Thermomechanical modeling of dislocation density increase during PVT growth of SiC crystals

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Outline

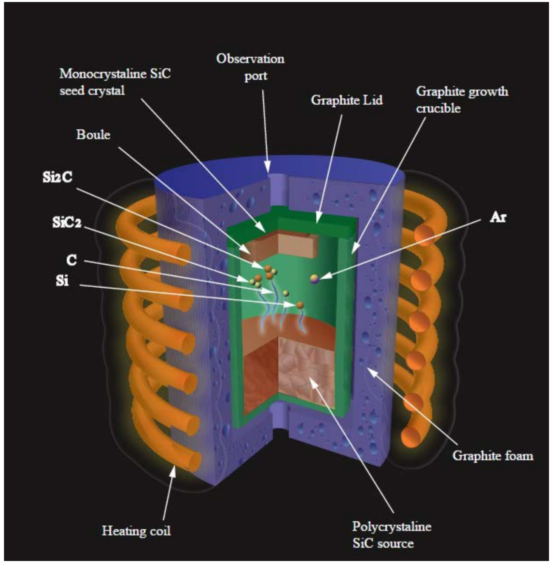
- Context and motivation : Physical Vapor Transport and dislocations
- Alexander-Haasen model & COMSOL implementation
- Cooling of a mono-crystal and increase of dislocation density
- Prospects : crystal growth and 3D modeling
- Conclusion

- Physical Vapor Transport growth of single SiC crystals

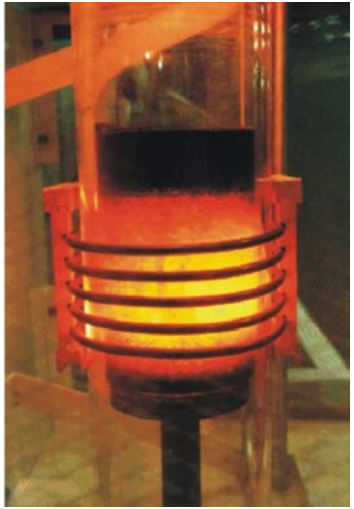
Induction heating
Very high temperatures (2300 °C)

Applications : abrasives, **wafers for power electronic devices** …


(Wikipedia)

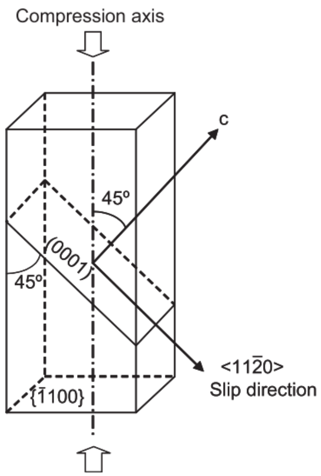


(Wikipedia)

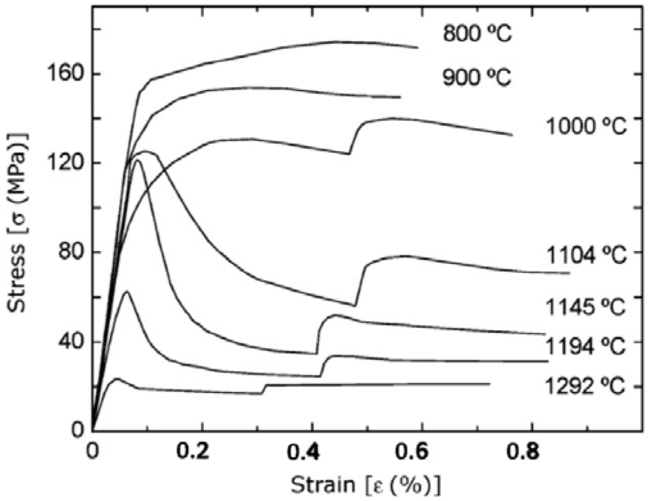

LMGP PVT reactor

Thermal gradients ⇒ Thermal stresses ⇒ Plasticity (T=2300 °C !) ⇒ Dislocation density increase

- Mechanical behavior of SiC at very high temperature



Single hcp crystal
Dislocations glide along basal plane (0001)



Lara et al., *Ceram. Int.* **38,** 1381–1390 (2012).

