Continuum single crystal plasticity

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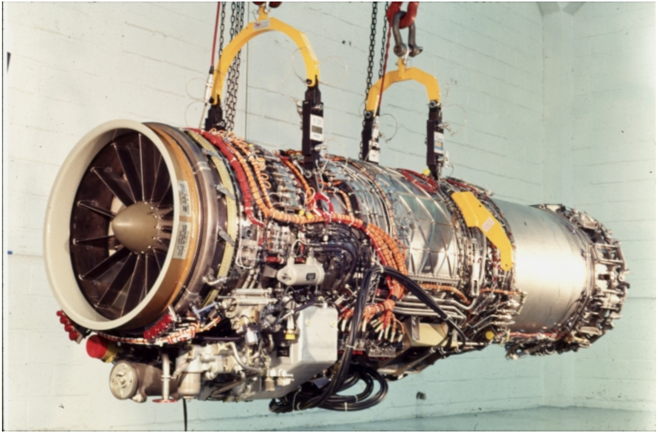
Plan

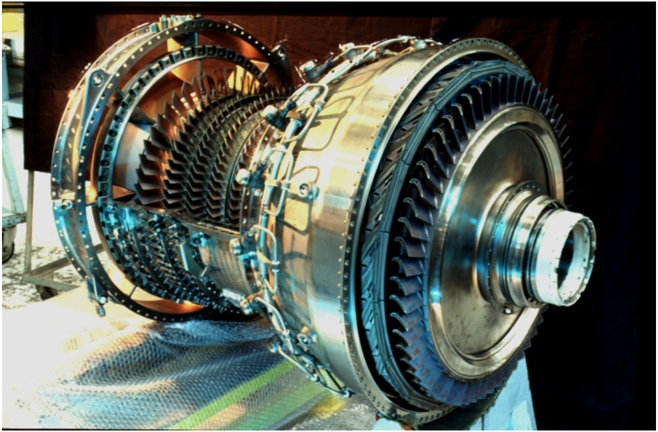
Plan

Single crystals in industrial components



jet engine (source: SNECMA)

Single crystals in industrial components

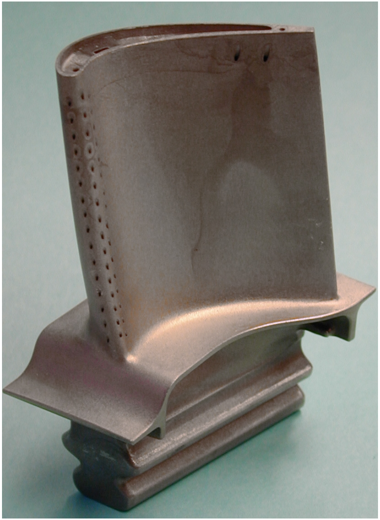


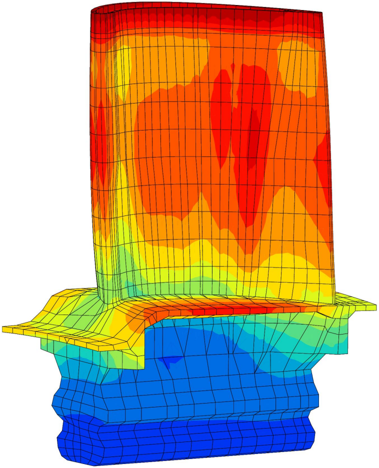
compressor / combustion chamber / high pressure turbine

Single crystals in industrial components

single crystal nickel base superalloy turbine blades

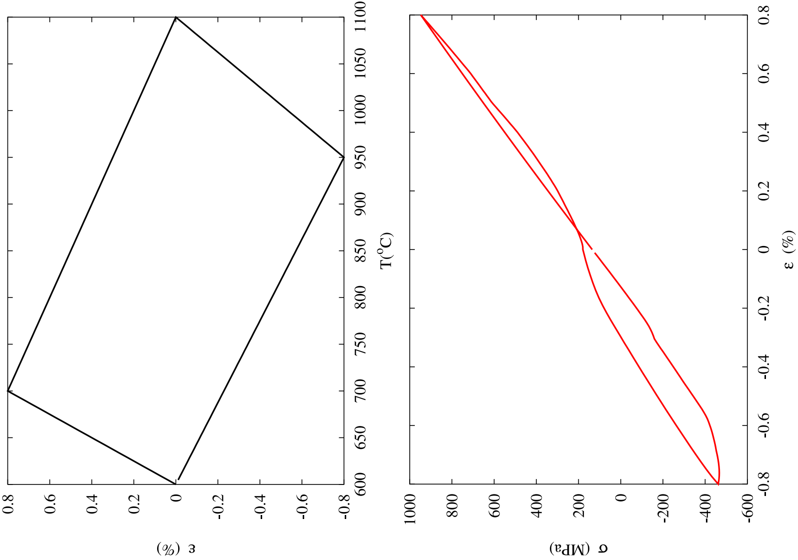
Thermomechanics of single crystal component





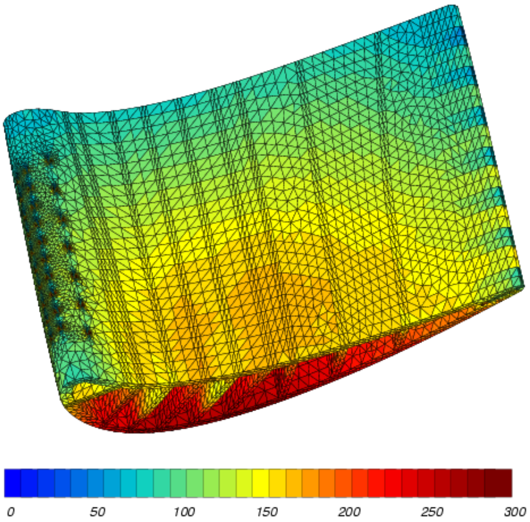
temperature field in a single crystal turbine blade

Thermomechanics of single crystal component



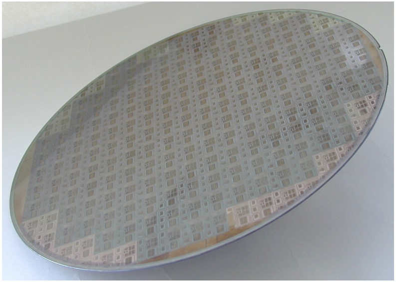
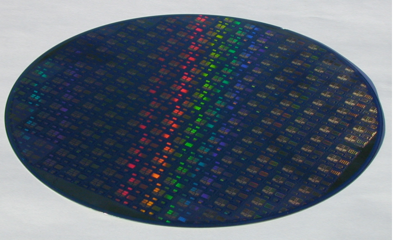
Cyclic loading of multi-perforated single crystal blades

Thermomechanics of single crystal component



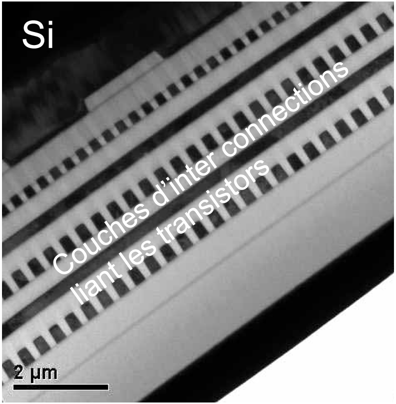
Cyclic loading of multi-perforated single crystal blades

