Theory and application of a computational framework for crystal plasticity

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goal

predicting the solid mechanics of metals in structural applications goal

predicting the solid mechanics of metals in structural applications



from http://courses.eas.ualberta.ca/eas421/lecturepages/microstructurediags.html

deep drawing simulation



rand1

Equivalent Von Mises Stress

deep drawing simulation



rand1

Equivalent Von Mises Stress

examples













VAW aluminium AG

University Gent, Belgium





PART I

Background on Crystalline Solids







face centered cubic



hexagonal close packed body centered cubic

crystal lattice structures





face centered cubic



hexagonal close packed body centered cubic











inherently anisotropic due to underlying mechanisms:

- dislocation slip
- mechanical twinning
- displacive phase transformation







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dislocation – dislocation interaction



dislocation structure



Figure 5. TEM of different regions of steel drawn in 2 passes (8° e 20%), and cyclically twisted (11.2% per cycle, 10 cycles).











displacive transformation



320 340 360 380 400 420 440

polycrystalline surface

3D soap foam









macroscopic response is isotropic only for random distribution of crystallite orientations



macroscopic response is isotropic only for random distribution of crystallite orientations

texture causes anisotropy plastic deformation alters texture



PART II

Background in Continuum Mechanics




local expansion of deformation map:

$$x = \psi(X) + \operatorname{Grad} \psi(X)|_{X_0} (X - X_0) + o(X - X_0)$$

= $x_0 + \operatorname{Grad} x|_{x_0} (X - X_0) + o(X - X_0)$

$$\mathrm{d}x \quad = \quad \mathrm{Grad}\,x\,\mathrm{d}X + o(\mathrm{d}X)$$

 $\mathrm{d}x = \mathbf{F}\,\mathrm{d}X$

deformation gradient:

$$\mathbf{F}(X,t) = (\operatorname{Grad} \psi)(X,t)$$
$$\mathbf{F}^{-1}(x,t) = (\operatorname{grad} \Psi)(x,t)$$

strain measures



strain measures: change of length dx = 1 dsdX = L dS

$$\begin{aligned} l \, ds \cdot l \, ds &= \mathbf{F}L \, dS \cdot \mathbf{F}L \, dS \\ \left(\frac{ds}{dS}\right)^2 &= \mathbf{F}L \cdot \mathbf{F}L \\ &= L \cdot \mathbf{F}^T \mathbf{F}L \\ &= L \cdot \mathbf{C}L \\ &\text{right Cauchy-} \\ &\text{Green tensor} \end{aligned} \qquad \begin{aligned} L \, dS \cdot L \, dS &= \mathbf{F}^{-1}l \, ds \cdot \mathbf{F}^{-1}l \, ds \\ \left(\frac{ds}{dS}\right)^2 &= \left(\mathbf{F}^{-1}l \cdot \mathbf{F}^{-1}l\right)^{-1} \\ &= \left(l \cdot \mathbf{F}^{-T} \mathbf{F}^{-1}L\right)^{-1} \\ &= \left(l \cdot (\mathbf{F} \mathbf{F}^T)^{-1}L\right)^{-1} \\ &= \left(l \cdot \mathbf{B}^{-1}l\right)^{-1} \end{aligned}$$

strain measures: change of angle

$$dy = \mathbf{m} du$$
$$dY = \mathbf{M} dU$$

$$\cos \theta = l \cdot m$$

= $\mathbf{F}L \frac{\mathrm{d}S}{\mathrm{d}s} \cdot \mathbf{F}M \frac{\mathrm{d}U}{\mathrm{d}u}$
= $L \cdot \mathbf{C}M \frac{\mathrm{d}S}{\mathrm{d}s} \frac{\mathrm{d}U}{\mathrm{d}u}$

polar decomposition of deformation gradient

$\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{V}\mathbf{R}$

where **R**: rotation (proper orthogonal tensor) and **U**, **V**: symmetric, positive definite (stretch) tensor