Highly anisotropic viscoplasticity

- Alexander-Haasen model : viscoplasticity with internal variable

Shear strain rate / s^{-1}

$$\dot{\gamma}^{vp} = Nm\, b\, v_0\, \tau_{eff}^{\ n} \exp\left(\frac{-Q}{k_B T}\right)$$

Effective stress $\tau_{eff} = \tau - D\sqrt{Nm}$

(mobile) dislocation density / m^{-2}

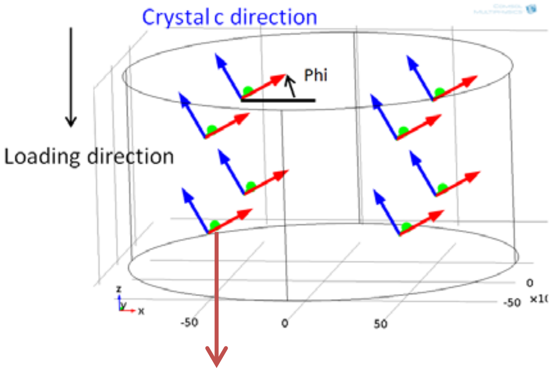
$$\frac{\partial Nm}{\partial t} = K v_0 Nm\, \tau_{eff}^{\ n+\lambda} \exp\left(\frac{-Q}{k_B T}\right)$$

5 parameters to be fitted

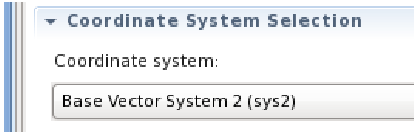
v_0 ; n ; Q ; K ; λ

Alexander-Haasen model : COMSOL implementation

Calibration compression test (3D)



Coordinate system associated with behavior law



NB : nonlinear structural materials module is required

Alexander-Haasen model : COMSOL implementation

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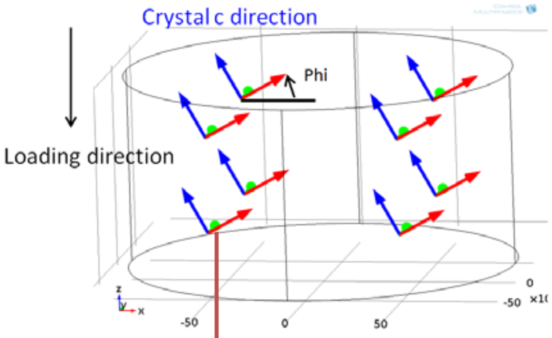

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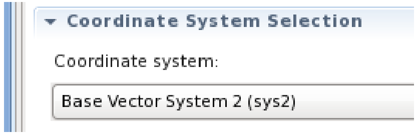
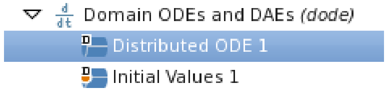
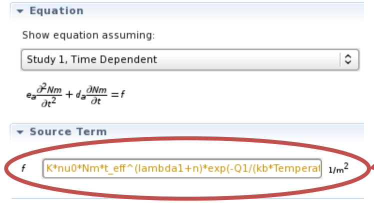


- Domain ODE governing dislocation density rate





$$\frac{\partial Nm}{\partial t} = K \nu_0 Nm \tau_{eff}^{n+\lambda} \exp\left(\frac{-Q}{k_B T}\right)$$

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Alexander-Haasen model : COMSOL implementation

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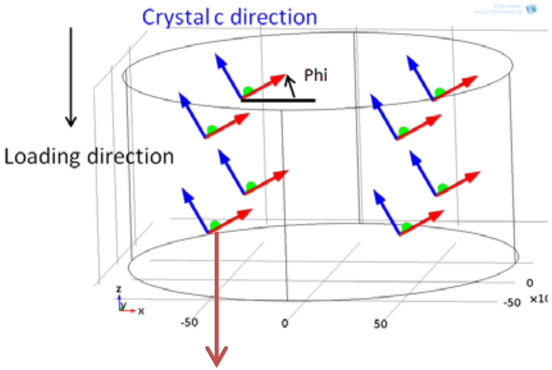

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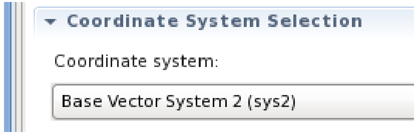

