PLASTICITÉ CRISTALLINE ET TRANSITION D'ÉCHELLE : CAS DU MONOCRISTAL

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Lionel MARCIN (Safran Tech/M&P), lionel.marcin@safrangroup.com



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Outline



1. Introduction & motivation
2. Physical origins of crystal slip
Experimental observations
Taylor's paradox
Dislocations
3. Continuum crystal plasticity
The schmid law

Geometry of slip and Schmid factors in FCC crystals Constitutive rules for single crystal plasticity Example of monocrystal behaviour Example of FE computation



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Deformation of crystalline materials : a multiscale problem



Espace (cm) / Échelles

Plastic deformation results in the motion of lots of defects in the crystal lattice (dislocations) \rightarrow continuum scale (> µm)



Integrated Computational Materials Engineering



Local values (as opposed to mean values) are crucial when studying deformation and fracture \rightarrow model for crystal plasticity needed.



Such applications in aeronautic (Safran sources)





Such applications in electronics (Single crystal)









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A brief history

V.Volterra	G.I. Taylor	M. Polanyi	E. Orowan	P.B. Hirsch
1860 - 1940	1886 - 1975	1891 - 1976	1891 - 1976	1920 -

The early of the history of dislocation theory. 1907: Definition of Volterra's dislocation (or isolated defect) by the mathematician V. Volterra; 1934: Discovery of the concept of crystal dislocation introduced by Orowan, Polany and Taylor; 1956: First published observations of dislocations by transmission electron microscopy.



60 years of plastic slip in monocrystals



Cadmium monocrystal deformed under tension [Schmid and Boas, 1950]

mode mag 🖳 10 1 mm FTD SE 15 000 x

Fib fabricated micropillar deformed under compression [Shan et al., 2007]

Conclusion : Crystals deform by shear. Shear appear to be localized on the highest atomic density planes, the so-called *slip planes*.



Evidences of crystallographic slip in Ni-based superalloy



With each passage of a dislocation through a single crystal corresponds the appearance of a "walk" on the surface and a shift of the two parts. The set of these shifts generates the plastic deformation observable on the macroscopic scale



The concept of dislocation (1/2)



pure edge

pure screw

mixed dislocation



The concept of dislocation (2/2)

A dislocation can be represented by :

♦a line vector L

♦a Bürgers vector b

Dislocations may pre-exist and are created during plastic deformation.

The sum of the Burgers vector of created dislocations is equal to zero

A dislocation moves

- The motion is defined by a glide plane (L , b) and a glide direction g
- Screw dislocation don't have a single glide plane
- Edge dislocation do have a single glide plane
- Plastic deformation is associated to the flux of disloc-

The crystal is distorted around dislocations

- Dislocations are stress concentrators
- There is an elastic energy associated to dislocations





dislocated network

perfect network



Can we actually see dislocations ?



Microscope FEI TECNAI F20-ST Centre des Matériaux – MINES ParisTech

Bright field image Dislocation microstructure of deformed Ti-6242 alloy





Can we actually see dislocations ?

In 1cm3 of metal alloys (order of magnitude):

- 10m of dislocation in a single crystal alloy
- 10.000km in a polycrystal weakly hardened
- 10.000.000km in a highly hardened polycrystal

Bright field image Dislocation microstructure of deformed Ti-6242 alloy







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Tensile test apllied to SX - Resolved shear stress



Given a slip direction *I* contained in a slip plane with a normal vector *n*, the shear τ in the slip direction can be related to the applied tensile stress σ :

$$\tau = \frac{F\cos(\lambda)}{S/\cos(\chi)} = \sigma\cos(\lambda)\cos(\chi)$$

 $m = \cos(\lambda) \cos(\chi) 2 [0, 0.5]$ is called the **Schmid** factor.

Generalization, in tensorial form we have :

$$\tau = l_i \sigma_{ij} n_j$$



The critical resolved shear stress

Experiments of Schmid and Boas

◆No influence of the normal stress operating on the glide plane.

◆ A critical value of the resolved shear stress is required for the initiation of glide.





