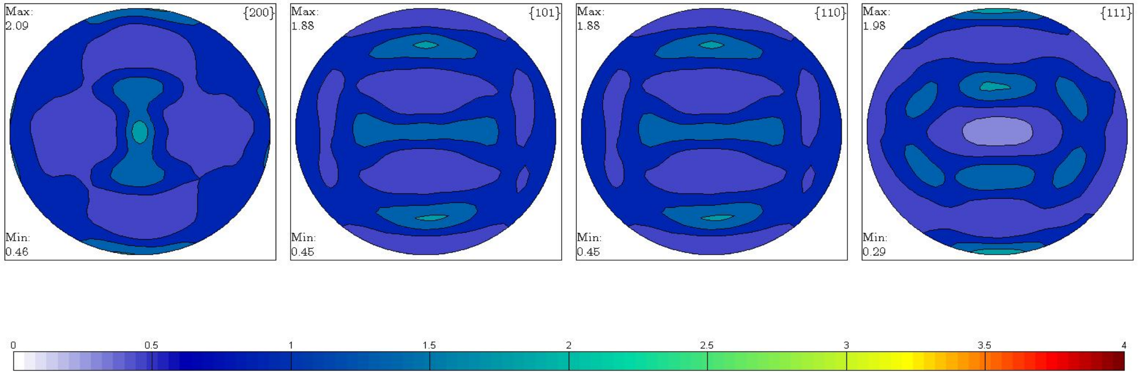
  Intel(R) Xeon(R) CPU E5-2680 v3 2.50GHz
- Software: Matlab 2013b, Mtex v3.5

Texture simulations results of Cu afte rolling up to 80% of thickness reduction
local computer: Intel i7 CPU