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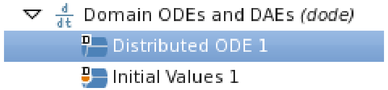
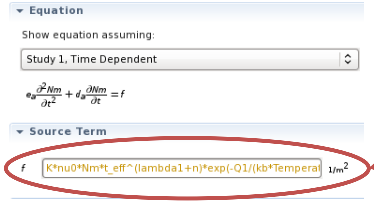
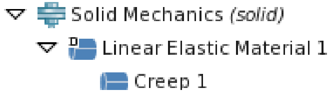
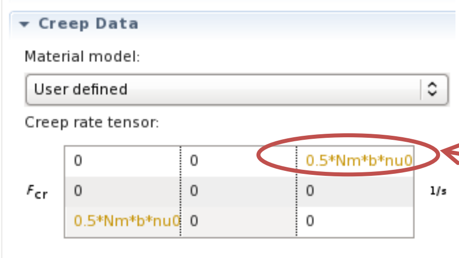




$$\frac{\partial Nm}{\partial t} = K \nu_0 Nm \tau_{eff}^{\, n+\lambda} \exp\left(\frac{-Q}{k_B T}\right)$$

- Anisotropic elasticity + creep strain rate



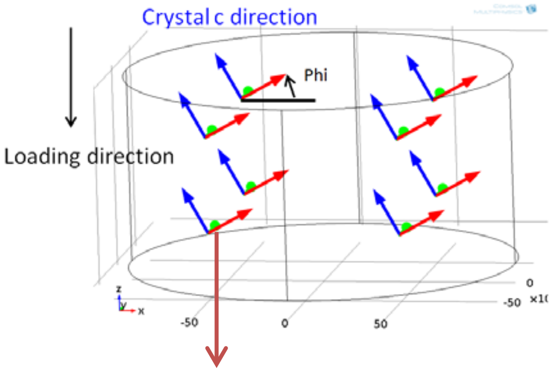


$$\dot{\gamma}^{vp} = Nm\, b\ \nu_0\ \tau_{eff}^{\ n}\ \exp\left(\frac{-Q}{k_B T}\right)$$

NB : nonlinear structural materials module is required

Alexander-Haasen model : calibration / validation

Calibration compression test (3D)



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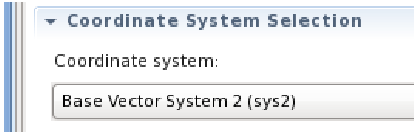

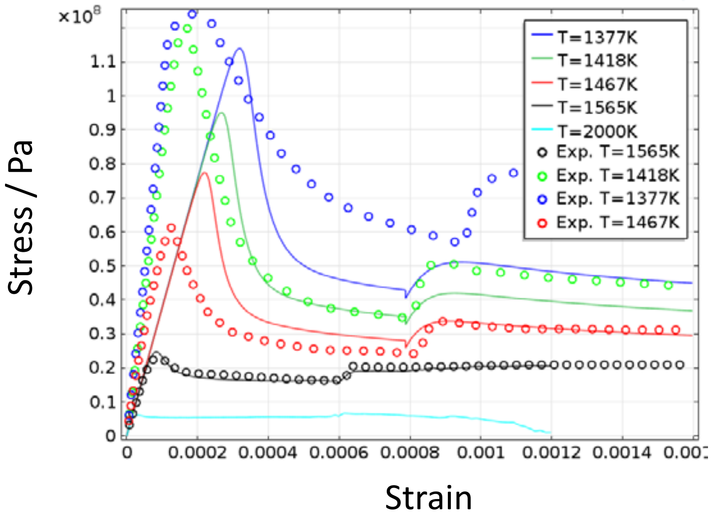

$$\nu_0 = 8.5\mathrm{E}\text{-}15\,;\; n = 2.8\;;\; Q = 3.3eV\;;\; K = 7\mathrm{E}\text{-}5\,;\; \lambda = 1.1$$

Gao et al., *Cryst. Growth Des.*, **14**, 1272-1278 (2014)