The critical resolved shear stress

Experiments of Schmid and Boas

◆No influence of the normal stress operating on the glide plane.

◆ A critical value of the resolved shear stress is required for the initiation of glide.





The critical resolved shear stress

More experimental data on critical resolved shear stress:

Mg data from [Schmid1950]

Zn data from [Jillson]

Cd data from [Andrade & Roscoe]





Some important crystalline structures

Face centered cubic



Body centered cubic

Hexagonal close packing





Slip systems in FCC crystals



Octaedral slip

4 slip planes {111} i.e. (111), (111), (111), (111) indicated by normals 3 slip directions of type <110> in each 111 plane

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\overline{1}1)$	$(1\overline{1}1)$	$(1\overline{1}1)$
direction	[101]	$[0\overline{1}1]$	$[\overline{1}10]$	[101]	[011]	[110]
number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\overline{1}11)$	$(11\overline{1})$	$(11\overline{1})$	$(11\overline{1})$
direction	$[0\overline{1}1]$	[110]	[101]	$[\overline{1}10]$	[101]	[011]



Tensile test in the direction [001]

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\overline{1}1)$	$(1\overline{1}1)$	$(1\overline{1}1)$
direction	$[\overline{1}01]$	$[0\overline{1}1]$	$[\overline{1}10]$	[101]	[011]	[110]
Schmid factor						
number	7	8	9	10	11	12
number name	7 A2	8 A6	9 A3	10 C5	11 C3	12 C1
number name plane	7 A2 (ī11)	8 A6 (111)	9 A3 (111)	10 C5 (111)	11 C3 (111)	12 C1 (111)



Tensile test in the direction [001]

Schmid factor $m^{s} = (\mathbf{n}^{s} \cdot \mathbf{t}) (\mathbf{l}^{s} \cdot \mathbf{t})$

8 active slip systems

3 5 number 2 4 6 B4 B2 B5 D4 D1 D6 name $(1\overline{1}1)$ $(1\overline{1}1)$ $(1\overline{1}1)$ plane 111)(111)(111)101] [011][110][101]direction [011][110] $\frac{1}{\sqrt{6}}$ $\frac{1}{\sqrt{6}}$ Schmid factor $\frac{1}{\sqrt{6}}$ $\frac{1}{\sqrt{6}}$ 0 0 number 8 9 10 11 12 C5 C3 A2 A6 A3 C1 name $(\bar{1}11)$ $(\bar{1}11)$ $(\overline{1}11)$ $(11\overline{1})$ $(11\overline{1})$ plane (111)direction [011][110]101 [110][101][011]Schmid factor $\frac{1}{\sqrt{6}}$ $\frac{1}{\sqrt{6}}$ 0 0 $\overline{\sqrt{6}}$ $\sqrt{6}$



Tensile test in the direction [111]

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\overline{1}1)$	$(1\overline{1}1)$	$(1\overline{1}1)$
direction	[101]	$[0\overline{1}1]$	$[\overline{1}10]$	[101]	[011]	[110]
Schmid factor						
number	7	8	9	10	11	12
number name	7 A2	8 A6	9 A3	10 C5	11 C3	12 C1
number name plane	7 A2 (ī11)	8 A6 (111)	9 A3 (Ī11)	10 C5 (111)	11 C3 (111)	12 C1 (111)
number name plane direction	7 A2 (111) [011]	8 A6 (111) [110]	9 A3 (111) [101]	10 C5 (111) [110]	11 C3 (111) [101]	12 C1 (111) [011]



Tensile test in the direction [111]

6 active slip systems

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\overline{1}1)$	$(1\overline{1}1)$	$(1\overline{1}1)$
direction	$[\overline{1}01]$	$[0\overline{1}1]$	$[\overline{1}10]$	$[\overline{1}01]$	[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
number name	7 A2	8 A6	9 A3	10 C5	11 C3	12 C1
number name plane	7 A2 (Ī11)	8 A6 (111)	9 A3 (Ī11)	10 C5 (111)	11 C3 (111)	12 C1 (111)
number name plane direction	7 A2 (ī11) [0ī1]	8 A6 (111) [110]	9 A3 (ī11) [101]	10 C5 (111) [110]	11 C3 (111) [101]	12 C1 (111) [011]