spectral decomposition of U, V

eigenvalues

 $\lambda_1,\lambda_2,\lambda_3$

eigenvectors

 $p_1, p_2, p_3 \text{ for } \mathbf{U}$ $q_1, q_2, q_3 \text{ for } \mathbf{V}$ $\mathbf{U} = \sum_{i=1}^{3} \lambda_i p_i \otimes p_i$ $\mathbf{V} = \sum_{i=1}^{3} \lambda_i q_i \otimes q_i$



relation between polar decomposition $\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{V}\mathbf{R}$ and Cauchy–Green tensors

$$\begin{split} \mathbf{C} &= \mathbf{F}^{\mathrm{T}} \mathbf{F} & \mathbf{B} &= \mathbf{F} \mathbf{F}^{\mathrm{T}} \\ &= (\mathbf{R} \mathbf{U})^{\mathrm{T}} (\mathbf{R} \mathbf{U}) & = (\mathbf{V} \mathbf{R}) (\mathbf{V} \mathbf{R})^{\mathrm{T}} \\ &= \mathbf{U}^{\mathrm{T}} \mathbf{R}^{\mathrm{T}} \mathbf{R} \mathbf{U} & = \mathbf{V} \mathbf{R} \mathbf{R}^{\mathrm{T}} \mathbf{V}^{\mathrm{T}} \\ &= \mathbf{U}^{2} & = \mathbf{V}^{2} \end{split}$$

interpretation of Cauchy–Green tensors



 $\mathbf{C}_{lphaeta}$ is the product of stretches along E_{lpha}, E_{eta} $e_{lpha} \cdot e_{eta}$ base vectors and the scalar product

relation of right Cauchy–Green tensor to small strain

- $\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}$
 - $= (\mathbf{I} + \operatorname{Grad} u)^{\mathrm{T}} (\mathbf{I} + \operatorname{Grad} u)$
 - $= \mathbf{I} + \operatorname{Grad} u + (\operatorname{Grad} u)^{\mathrm{T}} + \operatorname{Grad} u (\operatorname{Grad} u)^{\mathrm{T}}$
 - $\approx \mathbf{I} + (\operatorname{Grad} u)_{\operatorname{sym}}$
 - = I + 2 ϵ

$$\mathbf{E} = \frac{1}{2} (\mathbf{C} - \mathbf{I})$$
$$= \frac{1}{2} (\mathbf{U}^2 - \mathbf{I})$$
$$= \frac{1}{2} (\mathbf{F}^{\mathrm{T}} \mathbf{F} - \mathbf{I})$$

velocity gradient

$$\mathbf{L} = \operatorname{grad} v$$

$$= \operatorname{grad} \dot{x}$$

$$= (\operatorname{Grad} \dot{x}) \mathbf{F}^{-1}$$

$$= \left(\operatorname{Grad} \left[\frac{\partial}{\partial t} x \right] \right) \mathbf{F}^{-1}$$

$$= \left(\frac{\partial}{\partial t} \left[\operatorname{Grad} x \right] \right) \mathbf{F}^{-1}$$

$$= \left(\frac{\partial}{\partial t} \mathbf{F} \right) \mathbf{F}^{-1}$$

$$= \dot{\mathbf{F}} \mathbf{F}^{-1}$$

material time derivatives

$$\frac{\partial}{\partial t} (\mathrm{d}x) = \frac{\partial}{\partial t} (\mathbf{F} \,\mathrm{d}X)$$
$$= \frac{\partial \mathbf{F}}{\partial t} \,\mathrm{d}X + \mathbf{F} \frac{\partial \mathrm{d}X}{\partial t}$$
$$= \dot{\mathbf{F}} \,\mathrm{d}X$$
$$= \mathbf{L}\mathbf{F} \,\mathrm{d}X$$
$$(\mathrm{d}x) = \mathbf{L} \,\mathrm{d}x$$

material time derivatives

$$\frac{\partial}{\partial t} (dx) = \mathbf{L} dx$$
$$\frac{\partial}{\partial t} (l ds) = \mathbf{L} l ds$$
$$\frac{\partial}{\partial t} ds + l \frac{\partial ds}{\partial t} = \mathbf{L} l ds$$
$$l \cdot \dot{l} ds + l \cdot l (ds) = l \cdot \mathbf{L} l ds$$
$$(ds) = l \cdot \mathbf{L} l ds$$