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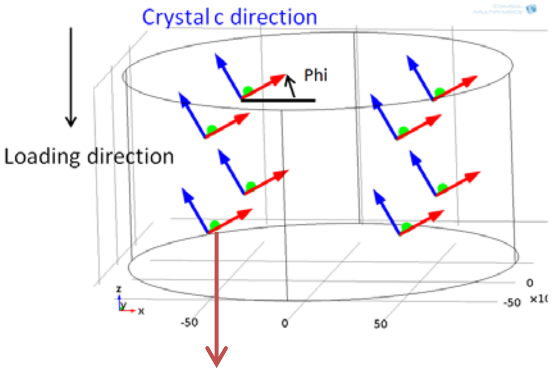

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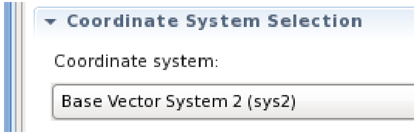
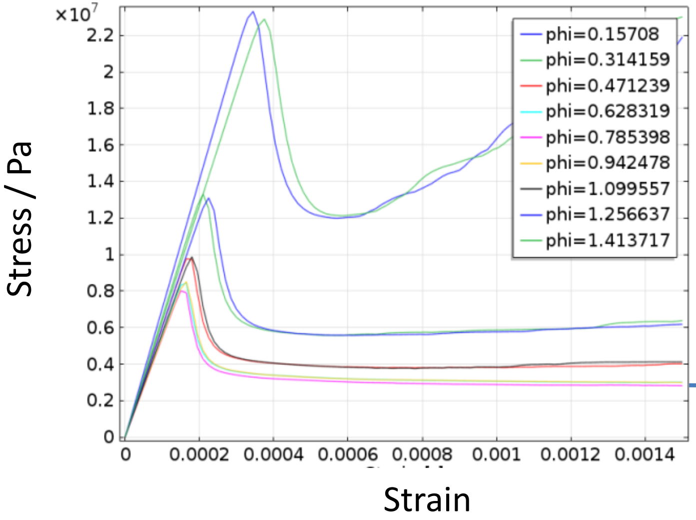


T = 2300 K



OK with Schmid law

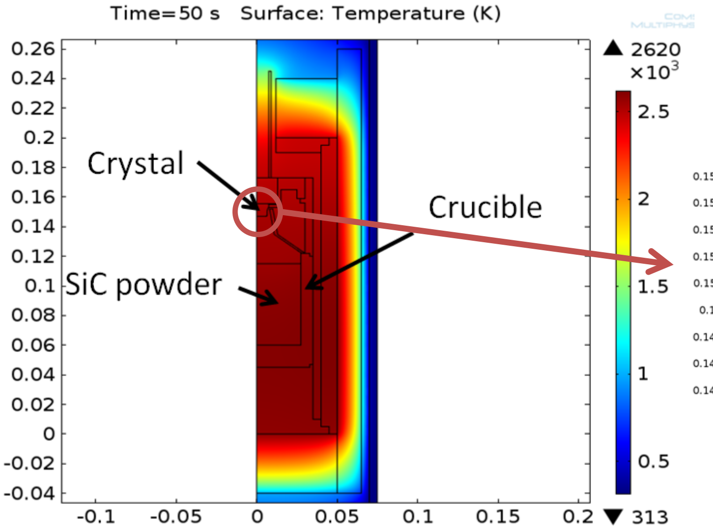
phi = pi/4

$$\nu_0 = 8.5\text{E-}15;\; n = 2.8\;;\; Q = 3.3eV\;;\; K = 7\text{E-}5;\; \lambda = 1.1$$

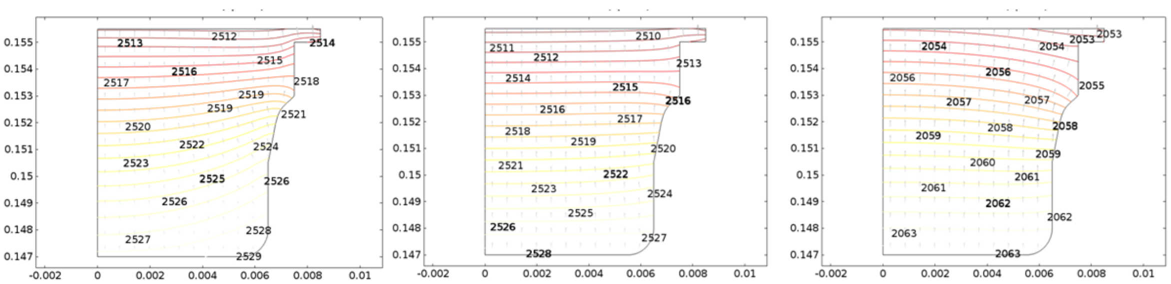
Gao et al., *Cryst. Growth Des.*, **14**, 1272-1278 (2014)