Tensile test in the direction [011]

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\overline{1}1)$	$(1\overline{1}1)$	$(1\overline{1}1)$
direction	$[\overline{1}01]$	$[0\overline{1}1]$	$[\overline{1}10]$	[101]	[011]	[110]
Schmid factor						
number	7	8	9	10	11	12
number name	7 A2	8 A6	9 A3	10 C5	11 C3	12 C1
number name plane	7 A2 (Ī11)	8 A6 (ī111)	9 A3 (Ī11)	10 C5 (111)	11 C3 (111)	12 C1 (111)
number name plane direction Schmid factor	7 A2 (ī11) [0ī1]	8 A6 (111) [110]	9 A3 (ī11) [101]	10 C5 (111) [110]	11 C3 (111) [101]	12 C1 (111) [011]



Tensile test in the direction [011]

4 active slip systems

number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\overline{1}1)$	$(1\overline{1}1)$	$(1\overline{1}1)$
direction	[101]	$[0\overline{1}1]$	$[\overline{1}10]$	[101]	[011]	[110]
Schmid factor	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0	0
number	7	8	9	10	11	12
number name	7 A2	8 A6	9 A3	10 C5	11 C3	12 C1
number name plane	7 A2 (ī11)	8 A6 (111)	9 A3 (Ī11)	10 C5 (111)	11 C3 (111)	12 C1 (111)
number name plane direction	7 A2 (111) [011]	8 A6 (111) [110]	9 A3 (ī11) [101]	10 C5 (111) [110]	11 C3 (111) [101]	12 C1 (111) [011]



First activated slip systems in tension according to Schmid law:



[001] tension

[111] tension

[110] tension





First activated slip systems in tension according to Schmid law:



[001] tension

8 slip systems : B4, C1, A2, D4, C3, B2, D1, A3 [111] tension

[110] tension



First activated slip systems in tension according to Schmid law:



[001] tension

8 slip systems : B4, C1, A2, D4, C3, B2, D1, A3

[111] tension

6 slip systems : D4, D1, C1, C5, B4, B5

[110] tension





First activated slip systems in tension according to Schmid law:



[001] tension

8 slip systems : B4, C1, A2, D4, C3, B2, D1, A3

[111] tension

6 slip systems : D4, D1, C1, C5, B4, B5

[110] tension

4 slip systems : B4, A3, B5, A6





Historical developments of the theory

- □ The initial foundations are laid out by the pioneering work of **Taylor** in 1938 [Taylor, 1938].
- The theory was since further developed by Bishop & Hill [Bishop and Hill, 1951], Kocks
 [Kocks and Brown, 1966, Kocks, 1970], Hill and Rice
 [Hill, 1966, Hill and Rice, 1972], Asaro and Rice
 [Asaro, 1975, Asaro and Rice, 1977], Havner [Havner, 1992],
 Cailletaud [Meric et al., 1991, Meric and Cailletaud, 1991].



Rate sensitive plastic slip

The Schmid law predicting an elastic-perfectly plastic behaviour cannot describe typical () curves. The plastic slip on a given slip system s (*ns*, *ls*) is rate sensitive and can be described by a power law.



Two main formulations exist in the literature : **Multiplicative**

$$\dot{\gamma}^s = \dot{\gamma}_0 (\frac{\tau^s}{\tau_0})^n sign(\tau^s)$$

Additive with threshold

 $\dot{\gamma}^{s} = \left\langle \frac{\left|\tau^{s}\right| - \tau_{0}}{K} \right\rangle sign(\tau^{s})$

 τ_0 is the critical resolved shear stress, $\dot{\gamma_0}$, *K* and *n* are parameters.