material time derivatives $i ds + l (ds)^{\cdot} = \mathbf{L} l ds$ $i ds + l (l \cdot \mathbf{L} l ds) = \mathbf{L} l ds$ $i = \mathbf{L} l - (l \cdot \mathbf{L} l) l$

material time derivatives

$$\frac{\partial}{\partial t} (\cos \theta) = \frac{\partial}{\partial t} (l \cdot m)
-\sin \theta \dot{\theta} = \dot{l} \cdot m + l \cdot \dot{m}
\dot{\theta} = |l \times m|^{-1}
[\{l \cdot \mathbf{L}l + m \cdot \mathbf{L}m\} (l \cdot m) - l \cdot \{(\mathbf{L} + \mathbf{L}^{\mathrm{T}}) m\}]$$

F specifies changes of size and shape while **L** describes the *rate* of those changes

additive decomposition of \boldsymbol{L}

$$\mathbf{L} = \frac{1}{2} \left(\mathbf{L} + \mathbf{L}^{\mathrm{T}} \right) + \frac{1}{2} \left(\mathbf{L} - \mathbf{L}^{\mathrm{T}} \right)$$
$$= \mathbf{D} + \mathbf{W}$$

symmetric skew-symmetric

interpretation of **D** and **W** using $\mathbf{F} = \mathbf{R}\mathbf{U} = \mathbf{V}\mathbf{R}$ $! L = (RU) \hat{u} (RU)^{-1}$ $= (\dot{R} U + R\dot{U})(U^{-1}R^{-1})$ $= \mathbf{R} \mathbf{H} \mathbf{R}^{\mathsf{T}} + \mathbf{R} \mathbf{H} \mathbf{U}^{-1} \mathbf{R}^{\mathsf{T}}$ $RR^{T} = I$ $\begin{array}{l} \mathbf{R} \hat{\mathbf{R}} \mathbf{R}^{\mathsf{T}} + \mathbf{R} \mathbf{R} \hat{\mathbf{R}}^{\mathsf{T}} &= 0 \\ \mathbf{R} \hat{\mathbf{R}} \mathbf{R}^{\mathsf{T}} + \mathbf{R} \hat{\mathbf{R}} \mathbf{R}^{\mathsf{T}} &= 0 \end{array}$

interpretation of **D** and **W** using $\mathbf{L} = \mathbf{E} \mathbf{F}^{! 1}$ $\mathbf{F} = \mathbf{R} \mathbf{U} = \mathbf{V} \mathbf{R}$ $! \ \mathbf{L} = \mathbf{E} \mathbf{R} \mathbf{V}^{\mathsf{T}} + \mathbf{R} \mathbf{U} \mathbf{V}^{! 1} \mathbf{R}^{\mathsf{T}}$

$$D = \frac{1}{2} R^{\dagger} \dot{\Psi} U^{\dagger} + U^{\dagger} \dot{\Psi} R^{T}$$
$$= \frac{1}{2} R^{\dagger} \dot{\Psi} U^{\dagger} + U^{\dagger} \dot{\Psi} R^{T} + R^{\dagger} R^{T}$$
$$W = \frac{1}{2} R^{\dagger} \dot{\Psi} U^{\dagger} + U^{\dagger} \dot{\Psi} R^{T} + R^{\dagger} R^{T}$$

suppose reference configuration equals current configuration:

$$F = R = U (= V) = I$$

rate of change of stretch ...