NB : nonlinear structural materials module is required

- Crystal shape and thermal field from thermo-chemical simulation[1]



Cooling

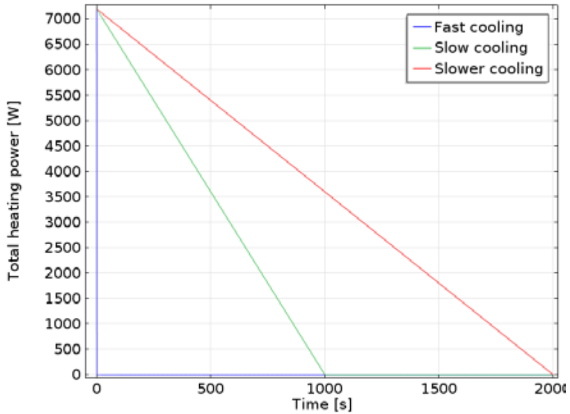


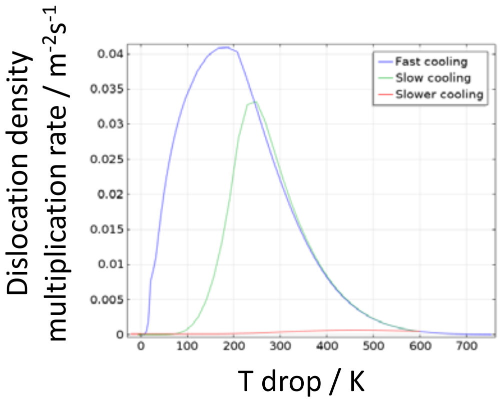
[1] Ariyawong, K. *et al.*, *Materials Science Forum*, **778-780**, 35-38 (2014).

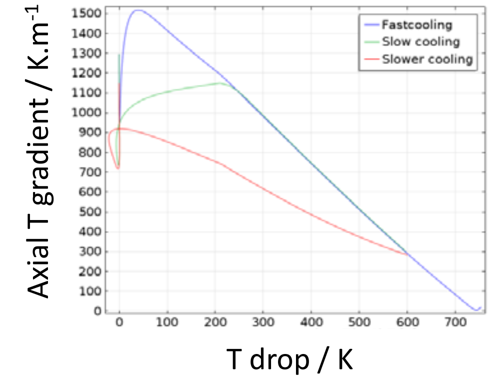
Time-dependant heat transfer simulation of the whole reactor
+
Time-dependant mechanical simulation of thermal stresses with temperature dependant behavior for the crystal

- Effect cooling velocity

Cooling profiles







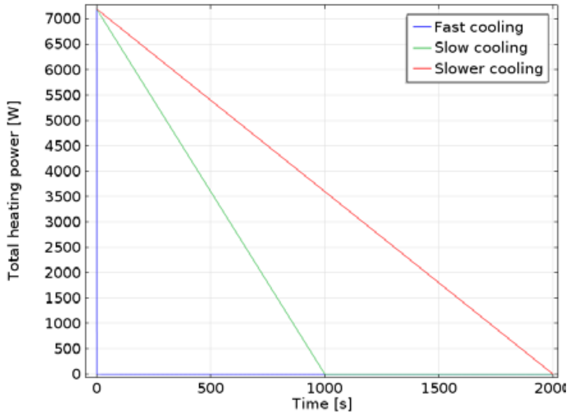
Dislocation density increase very low under 1800K