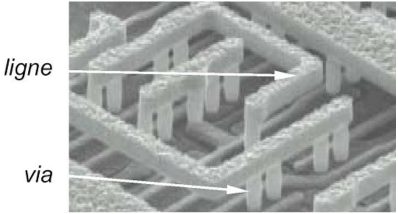
Micro-electromechanichal systems: MEMS

silicium wafer with chips

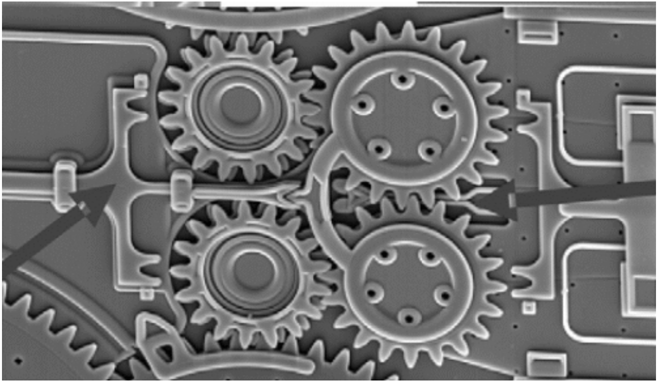
Micro-electromechanichal systems: MEMS





multilayered component / aluminium or copper interconnections

Nano–mechanics



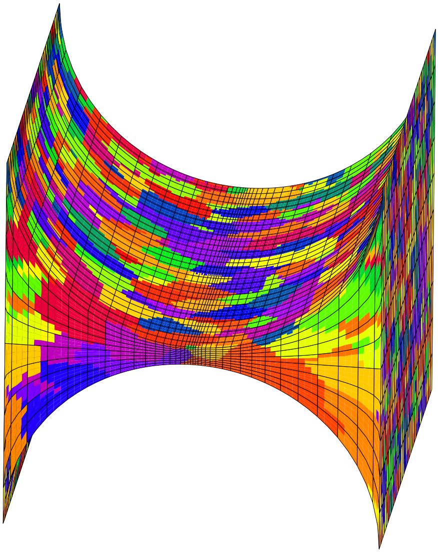
nanomachines

Multicrystalline part in a MEMS

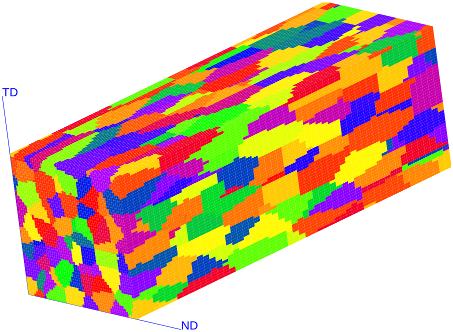
$d \sim L$

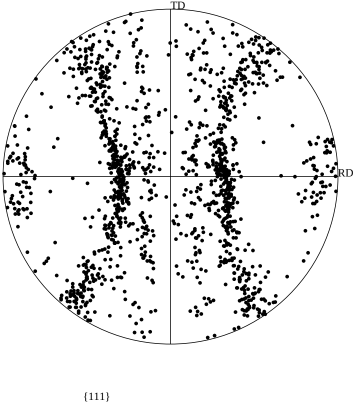
d grain size
L component size

- **fluctuations** of apparent properties
- stress and strain **gradients**



Predict polycrystal anisotropic behavior





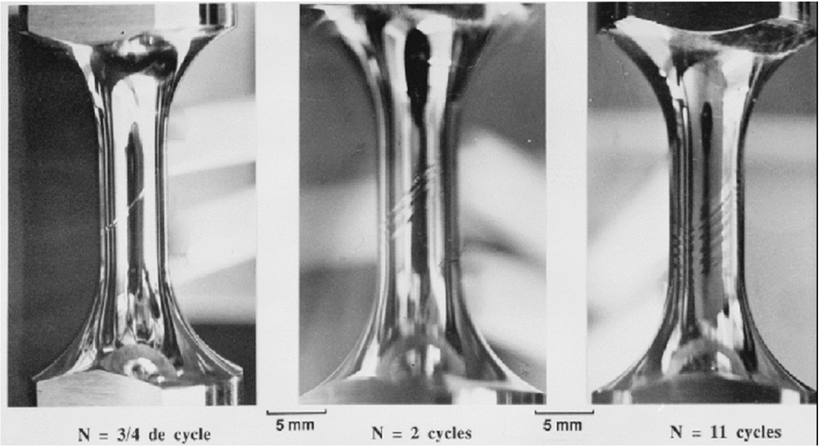
Metal forming: Rolling of a cuproberyllium alloy

Aims of microstructural mechanics

1. **Mechanical behaviour of heterogeneous materials**
   - ⋆ understanding of local deformation and fracture mechanisms
   - ⋆ influence of morphology of phases : computation of RVE
   - ⋆ homogenization methods and modelling effective properties :
     - ∗ test available estimations
     - ∗ prediction with a minimum of approximations, respecting bounds!
     - ∗ case of constituents with high contrast of properties
   - ⋆ additional information : variance of the fields, dispersion, local heterogeneity
2. **Computation of small structures**
   - ⋆ mini-samples, thin layers, coarse grain materials, MEMS
   - ⋆ zones of stress concentration
3. **Damage of materials** driven by extremal values, not by mean values...

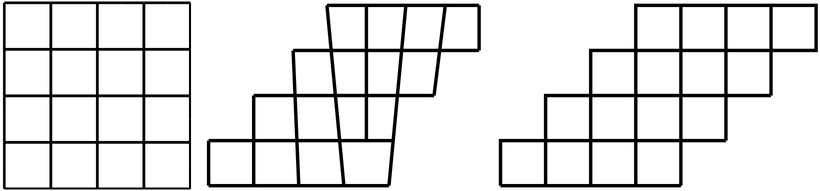
Plan

Slip bands in a single crystal during cyclic loading



[Hanriot, 1993]

Plastic slip of atomic planes...



... due to the motion of crystal linear defects: **dislocations**

Kinematics of plastic single slip

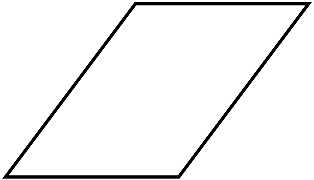
$$u_1 = \gamma\, x_2$$

$$F_{12} = \frac{\partial u_1}{\partial x_2} = \gamma$$

$$\underline{\mathbf{u}} = \gamma\, \underline{\mathbf{x}} . \underline{\mathbf{e}}_2\, \underline{\mathbf{e}}_1$$

continuous glide

$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{1}} + \gamma\, \underline{\mathbf{e}}_1 \otimes \underline{\mathbf{e}}_2$$



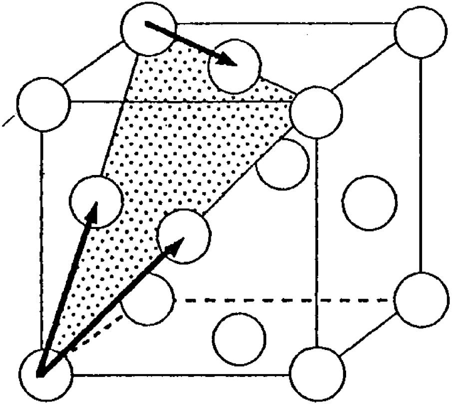
slip direction $\underline{\boldsymbol{\ell}}^{\,s}$
normal to the slip plane $\underline{\mathbf{n}}^{\,s}$
plastic deformation:

$$\underset{\sim}{\mathbf{P}} = \underset{\sim}{\mathbf{1}} + \gamma^s \underline{\boldsymbol{\ell}}^{\,s} \otimes \underline{\mathbf{n}}^{\,s}$$

small plastic strain:

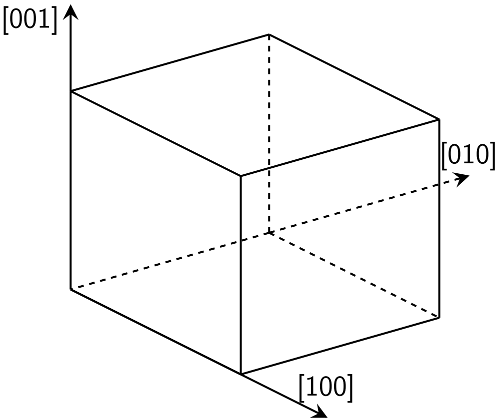
$$\underset{\sim}{\varepsilon}^p = \frac{\gamma^s}{2} (\underline{\boldsymbol{\ell}}^{\,s} \otimes \underline{\mathbf{n}}^{\,s} + \underline{\mathbf{n}}^{\,s} \otimes \underline{\boldsymbol{\ell}}^{\,s})$$

Cubic Face Centered (FCC) single crystals



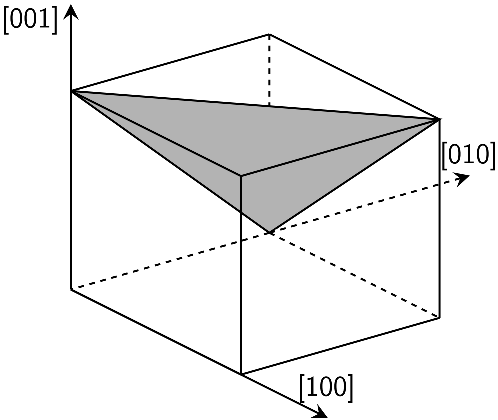
- slip directions a $\{111\}$–plane are indicated by arrows
- 4 slip planes $\{111\}$ i.e. $(111), (\bar{1}11), (1\bar{1}1), (11\bar{1})$
- 6 slip directions $<110>$ i.e. $[110], [\bar{1}10], [101], [\bar{1}01], [011], [01\bar{1}]$

Deformation mechanisms in FCC crystals



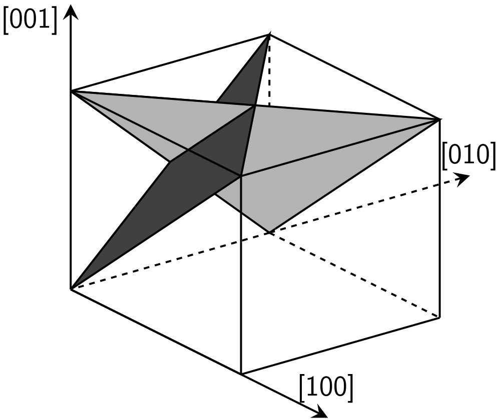
Deformation mechanisms in FCC crystals

Slip systems: $\{111\}\,\langle 110\rangle$

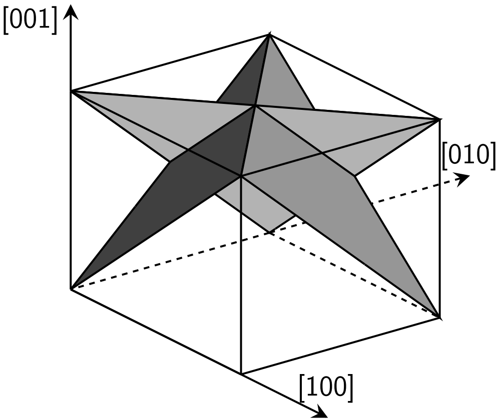


Deformation mechanisms in FCC crystals

Slip systems: $\{111\}\langle 110 \rangle$



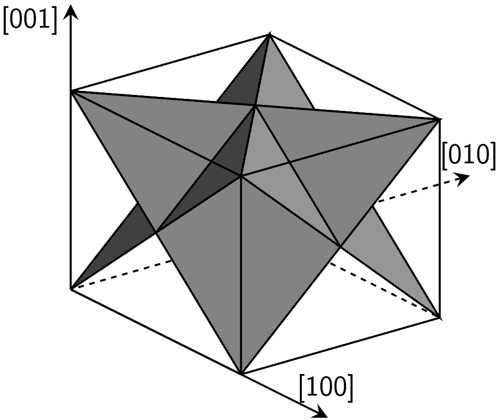
Deformation mechanisms in FCC crystals



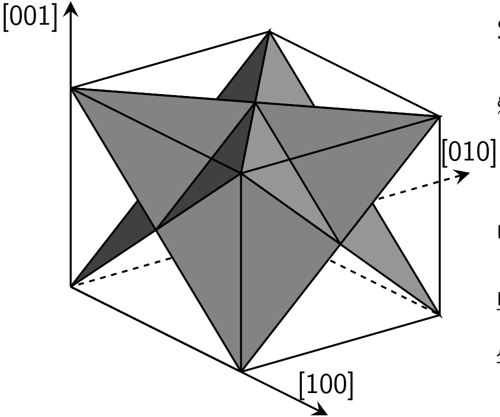
Slip systems: $\{111\}\,\langle 110 \rangle$

Deformation mechanisms in FCC crystals

Slip systems: $\{111\}\langle 110\rangle$



Deformation mechanisms in FCC crystals



Slip systems: $\{111\}\,\langle 110\rangle$

resolved shear stress: $\tau^s = \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\mathbf{m}}^s$

Schmid Law : $|\tau^s| = \tau_c$

$$\dot{\underset{\sim}{\varepsilon}}^p = \sum_{s=1}^{12} \underset{\sim}{\mathbf{m}}^s \dot{\gamma}^s$$

$$\underset{\sim}{\mathbf{m}}^s = \frac{1}{2}\left(\underline{\boldsymbol{\ell}}^{\,s} \otimes \underline{\mathbf{n}}^{\,s} + \underline{\mathbf{n}}^{\,s} \otimes \underline{\boldsymbol{\ell}}^{\,s}\right)$$

$\underline{\mathbf{n}}^{\,s}$: normal to the slip plane

$\underline{\boldsymbol{\ell}}^{\,s}$: slip direction

Plan

Plan

Slip systems in FCC crystals

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]

Simple tension for a single crystal specimen

tensile test in the direction $\underline{\mathbf{t}}$ $\quad \underset{\sim}{\boldsymbol{\sigma}} = \sigma \, \underline{\mathbf{t}} \otimes \underline{\mathbf{t}}, \quad \tau^s = \sigma \, (\underline{\mathbf{n}}^s . \underline{\mathbf{t}}) \, (\underline{\boldsymbol{\ell}}^s . \underline{\mathbf{t}})$

Schmid factor M^s $\quad \tau^s = M^s \, \sigma, \quad M^s = (\underline{\mathbf{n}}^s . \underline{\mathbf{t}}) \, (\underline{\boldsymbol{\ell}}^s . \underline{\mathbf{t}})$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]
Schmid factor						

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]
Schmid factor						

Simple tension for a single crystal specimen

tensile test in the direction [001]
Schmid factor $M^s = (\underline{\mathbf{n}}^s.\underline{\mathbf{t}})(\underline{\boldsymbol{\ell}}^s.\underline{\mathbf{t}})$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]
Schmid factor						

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]
Schmid factor						

Simple tension for a single crystal specimen

tensile test in the direction [001] **8 active slip systems**

Schmid factor $M^s = (\underline{\mathbf{n}}^s . \underline{\mathbf{t}})(\underline{\boldsymbol{\ell}}^s . \underline{\mathbf{t}})$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]
Schmid factor	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	0	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	0