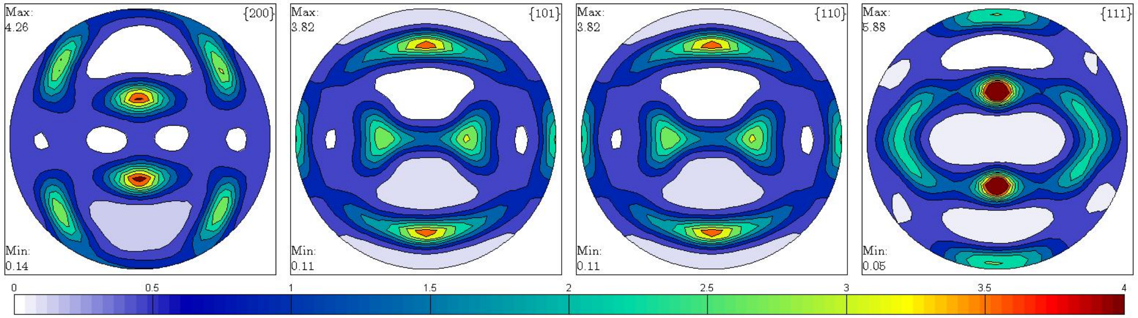




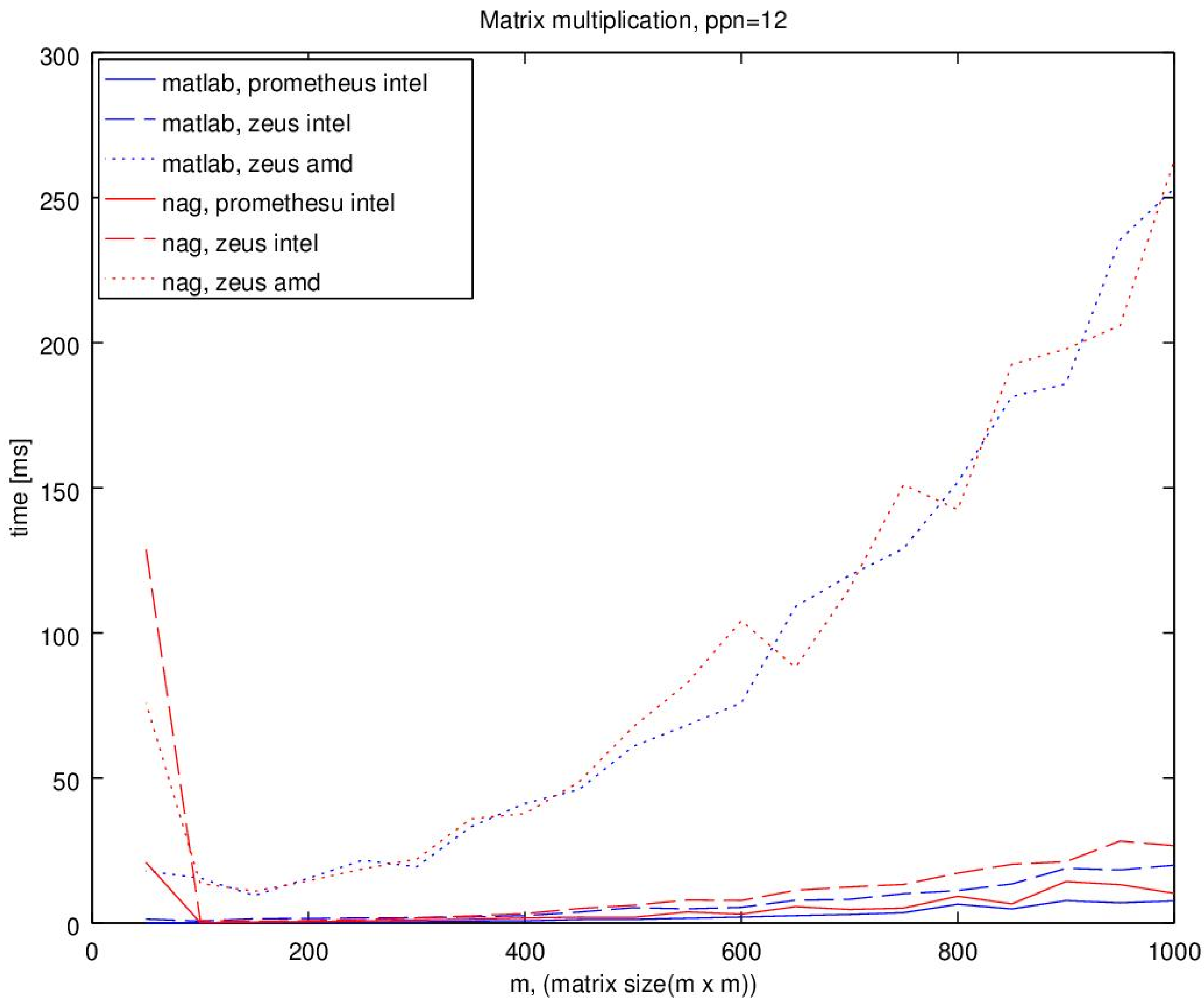
1000 elements
simulations time: 2 min i 48 s