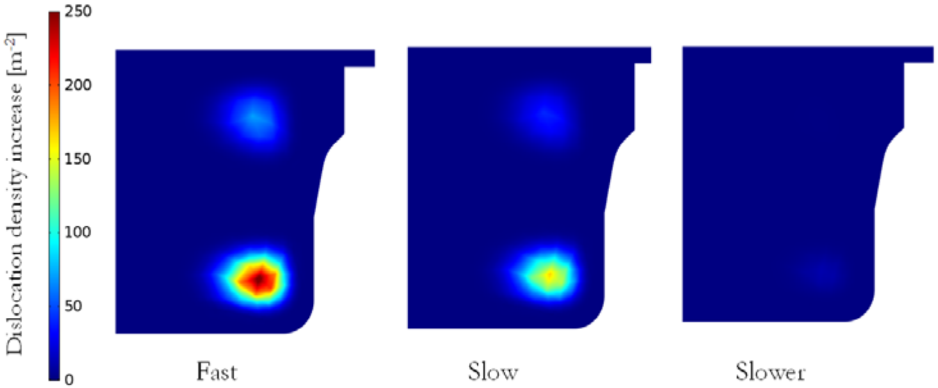
Slow cooling minimize axial temperature gradient

Induction heating = internal heat source

- Effect cooling velocity

Cooling profiles





Induction heating = internal heat source

Prospects : dynamic crystal growth simulation

Motivation : dislocations actually mainly develop during growth !

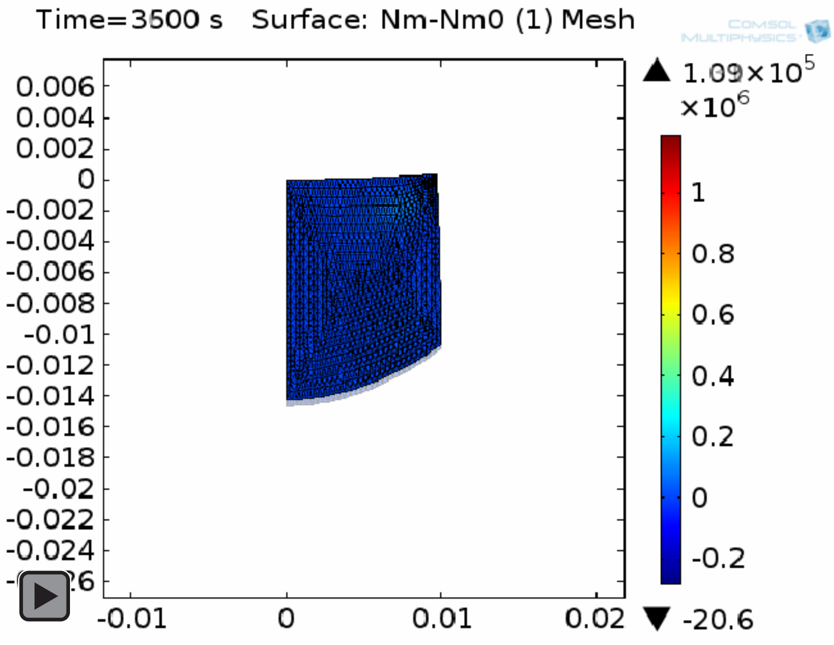
Thermo-chemical simulation[1]

↓

Growth velocity
Thermal field

↓

Deformed mesh node
with prescribed mesh velocity
+
Mechanical modeling (AH)



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Prospects : 3D modeling

Motivation : off-axis orientation of the crystal

2D axisymetric heat transfer simulation of the whole reactor

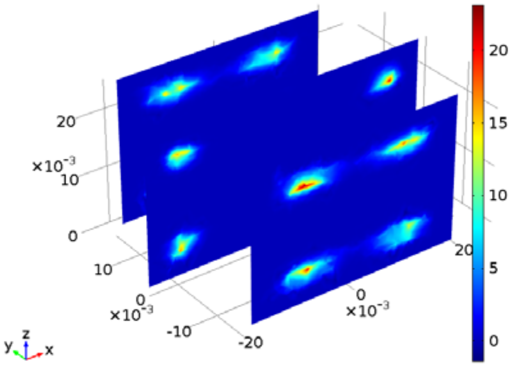
↓

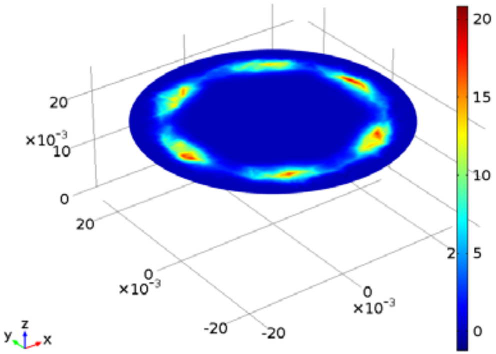
3D thermal field

↓

3D mechanical model
3 basal slip systems α
-> 3 additional ODE for $Nm^{(\alpha)}$