Basic ingredients of crystal plasticity



A collection of *N* slip systems Normal to slip plane *n^s* Direction of slip system *I^s*

Orientation tensor $\underline{m}^s = \frac{1}{2} (\vec{n}^s \otimes \vec{l}^s + \vec{l}^s \otimes \vec{n}^s)$ Resolved shear stress $\tau^s = \underline{\sigma} : \underline{m}^s = \underline{\sigma} : \frac{1}{2} (\vec{l}^s \otimes \vec{n}^s + \vec{n}^s \otimes \vec{l}^s)$ Yield function $f^s(\tau^s, \text{hardening variables}, ...) = 0$ Elastic behavior $\forall s, f^s < 0$ Shear strain rate $\dot{\gamma}^s = \dot{\gamma}^s(f^s)$



Small strain formalism and schmid law

□ Strain partition into elastic and plastic parts

$$\underline{\varepsilon} = \underline{\varepsilon}^e + \underline{\varepsilon}^p$$

Resolved shear stress, computed by means of the *orientation tensor*, *m^s*, using the vector normal to the slip plane, *n^s*, and the slip direction, *l^s*

$$\tau^{s} = \underline{\sigma} : \underline{m}^{s} \qquad \underline{m}^{s} = \frac{1}{2} (\vec{l}^{s} \otimes \vec{n}^{s} + \vec{n}^{s} \otimes \vec{l}^{s})$$

□ A yield function *f s* is defined on each slip system *s* (here with additive hardening)

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

Viscoplastic flow Shear strain rate s deduced from resolved shear stress s and from the value of the kinematic (Xs) and isotropic (Rs) variables :

$$\dot{\gamma}^{s} = \left\langle \frac{\left| \tau^{s} - x^{s} \right| - r^{s}}{K^{s}} \right\rangle^{n^{s}} sign(\tau^{s} - x^{s})$$



Single crystal model

□ Viscoplastic potential [Mandel, 1972]

$$\Omega(\underline{\sigma},...) = \sum_{s} \frac{K}{n+1} \left\langle \frac{f^{s}}{K} \right\rangle^{n+1}$$

□ Viscoplastic strain rate (from the viscoplastic potential)

$$\underline{\dot{\varepsilon}}^{p} = \sum_{s} \frac{\partial \Omega}{\partial \underline{\sigma}} = \sum_{s} \frac{\partial \Omega}{\partial f^{s}} \frac{\partial f^{s}}{\partial \underline{\sigma}} = \sum_{s} \dot{v}^{s} \underline{m}^{s} \eta^{s} = \sum_{s} \dot{\gamma}^{s} \underline{m}^{s}$$

 \Box Hardening rules : X^s and R^s computed by means of state variables s and r^s

$$X^{s} = c\alpha^{s} \qquad \dot{\alpha}^{s} = (\eta^{s} - d\alpha^{s})\dot{v}^{s}$$
$$R^{s} = r_{0} + Q\sum_{j} h_{sj}r^{j} \qquad \dot{r}^{j} = (1 - br^{j})\dot{v}^{j}$$



Interaction matrix

	<i>B</i> 4	B2	<i>B</i> 5	D4	D1	D6	A2	<i>A</i> 6	A3	<i>C</i> 5	С3	C1
<i>B</i> 4	h_1	<i>h</i> ₂	<i>h</i> ₂	h_4	h_5	h_5	h_5	h_6	<i>h</i> 3	h_5	h ₃	h_6
<i>B</i> 2		h_1	<i>h</i> 2	h_5	h_3	h_6	<i>h</i> 4	h_5	h_5	h_5	h_6	<i>h</i> 3
<i>B</i> 5			h_1	h_5	h_6	h_3	h_5	<i>h</i> 3	h_6	h_4	h_5	h_5
D4				h_1	<i>h</i> ₂	<i>h</i> ₂	h_6	h_5	<i>h</i> 3	h_6	h ₃	h_5
D1					h_1	h_2	h ₃	h_5	h_6	h_5	h_5	h_4
<i>D</i> 6						h_1	h_5	<i>h</i> 4	<i>h</i> 5	h ₃	h_6	h_5
A2							h_1	h_2	<i>h</i> ₂	h_6	h_5	h_3
<i>A</i> 6								h_1	<i>h</i> ₂	h ₃	h_5	h_6
A3									h_1	h_5	h_4	h_5
<i>C</i> 5										h_1	h_2	h_2
С3											h_1	h_2
<i>C</i> 1												h_1

simplified version (Taylor model)

h1 = h2 = h3 = h4 = h5 = h6 = 1



Example of monocrystal behaviour

Stress–strain curves simulated for a β -titane monocrystal under tension in different directions.