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]
Schmid factor	$\frac{1}{\sqrt{6}}$	0	$\frac{1}{\sqrt{6}}$	0	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$

Simple tension for a single crystal specimen

tensile test in the direction [111]
Schmid factor $M^s = (\underline{\mathbf{n}}^{\,s}.\underline{\mathbf{t}})\,(\underline{\boldsymbol{\ell}}^{\,s}.\underline{\mathbf{t}})$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]
Schmid factor						

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]
Schmid factor						

Simple tension for a single crystal specimen

tensile test in the direction [111] **6 active slip systems**

Schmid factor $M^s = (\underline{\mathbf{n}}^{\,s}.\underline{\mathbf{t}}\,)\,(\underline{\boldsymbol{\ell}}^{\,s}.\underline{\mathbf{t}}\,)$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	$[011]$	$[110]$
Schmid factor	0	0	0	0	$\frac{2}{3\sqrt{6}}$	$\frac{2}{3\sqrt{6}}$

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	$[110]$	$[101]$	$[\bar{1}10]$	$[101]$	$[011]$
Schmid factor	0	$\frac{2}{3\sqrt{6}}$	$\frac{2}{3\sqrt{6}}$	0	$\frac{2}{3\sqrt{6}}$	$\frac{2}{3\sqrt{6}}$

Simple tension for a single crystal specimen

tensile test in the direction [011]
Schmid factor $M^s = (\underline{\mathbf{n}}^{\,s}.\underline{\mathbf{t}}\,)\,(\underline{\boldsymbol{\ell}}^{\,s}.\underline{\mathbf{t}}\,)$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]
Schmid factor						

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]
Schmid factor						

Simple tension for a single crystal specimen

tensile test in the direction [011] **4 active slip systems**

Schmid factor $M^s = (\underline{\mathbf{n}}^{\,s}.\underline{\mathbf{t}})\,(\underline{\boldsymbol{\ell}}^{\,s}.\underline{\mathbf{t}})$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]
Schmid factor	$\frac{1}{\sqrt{6}}$	0	$\frac{1}{\sqrt{6}}$	0	0	0

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]
Schmid factor	0	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	0	0	0

Simple tension for a single crystal specimen

tensile test in the direction [012]

Schmid factor $M^s = (\underline{\mathbf{n}}^{\,s}.\underline{\mathbf{t}})\,(\underline{\boldsymbol{\ell}}^{\,s}.\underline{\mathbf{t}})$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	$[011]$	$[110]$
Schmid factor						

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	$[110]$	$[101]$	$[\bar{1}10]$	$[101]$	$[011]$
Schmid factor						

Simple tension for a single crystal specimen

tensile test in the direction [012] **2 active slip systems**

Schmid factor $M^s = (\underline{\mathbf{n}}^s . \underline{\mathbf{t}})(\underline{\boldsymbol{\ell}}^s . \underline{\mathbf{t}})$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]
Schmid factor	$\frac{\sqrt{6}}{5}$	$\frac{1}{5}\sqrt{\frac{3}{2}}$	$\frac{1}{5}\sqrt{\frac{3}{2}}$	$\frac{1}{5}\sqrt{\frac{2}{3}}$	$\frac{1}{5}\sqrt{\frac{3}{2}}$	$\frac{1}{5\sqrt{6}}$

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]
Schmid factor	$\frac{1}{5}\sqrt{\frac{3}{2}}$	$\frac{1}{5}\sqrt{\frac{2}{3}}$	$\frac{\sqrt{6}}{5}$	$-\frac{1}{5\sqrt{6}}$	$-\frac{1}{5}\sqrt{\frac{2}{3}}$	$-\frac{1}{5}\sqrt{\frac{3}{2}}$

Simple tension for a single crystal specimen

tensile test in the direction [123]
Schmid factor $M^s = (\underline{\mathbf{n}}^{\,s}.\underline{\mathbf{t}}\,)\,(\underline{\boldsymbol{\ell}}^{\,s}.\underline{\mathbf{t}}\,)$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	$[011]$	$[110]$
Schmid factor						

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	$[110]$	$[101]$	$[\bar{1}10]$	$[101]$	$[011]$
Schmid factor						

Simple tension for a single crystal specimen

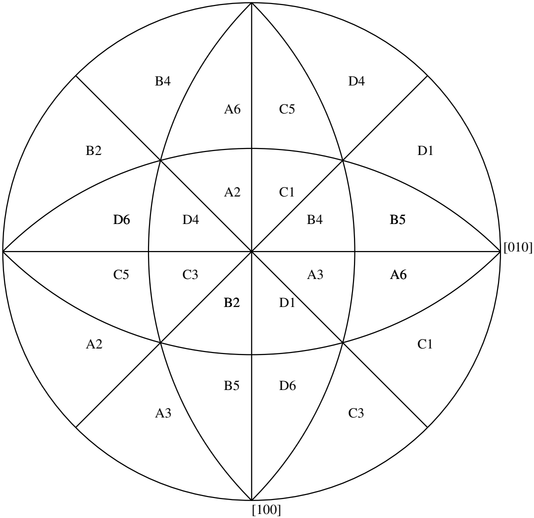
tensile test in the direction [123] **1 active slip system**

Schmid factor $M^s = (\underline{\mathbf{n}}^{\,s}.\underline{\mathbf{t}}\,)(\underline{\boldsymbol{\ell}}^{\,s}.\underline{\mathbf{t}}\,)$

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]
Schmid factor	$\frac{\sqrt{6}}{7}$	$\frac{\sqrt{6}}{14}$	$\frac{\sqrt{6}}{14}$	$\frac{1}{7}\sqrt{\frac{2}{3}}$	$\frac{5}{7\sqrt{6}}$	$\frac{\sqrt{6}}{14}$

number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]
Schmid factor	$\frac{1}{7}\sqrt{\frac{2}{3}}$	$\frac{\sqrt{6}}{7}$	$\frac{4}{7}\sqrt{\frac{2}{3}}$	0	0	0

Simple tension for a single crystal specimen



firs activated slip systems in tension according to Schmid law

Yield surface single crystals

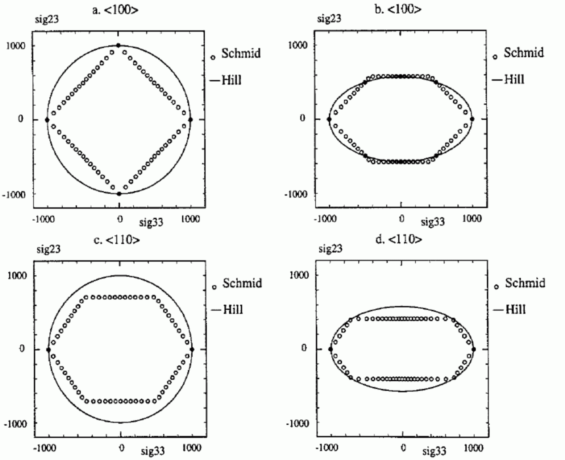


Fig. 1. Theoretical yield surfaces predicted by Schmid and Hill criteria (stresses in MPa). (a) Octahedral slip only, coordinate system ⟨100⟩, ⟨010⟩, ⟨001⟩. (b) Octahedral and cube slip, coordinate system ⟨100⟩, ⟨010⟩, ⟨001⟩. (c) Octahedral slip only, coordinate system ⟨110⟩, ⟨$\bar{1}$10⟩, ⟨001⟩. (d) Octahedral and cube slip, coordinate system ⟨110⟩, ⟨$\bar{1}$10⟩, ⟨001⟩.