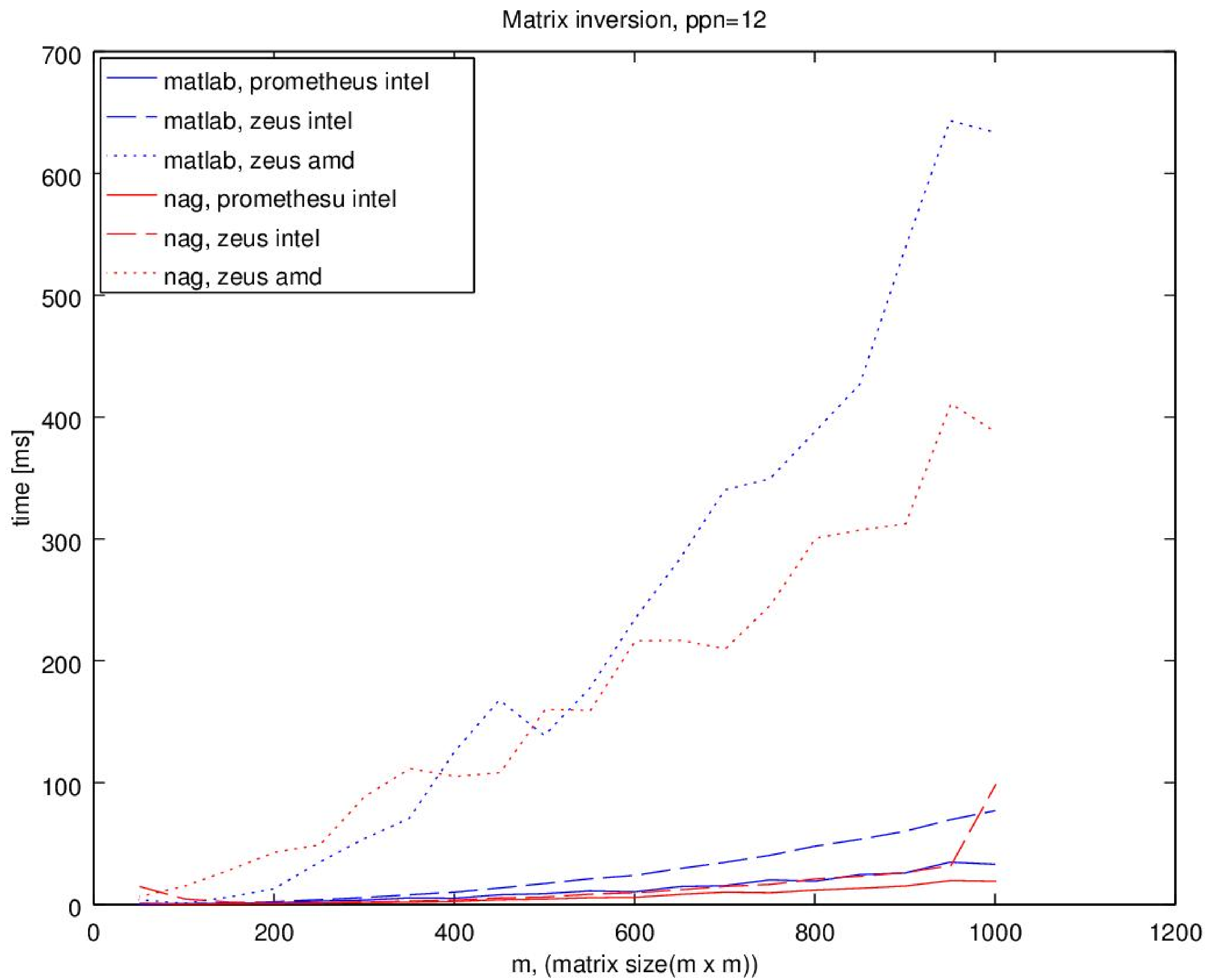
10 000 elements
simulations time: 27 min i 39 s