$$D = \frac{1}{2} R \stackrel{!}{\Psi} \stackrel{\Psi}{U} \stackrel{!}{}^{1} + U \stackrel{!}{\Psi} \stackrel{\Psi}{W} R^{T} = \stackrel{\Psi}{\Psi}_{0}$$

$$W = \frac{1}{2} R \stackrel{\Psi}{\Psi} \stackrel{\Psi}{U} \stackrel{!}{}^{1} ! U \stackrel{!}{\Psi} R^{T} + \stackrel{\Psi}{R} R^{T} = \stackrel{\Psi}{R}_{0}$$

rate of change of rotation while passing through current configuration

$$\frac{(ds)\dot{u}}{ds} = I \dot{a}LI$$
$$= I \dot{a}DI$$

 \mathbf{D}_{ii} : rate of extension along base vector \mathbf{e}_i



$$I^{U} = II I m I^{!1}$$

{I áLI + m áLm} (I ám) "I á L + L^T m[%]
with I ám = 0
" $\frac{1}{2}I^{U} = I$ áD m e_{3}

 e_2

 \mathbf{D}_{ij} : half the rate of decrease in angle between base vectors \mathbf{e}_i and \mathbf{e}_j

spectral decomposition of D results in three principal stretchings v_i and their respective (orthogonal) axes r_i

rate of angular change is zero, thus principal axes perform (rigid) rotation

principal axes $r_{\rm i}$ perform (rigid) rotation

$$\dot{\mu} = LI! (I \acute{a}LI)I$$

"
$$\mathbf{i}_{i} = (\mathbf{D} + \mathbf{W})\mathbf{r}_{i} ! (\mathbf{r}_{i} \mathbf{\Delta} \mathbf{D} \mathbf{r}_{i})\mathbf{r}_{i}$$

$$= !_{i} r_{i} + W r_{i} ! (r_{i} \acute{a}!_{i} r_{i}) r_{i}$$

$$=$$
 W r_i

 $= w \# r_i$

equilibrium

Cauchy stress tensor

$$t_{(n)} = ! n$$



angular momentum balance



! ^T = !

equilibrium

linear momentum balance $\frac{d}{dt} \left[\begin{array}{c} x \\ x \\ dt \end{array} \right] \times (dv) = \left[\begin{array}{c} y \\ y \\ r \\ r \end{array} \right] \left[\begin{array}{c} b \\ dv \\ r \\ r \\ r \\ r \\ r \end{array} \right]$



equilibrium

linear momentum balance $\frac{d}{dt} \left[\begin{array}{c} x \\ x \\ \end{array} \right] x (dv) = \left[\begin{array}{c} y \\ \end{array} \right] t (bdv) + \left[\begin{array}{c} x \\ \end{array} \right] t (n) da \\ y \\ \end{array}$

$$e_3$$

div !
$$dv = 0$$



Cauchy!first Piola-Kirchhoff $P = J!F!^{T} = FS$ second Piola-Kirchhoff $S = JF!^{1}!F!^{T}$

$$P_{int} = \begin{array}{c} ! : L dv = \begin{array}{c} ! : D dv \\ \\ !^{v} & v \end{array}$$
$$= \begin{array}{c} P : F^{i} dV \\ \\ !^{v} \\ \\ \\ S : E^{i} dV \\ \\ \end{array}$$

A: $(BC) = (B^TA): C = (AC^T): B$ useful for derivation



finite strain plasticity

multiplicative decomposition of deformation gradient

$F = F^{!}F^{p} !' \qquad F^{!} = FF^{p''}$

multiplicative decomposition of deformation gradient

$$F = F^{!}F^{p} !' F^{!} = FF^{p''}$$

plastic velocity	μρ π-μρ μ 1		
gradient		!	

plastic velocity

elastic Green's

Lagrangian strain

gradient

multiplicative
decomposition of
deformation gradient

$$F = F^{!}F^{p} \quad !' \qquad F^{!} = FF^{p''} \quad !'$$

$$L^{p} = F^{ip}F^{p!} \quad !' \qquad F^{ip} = L^{p}F^{p}$$

$$E = \frac{1}{2} \quad F^{!T}F^{!} \quad !$$

multiplicative decomposition of deformation gradient	F = F [!] F ^p	!'	F [!] = FF ^{p" 1}	
plastic velocity gradient	L ^p = É ^{úp} F ^{p! 1}	!'	μ ^{μρ} = L ^ρ F ^ρ	
elastic Green's Lagrangian strain	$E = \frac{1}{2}^{+1}$	F ^{! T} F [!]	!	
work-conjugate second Piola– Kirchhoff stress	$S = C : E = \frac{1}{2}C$: : F ^{p!}	^T F ^T FF ^{p!1} !	I