Plan

Main equations of continuum thermodynamics

- energy principle (local form)

$$\rho \dot{e} = \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\mathbf{D}} + \rho r - \operatorname{div} \underline{\mathbf{q}}$$

- entropy principle (local form)

$$\rho \dot{s} + \operatorname{div}\left(\frac{\underline{\mathbf{q}}}{T}\right) - \frac{\rho r}{T} \geq 0$$

- Clausius-Duhem inequality

$$-\rho(\dot{e} - T\dot{s}) + \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\mathbf{D}} - \frac{\underline{\mathbf{q}}}{T}.\mathrm{grad}\, T \geq 0$$

Helmholtz free energy density $\psi = e - Ts$

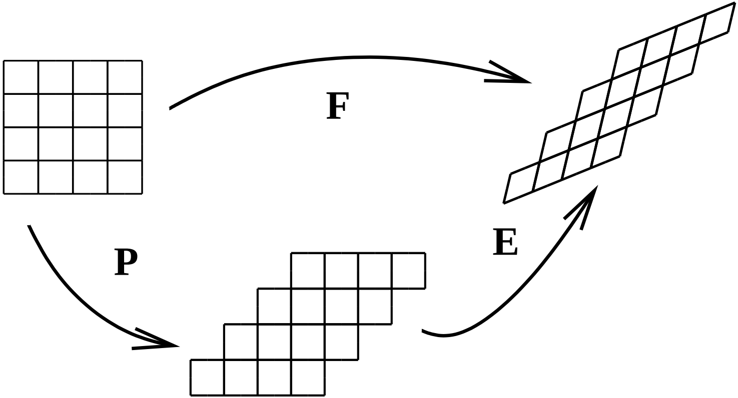
$$-\rho(\dot{\psi} + s\dot{T}) + \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\mathbf{D}} - \frac{\underline{\mathbf{q}}}{T}.\mathrm{grad}\, T \geq 0$$

- intrinsic and thermal dissipation

$$D^{th} = -\frac{\underline{\mathbf{q}}}{T}.\mathrm{grad}\, T$$

$$D^{i} = -\rho(\dot{\Psi} + s\dot{T}) + \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\mathbf{D}}$$

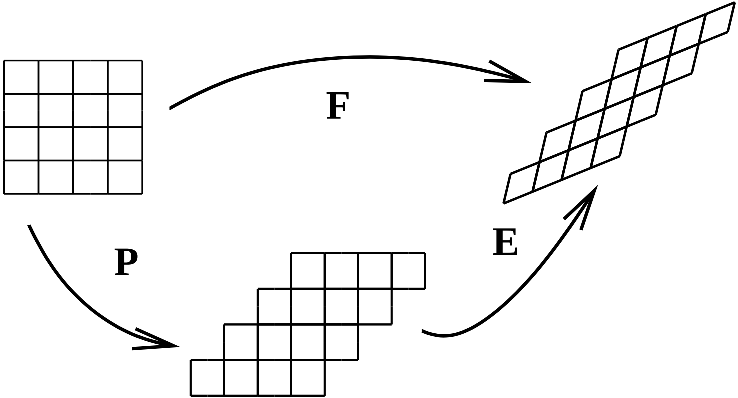
Multiplicative decomposition of the deformation gradient



$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{E}} \cdot \underset{\sim}{\mathbf{P}}$$

isoclinic intermediate configuration according to [Mandel, 1973]

Multiplicative decomposition of the deformation gradient



$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{R}} \cdot \underset{\sim}{\mathbf{U}}, \quad \underset{\sim}{\mathbf{E}} = \underset{\sim}{\mathbf{R}}^e \cdot \underset{\sim}{\mathbf{U}}^e, \quad \underset{\sim}{\mathbf{P}} = \underset{\sim}{\mathbf{R}}^p \cdot \underset{\sim}{\mathbf{U}}^p$$

$\underset{\sim}{\mathbf{U}}^e$ / $\underset{\sim}{\mathbf{U}}^p$: elastic/plastic stretch tensors

$\underset{\sim}{\mathbf{R}}^e$ / $\underset{\sim}{\mathbf{R}}^p$: elastic (lattice) /plastic rotation tensors

Elastoviscoplastic anisotropic materials

- elastic strain and stress tensor with respect to the isoclinic configuration

$$\underset{\sim}{\mathbf{E}}^e = \frac{1}{2}(\underset{\sim}{\mathbf{E}}^T.\underset{\sim}{\mathbf{E}} - \underset{\sim}{\mathbf{1}}), \quad \underset{\sim}{\mathbf{\Pi}}^e = \frac{\rho_i}{\rho}\underset{\sim}{\mathbf{E}}^{-1}.\underset{\sim}{\boldsymbol{\sigma}}.\underset{\sim}{\mathbf{E}}^{-T}$$

- power of internal forces

$$\frac{1}{\rho}\underset{\sim}{\boldsymbol{\sigma}} : (\dot{\underset{\sim}{\mathbf{F}}}.\underset{\sim}{\mathbf{F}}^{-1}) = \frac{1}{\rho_i}(\underset{\sim}{\mathbf{\Pi}}^e : \dot{\underset{\sim}{\mathbf{E}}}^e + (\underset{\sim}{\mathbf{E}}^T.\underset{\sim}{\mathbf{E}}.\underset{\sim}{\mathbf{\Pi}}^e) : (\dot{\underset{\sim}{\mathbf{P}}}.\underset{\sim}{\mathbf{P}}^{-1}))$$

- Clausius–Duhem inequality

$$\rho(\frac{\underset{\sim}{\mathbf{\Pi}}^e}{\rho_i} - \frac{\partial\Psi}{\partial\underset{\sim}{\mathbf{E}}^e}) : \dot{\underset{\sim}{\mathbf{E}}}^e - \rho(s + \frac{\partial\Psi}{\partial T})\dot{T} + D^{res} \geq 0$$

- State variables: $(\underset{\sim}{\mathbf{E}}^e, T, \alpha)$, internal variables α
- State functions : internal energy density $e(\underset{\sim}{\mathbf{E}}^e, s, \alpha)$
  Helmholtz free energy density $\psi(\underset{\sim}{\mathbf{E}}^e, T, \alpha) = e - Ts$

Standard elastoviscoplastic materials

- exploitation of the second principle
  state laws

$$\underset{\sim}{\mathbf{\Pi}}^e = \rho_i \frac{\partial \Psi}{\partial \underset{\sim}{\mathbf{E}}^e}, \quad X = \rho_i \frac{\partial \Psi}{\partial \alpha}, \quad s = -\frac{\partial \Psi}{\partial T}$$

- residual dissipation:

$$D^{res} = \underset{\sim}{\mathbf{M}} : (\dot{\underset{\sim}{\mathbf{P}}}.\underset{\sim}{\mathbf{P}}^{-1}) - X\dot{\alpha} \geq 0$$

  Mandel stress tensor:

$$\underset{\sim}{\mathbf{M}} := \underset{\sim}{\mathbf{E}}^T.\underset{\sim}{\mathbf{E}}.\underset{\sim}{\mathbf{\Pi}}^e = \underset{\sim}{\mathbf{C}}^e.\underset{\sim}{\mathbf{\Pi}}^e$$

- assume the existence of a convex dissipation potential
  $\Omega(\underset{\sim}{\mathbf{M}}, X)$

$$\dot{\underset{\sim}{\mathbf{P}}}.\underset{\sim}{\mathbf{P}}^{-1} = \frac{\partial \Omega}{\partial \underset{\sim}{\mathbf{M}}}, \quad \dot{\alpha} = -\frac{\partial \Omega}{\partial X}$$