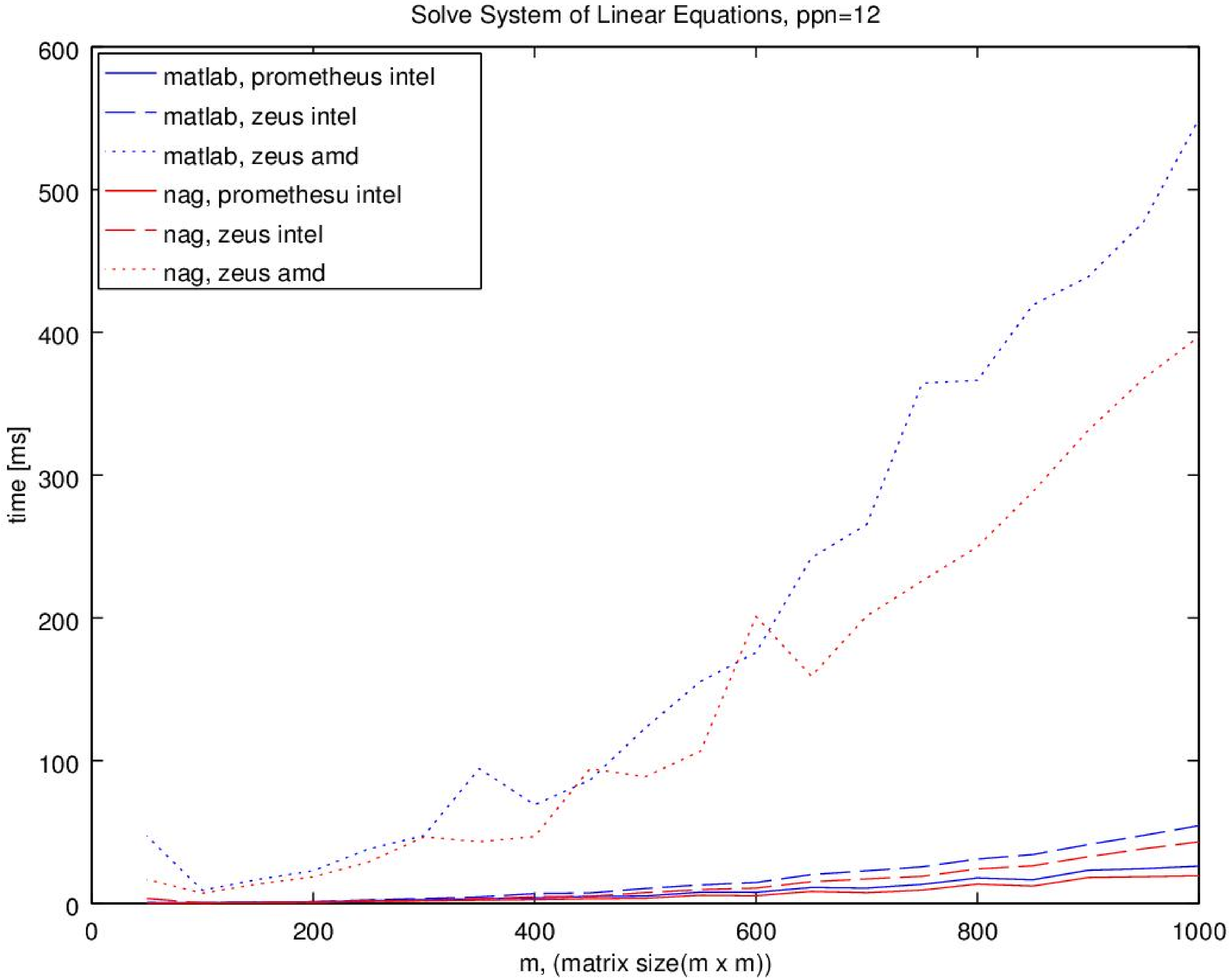
100 000
simulations time: 284 min i 15 s



Matrix multiplication, ppn=12
matlab, prometheus intel
matlab, zeus intel
matlab, zeus amd
nag, promethesu intel
nag, zeus intel
nag, zeus amd
time [ms]
m, (matrix size(m x m))
0
50
100
150
200
250
300
0
200
400
600
800
1000



Matrix inversion, ppn=12
matlab, prometheus intel
matlab, zeus intel
matlab, zeus amd
nag, promethesu intel
nag, zeus intel
nag, zeus amd
time [ms]
0
100
200
300
400
500
600
700
0
200
400
600
800
1000
1200
m, (matrix size(m x m))



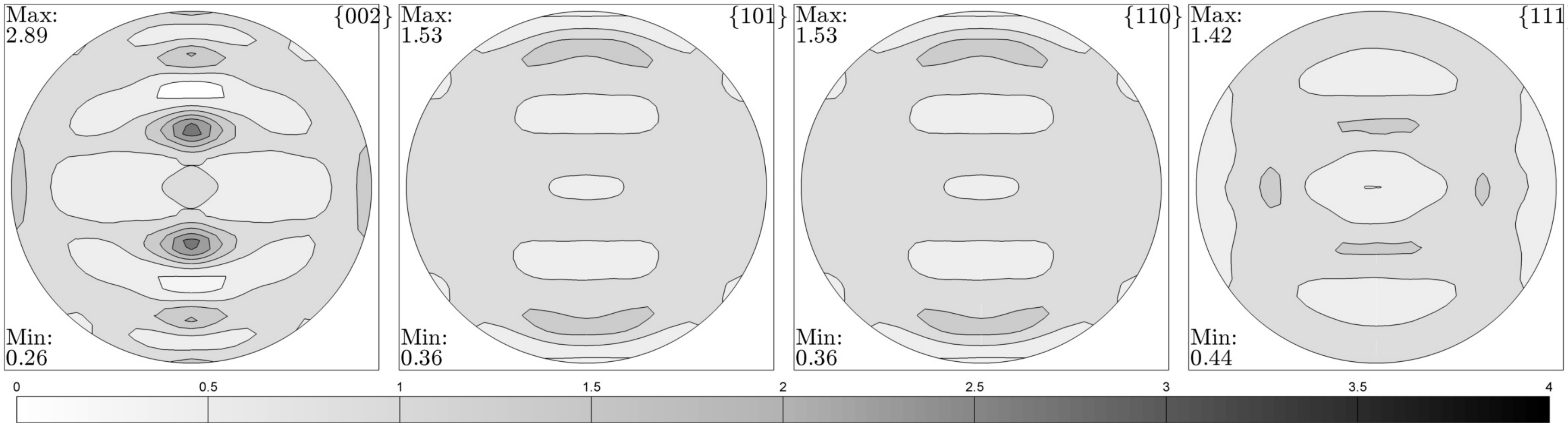
Solve System of Linear Equations, ppn=12
matlab, prometheus intel
matlab, zeus intel
matlab, zeus amd
nag, promethesu intel
nag, zeus intel
nag, zeus amd
time [ms]
m, (matrix size(m x m))
0
100
200
300
400
500
600
0
200
400
600
800
1000