Example of monocrystal behaviour

Stress-strain curves simulated for a nickel bas superalloys monocrystal under tension in different directions at 650 °C.



Temperature : 650 °C

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Yield surface





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Z-sim input file to compute the yield surface

```
****simulate
***test polysurf
 **load
  *segment 1
   time sig11 sig22 sig33 sig12 sig23 sig31
   0.0 0. 0. 0. 0. 0. 0.
   0.01 0. 1. 0. 0. 0. 0.
 **model
  *file ti mat
  *rotation euler x1 1, 0, 0, x2 1, 1, 1,
  *integration runge_kutta 1.e-4
 **output
 **yield_surface ps-11-12.test
  *degrees 1.
  *factor 1.e9
  *find offset 1.e-1
  *component sig11 sig12
  *time 0.0
****return
```







Crack in Ni based superalloy single crystals





Crack in Ni based superalloy single crystals

Comparison with experiments [Flouriot et al., 2003]









Cubic elasticity $\underline{\sigma} = \underline{\underline{C}} : \underline{\underline{c}}^{e}$

Resolved shear stress $\tau^s = \underline{\sigma} : \underline{m}^s$

Viscous flow $\dot{\gamma}^s = \varepsilon_0^s \sinh\left(\left\langle \frac{\left|\tau^s - x^s\right| - r^s}{K^s}\right\rangle^{n^s}\right) sign(\tau^s - x^s)$

Plastic strain rate $\underline{\dot{\varepsilon}}^{p} = \sum \dot{\gamma}^{s} \underline{m}^{s}$

Orientation tensor $\underline{\underline{m}}^{s} = \frac{1}{2}(\vec{n}^{s} \otimes \vec{l}^{s} + \vec{l}^{s} \otimes \vec{n}^{s})$ **Kinematic hardening restoration** $\dot{x}^{s} = C^{s}\dot{\gamma} - D^{s}x^{s}|\dot{\gamma}^{s}| - \left(\frac{|x^{s}|}{M^{s}}\right)^{m^{s}}sign(x^{s})$



saturation of viscosity



Use of sinh instead of power law (Norton-Hoff)

Goals : the use of a "sinh" form limits the increase of the viscous stress when the strain rate increases



Comparison between simulations and experiments for some isothermal cyclic strain tests.



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Concerning creep tests, the introduction of a static recovery term enables to simulate with quite good accuracy the secondary creep



Comparison between simulations and experiments for some creep tests.



Long term relaxation at 950°C



Hysteritic loop at 950 °C



Comparison between simulations and experiments for some hysteresis loops performed along <011> and <111> crystallographic directions



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Simulation of the evolution of the 0,2% yield stress with temperature for three strain rates in the <001> direction



In a second step, in order to test the material under conditions closer than those observed in service, specific tests were developed called: thermomechanical tests. In such tests, the material is simultaneously subjected to mechanical strain and temperature, both, evolving during the cycle.



Comparison between simulations and experiments for some anisothermal test



Synthèse avantage/inconvénient des différents modèles de comportement

	Modèle isotrope à 2 Potentiels de Norton	Modèle anisotrope cristallographique initial à 1 Potentiel de Norton	Modèle « Sinh+restauration »
Anisotrope cristalline	NON	OUI	OUI
Prise en compte de la restauration statique de l'écrouissage	NON	NON	OUI
Prise en compte du fluage	OUI mais <u>uniquement</u> dans la direction <001> du monocristal	NON	OUI
Saturation de la viscosité	NON	NON	OUI



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