Plan

Template for a single crystal model

- state variables: elastic strain $\underset{\sim}{\varepsilon}^e$, "dislocation density" ϱ^s, internal structure α^s
- free energy

$$\rho\psi(\underset{\sim}{\varepsilon}^e, \varrho^s, \alpha^s) = \frac{1}{2}\underset{\sim}{\varepsilon}^e : \underset{\approx}{\mathbf{c}} : \underset{\sim}{\varepsilon}^e + r_0 \sum_{s=1}^{N} \varrho^s + \frac{1}{2} q \sum_{r,s=1}^{N} h^{rs} \varrho^r \varrho^s + \frac{1}{2} c \sum_{s=1}^{N} \alpha^{s2}$$

- state laws

Template for a single crystal model

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- state laws

$$\begin{aligned} \underset{\sim}{\boldsymbol{\sigma}} &= \rho \frac{\partial \psi}{\partial \underset{\sim}{\varepsilon}^e} = \underset{\approx}{\mathbf{c}} : \underset{\sim}{\varepsilon}^e \\ r^s &= \rho \frac{\partial \psi}{\partial \varrho^s} = r_0 + q \sum_{r=1}^{N} h^{sr} \varrho^r \\ x^s &= \rho \frac{\partial \psi}{\partial \alpha^s} = c\alpha^s \end{aligned}$$

Template for a single crystal model

- resolved shear stress on slip system s

$$\tau^s = (\underset{\sim}{\boldsymbol{\sigma}}.\underline{\mathbf{n}}^s).\underline{\boldsymbol{\ell}}^s = \underset{\sim}{\boldsymbol{\sigma}} : (\underline{\boldsymbol{\ell}}^s \otimes \underline{\mathbf{n}}^s) = \underset{\sim}{\boldsymbol{\sigma}} : (\underline{\boldsymbol{\ell}}^s \overset{sym}{\otimes} \underline{\mathbf{n}}^s)$$

- multimechanism crystal plasticity yield criterion: **Schmid law**

$$f^s = |\tau^s - x^s| - r^s$$

yield limit r^s, internal stress (back–stress) x^s,
for each system s

- dissipation potential $\quad \Omega(\underset{\sim}{\boldsymbol{\sigma}}, r^s, x^s) = \dfrac{K}{n+1} \sum_{s=1}^{N} \langle \dfrac{f^s}{K} \rangle^{n+1}$

- flow and hardening rules

Template for a single crystal model

- resolved shear stress on slip system s

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- flow and hardening rules

$$\dot{\underset{\sim}{\boldsymbol{\varepsilon}}}^p = \frac{\partial \Omega}{\partial \underset{\sim}{\boldsymbol{\sigma}}} = \sum_{s=1}^{N} \dot{\gamma}^s \underline{\boldsymbol{\ell}}^s \overset{sym}{\otimes} \underline{\mathbf{n}}^s, \quad \dot{\varrho}^s = -\frac{\partial \Omega}{\partial r^s} = \dot{v}^s, \quad \dot{\alpha}^s = -\frac{\partial \Omega}{\partial x^s} = \dot{\gamma}^s$$

with

$$\dot{v}^s = \langle \frac{f^s}{K} \rangle^n, \quad \dot{\gamma}^s = \dot{v}^s \,\mathrm{sign}(\tau^s - x^s)$$

Nonlinear hardening rules

- nonlinear isotropic hardening

$$\varrho^s = 1 - \exp(-bv^s)$$

$$r^s = r_0 + q \sum_{r=1} h^{sr}(1 - \exp(-bv^s))$$

- nonlinear kinematic hardening

$$\dot{\alpha}^s = \dot{\gamma}^s - d\dot{v}^s \alpha^s$$

monotonic loading:

$$x^s = \frac{c}{d}(\pm 1 - \exp(-dv^s))$$

Interaction matrix

- **latent** hardening (two activated slip systems)

$$r^2 = r_0 + h_1 \varrho^1 + h_2 \varrho^2$$

- Taylor hardening $h^{rs} = 1, \quad \forall r, s$
- interaction matrix for FCC crystals

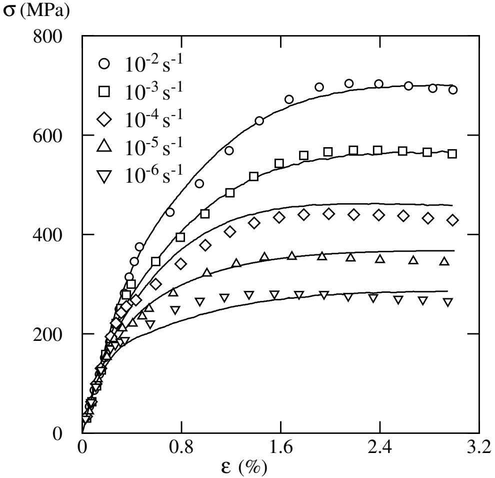
Interaction matrix

	$B4$	$B2$	$B5$	$D4$	$D1$	$D6$	$A2$	$A6$	$A3$	$C5$	$C3$	$C1$
$B4$	h_1	h_2	h_2	h_4	h_5	h_5	h_5	h_6	h_3	h_5	h_3	h_6
$B2$		h_1	h_2	h_5	h_3	h_6	h_4	h_5	h_5	h_5	h_6	h_3
$B5$			h_1	h_5	h_6	h_3	h_5	h_3	h_6	h_4	h_5	h_5
$D4$				h_1	h_2	h_2	h_6	h_5	h_3	h_6	h_3	h_5
$D1$					h_1	h_2	h_3	h_5	h_6	h_5	h_5	h_4
$D6$						h_1	h_5	h_4	h_5	h_3	h_6	h_5
$A2$							h_1	h_2	h_2	h_6	h_5	h_3
$A6$								h_1	h_2	h_3	h_5	h_6
$A3$									h_1	h_5	h_4	h_5
$C5$										h_1	h_2	h_2
$C3$											h_1	h_2
$C1$												h_1

simplified version: $h_1 = 1, \quad h_2 = h_3 = h_4 = h_5 = h_6 = h$

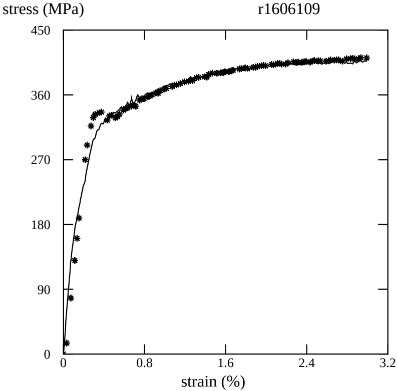
Plan

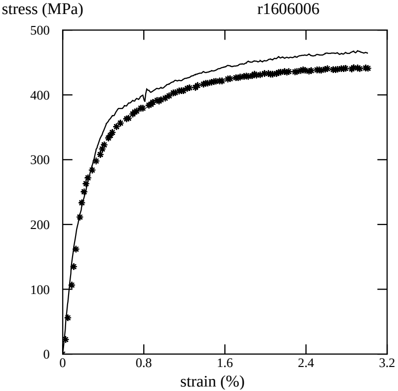
Identification of material parameters



Nickel-base single crystal superalloy at 950°C: tensile tests

Identification of material parameters

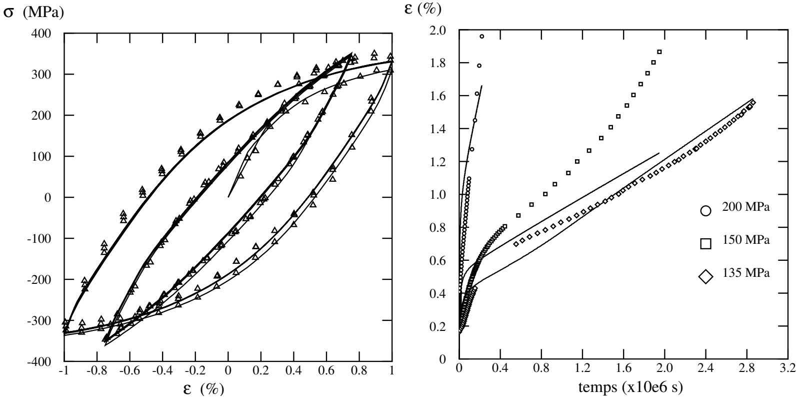




$< 111 >$–oriented single crystal SC16 at 950°C ($\dot{\varepsilon} = 10^{-3}s^{-1}$)