Comparison of calculations time on Prometheus and Zeus supercomputers

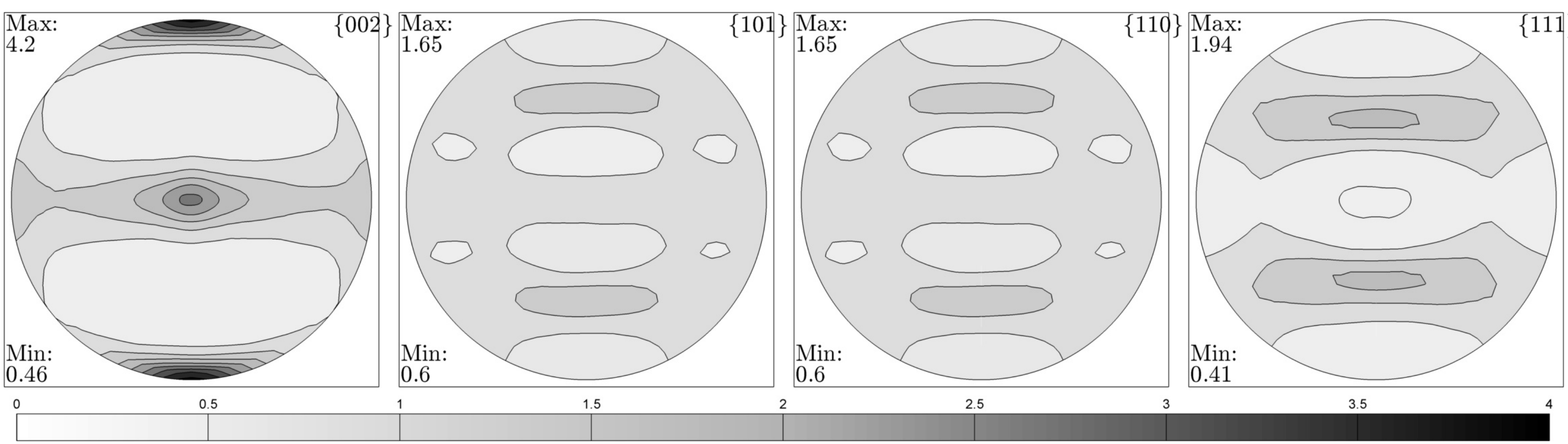
- Calculations steps : 15
- Number of elements : 100 000
- Number of cores : 12
- Calculations time hh:mm:ss

Prometheus Intel(R) Xeon(R) CPU E5-2680 v3 2.50GHz	00:28:52
Zeus Intel(R) Xeon(R) CPU X5650 2.67GHZ	00:59:37
Zeus AMD Opteron(TM) Processor 6276	2:26:50

Texture simulations results of Mg afte rolling up to 80% of thickness reduction



Deformation in soft slip systems



Deformation in hard slip systems

Conclusions

- Parallel Computing Toolbox and NAG toolbox for Matlab decreased significantly time needed for simulations of texture evolution in metals using Prometheus and Zeus supercomputers.

- The choice of adequate tool for parallel computations is dependent on the complexity and scalability of the given problem

- In the further work visco-plastic model will be implemented. The visco-plastic model is based on the minimization of non-linear equations.

Thank you for your attention