fully-implicit formulation of rate of change of plastic deformation gradient

$$\mathbf{F}^{ip} = \frac{F^{p}(!)! F^{p}(t)}{! t} = L^{p}(!)F^{p}(!)$$

fully-implicit formulation of rate of change of plastic deformation gradient

$$\mathbf{F}^{ip} = \frac{F^{p}(!)! F^{p}(t)}{! t} = L^{p}(!)F^{p}(!)$$

after rearranging

$$F^{p! 1}(!) = F^{p! 1}(t)[I! ! t_{\mu}L^{p}(!)]$$

$$F^{p! T}(!) = I! ! tL^{pT}(!) F^{p! T}(t)$$




with

combination of

$$S = C : E = \frac{1}{2}C : F^{p!T}F^{T}FF^{p!1} | I$$

finite strain plasticity

elasto-plastic consistency



material constitutive law

depends on stress **S** and internal state variables **s**

$$L^{p}(!) = L^{p}(S, s)$$

$$\mathbf{\hat{s}}(!) = \mathbf{\hat{s}}(S, s)$$

two-level predictor-corrector scheme



 $r_n = [s_n ! s(t)]! ! t s(s_n, s_n)$



 $\frac{! R_{ij}}{! L_{kl}^{p}} = \frac{! L_{kl}^{p}}{! L_{kl}^{p}}! \frac{! L_{ij}^{p}}{! S_{ij}} \frac{! S_{ij}}{! S_{ij}}$ $= \frac{! L_{kl}^{p}}{! L_{kl}^{p}}! \frac{! L_{ij}^{p}}{! S_{ij}} \frac{! S_{ij}}{! S_{ij}}$ $\frac{!S}{!L^{p}} = \frac{1}{2} C: B^{T}AB! I^{W}_{,L^{p}} = \frac{1}{2} C: B^{T}AB! I^{W}_{,L^{p}} + B^{T}AB! I^{S}_{,L^{p}} + B^{T}AB + B^{T}AB + B^{T}AB + B^{T}AB + B^{T}AB + B^{T}AL^{p}_{,L^{p}} + B^{T}AB + B^{T}AL^{p}_{,L^{p}} + B^{T}AB + B^{T}AL^{p}_{,L^{p}} + B^{T}AB + B^{T}AL^{p}_{,L^{p}} + B^{T}AB + B^{T}AB + B^{T}AL^{p}_{,L^{p}} + B^{T}AB + B^{$



finite strain plasticity

<u>' S</u> = $\begin{array}{rcl} & & & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$ $= \frac{1}{2} C : \begin{bmatrix} 0 \\ B^{T}, L^{p} \\ AB \\ I \end{bmatrix} + \begin{bmatrix} 0 \\ B^{T} \\ B^{T}, L^{p} \\ I \end{bmatrix} + \begin{bmatrix} 0 \\ B^{T} \\ B^{T} \\ I \end{bmatrix} + \begin{bmatrix} 0 \\ B^{T} \\ I$ $\frac{! S_{ij}}{! L_{kl}^{p}} = ! \frac{! t}{2} C_{ijmn} \qquad \frac{! L_{mq}^{p}}{! L_{kl}^{p}} A_{qp} B_{pn} + B_{mp}^{T} A_{pq} \frac{! L_{qn}^{p}}{! L_{kl}^{p}}$ = $\frac{!}{2} \frac{t}{C_{ijmn}} \int_{qk}^{qk} (AB)_{qn} + (B^{T}A)_{mq} \int_{qk}^{qk} (B^{T}A)_{mq} \int_{qk$ % = $! \frac{!}{2} C_{ijln} (AB)_{kn} + C_{ijml} (B^T A)_{mk}$