$< 011 >$–oriented single crystal SC16 at 950°C ($\dot{\varepsilon} = 10^{-3}s^{-1}$)

Identification of material parameters



Nickel-base single crystal superalloy at 950°C: cyclic and creep tests

Identification of material parameters

slip systems	k MPa$^{1/n}$	n	r_o MPa	q MPa	b	c MPa	d	M	m
octahedral	700	4.7	4.6	3.9	3.7	96536	1050	314	5
cubic	1172	2.4	17.3	-4.4	2.7	77081	1056	155	10

Nickel-base single crystal superalloy at 950°C: values of parameters

Plan

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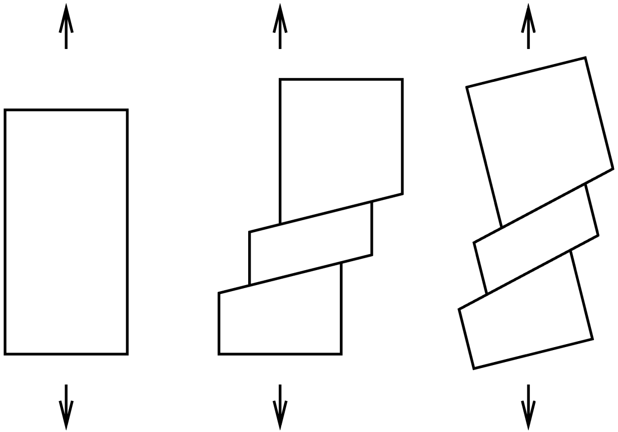
Lattice rotation concept



tensile specimen plastic slip superimposed rigid body motion

For small elastic strain (usual in metals), lattice rotation is given by the rotation part in the polar decomposition of the elastic deformation

$$\underset{\sim}{\mathbf{E}} = \underset{\sim}{\mathbf{V}}^e . \underset{\sim}{\mathbf{R}}^e = \underset{\sim}{\mathbf{R}}^e . \underset{\sim}{\mathbf{U}}^e$$

Plan

Kinematics of simple glide

$$\left\{ \begin{array}{l} x_1 = X_1 + \gamma X_2 \\ x_2 = X_2 \\ x_3 = X_3 \end{array} \right. , \quad \underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{1}} + \gamma \underline{\mathbf{e}}_1 \otimes \underline{\mathbf{e}}_2, \quad [\underset{\sim}{\mathbf{F}}] = \left[\begin{array}{ccc} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right]$$

Simple glide

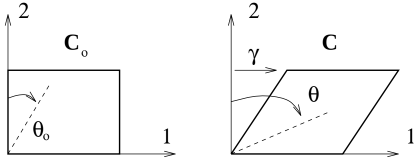
$$\underset{\sim}{\mathbf{U}} = \begin{bmatrix} \dfrac{1}{\sqrt{1+(\gamma/2)^2}} & \dfrac{\gamma}{2\sqrt{1+(\gamma/2)^2}} & 0 \\ \dfrac{\gamma}{2\sqrt{1+(\gamma/2)^2}} & \dfrac{1+\gamma^2/2}{\sqrt{1+(\gamma/2)^2}} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\underset{\sim}{\mathbf{V}} = \begin{bmatrix} \dfrac{1+\gamma^2/2}{\sqrt{1+(\gamma/2)^2}} & \dfrac{\gamma}{2\sqrt{1+(\gamma/2)^2}} & 0 \\ \dfrac{\gamma}{2\sqrt{1+(\gamma/2)^2}} & \dfrac{1}{\sqrt{1+(\gamma/2)^2}} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\underset{\sim}{\mathbf{R}} = \begin{bmatrix} \dfrac{1}{\sqrt{1+(\gamma/2)^2}} & \dfrac{\gamma}{2\sqrt{1+(\gamma/2)^2}} & 0 \\ \dfrac{-\gamma}{2\sqrt{1+(\gamma/2)^2}} & \dfrac{1}{\sqrt{1+(\gamma/2)^2}} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

eigenrotation around axis $\underline{\mathbf{e}}_3$ with angle $\tan\theta = -\frac{\gamma}{2}$

Rotation of material lines



$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{1}} + \gamma \underline{\mathbf{e}}_1 \otimes \underline{\mathbf{e}}_2$$

rotation of material lines:

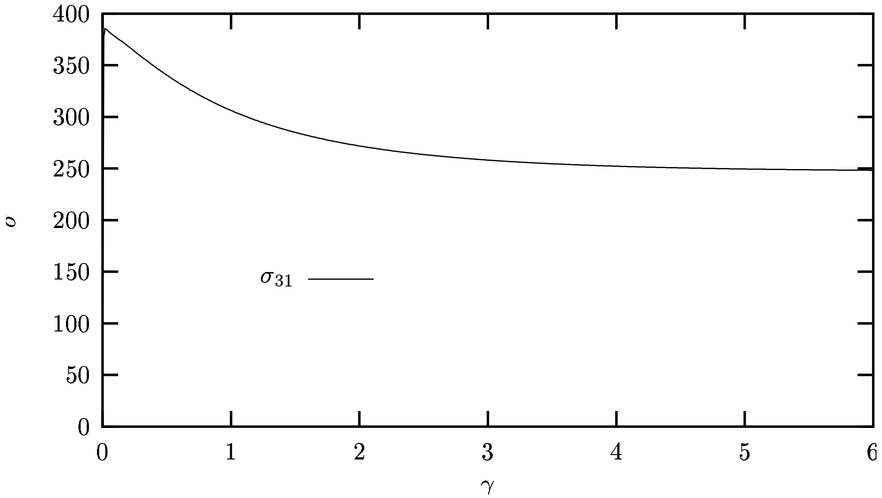
$$\tan\theta = \tan\theta_0 \; + \; \gamma, \quad \dot{\theta} \; = \; \frac{\dot{\gamma}}{1 \; + \; (\tan\theta_0 \; + \; \gamma)^2}$$

$$< \dot{\theta}_L > = \frac{\dot{\gamma}}{\pi} \int_{-\pi/2}^{\pi/2} \frac{1}{1 \; + \; (\tan\theta_0 \; + \; \gamma)^2} \, d\theta_0 \; = \; \frac{\dot{\gamma}}{2(1 + \frac{\gamma^2}{4})}$$

$$< \dot{\theta}_e > = \frac{\dot{\gamma}}{\pi} \int_{-\pi/2}^{\pi/2} \frac{1}{1 \; + \; \tan^2\theta} \, d\theta \; = \; \frac{\dot{\gamma}}{2}$$

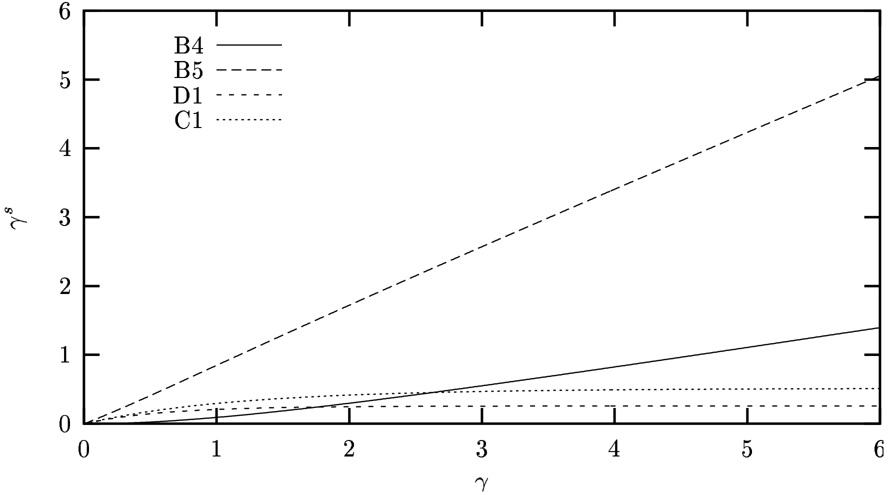
the corotational frame rotates without stopping! the eigen rotation stops progressively...

Simple glide for single crystals



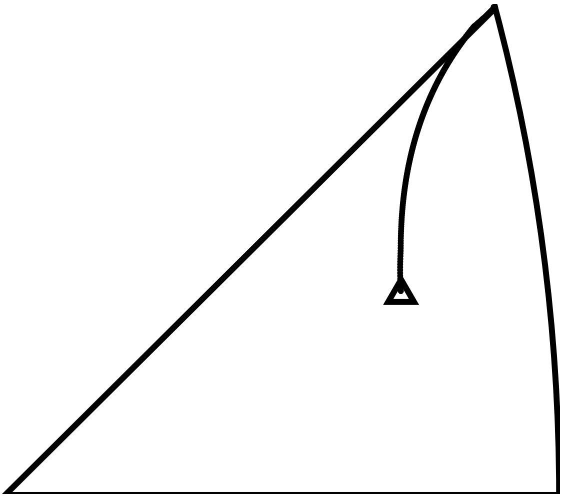
$\underline{\mathbf{e}}_1 = [2\bar{1}0] / \underline{\mathbf{e}}_2 = [123]$

Simple glide for single crystals



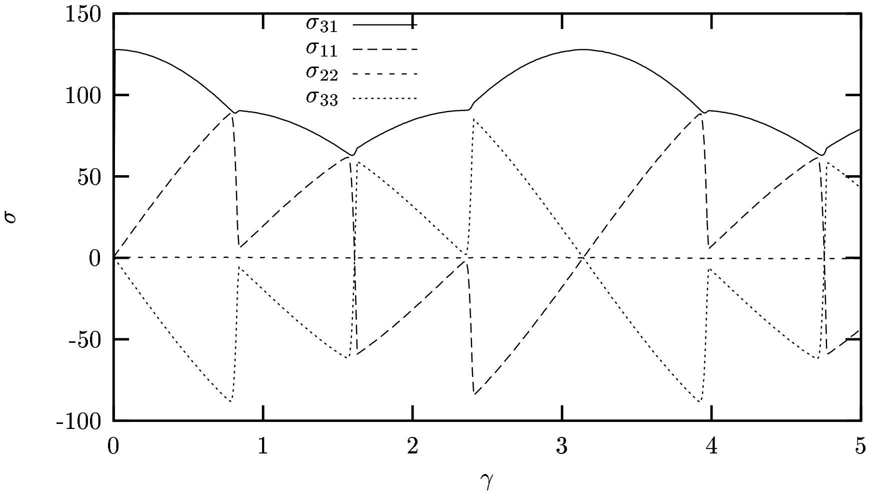
$\underline{\mathbf{e}}_1 = [2\bar{1}0] / \underline{\mathbf{e}}_2 = [123]$

Simple glide for single crystals



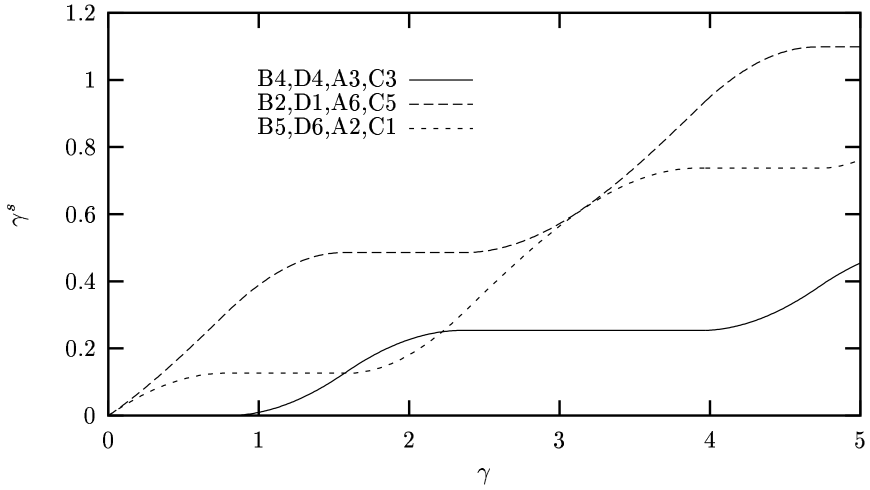
$\underline{\mathbf{e}}_1 = [2\bar{1}0] / \underline{\mathbf{e}}_2 = [123]$

Simple glide for single crystals



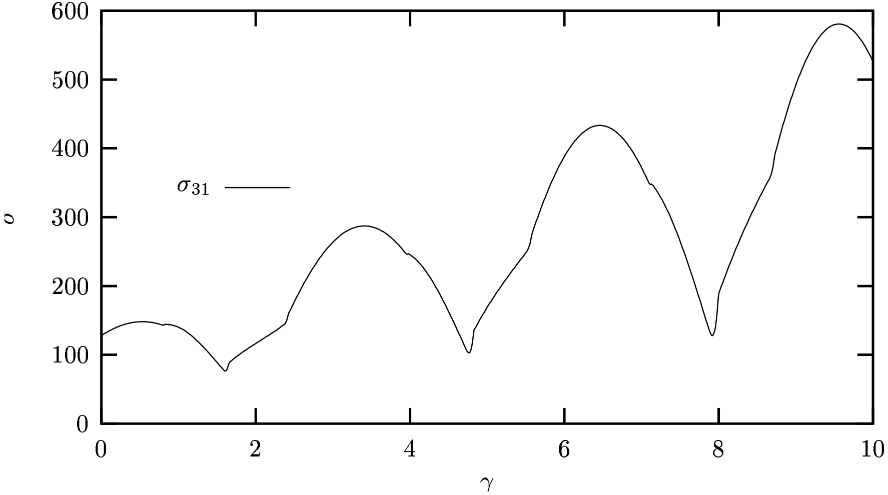
simple glide $\neq$ simple shear! $\underline{\mathbf{e}}_1 = [100]/\underline{\mathbf{e}}_2 = [001]$

Simple glide for single crystals



$\underline{\mathbf{e}}_1 = [100]/\underline{\mathbf{e}}_2 = [001]$

Simple glide for single crystals



$\underline{\mathbf{e}}_1 = [100] / \underline{\mathbf{e}}_2 = [001]$

Plan

Torsion of a single crystal