Cylindrical crystal with simple convection cooling on top





Dislocation density increase after 50s cooling / m^{-2}

Prospects : 3D modeling

Motivation : off-axis orientation of the crystal

2D axisymetric heat transfer simulation of the whole reactor

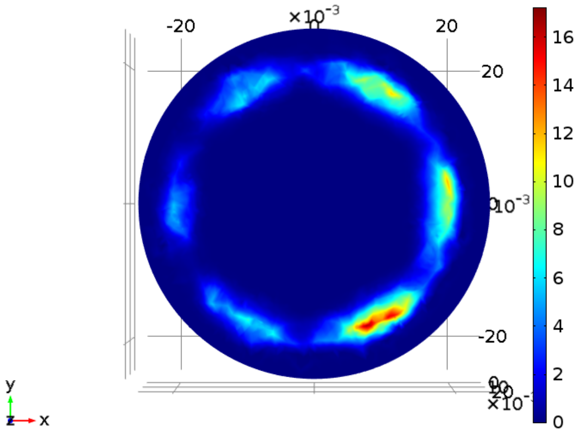
↓

3D thermal field

↓

3D mechanical model
3 basal slip systems α
-> 3 additional ODE for $Nm^{(\alpha)}$

Off-axis cylindrical crystal with simple convection cooling on top



8° disorientation

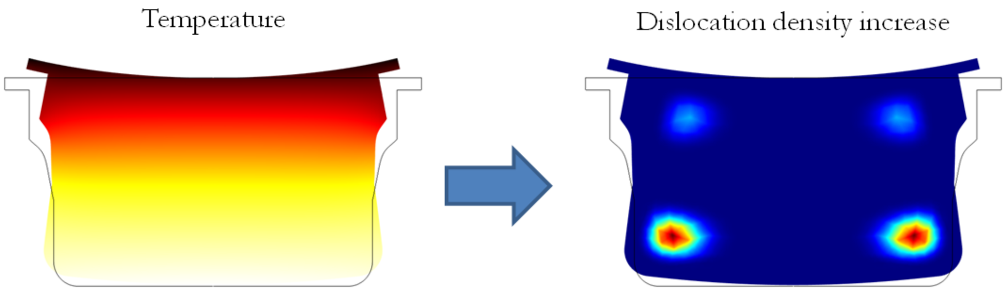
Dislocation density increase after 50s cooling / m^{-2}

- COMSOL implementation of AH model for crystal plasticity (basal slip systems)
  Additional domain ODE + user-defined creep law

- Dislocation density is tracked with an internal variable Nm

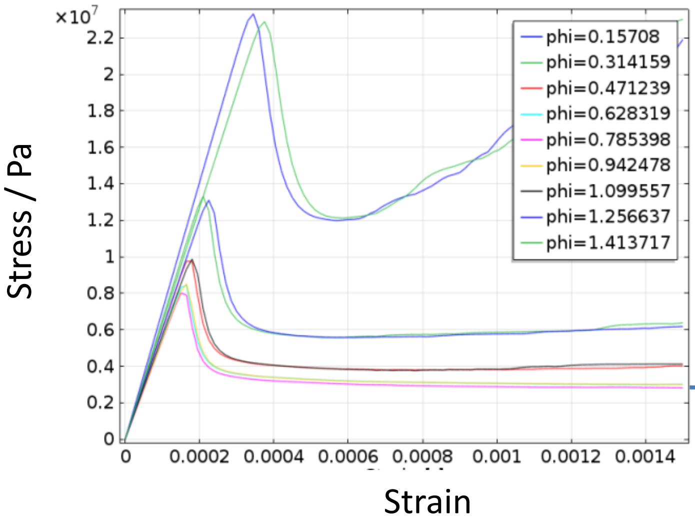
- Effect of cooling velocity can be studied

- Two directions for future work : (1) simulation of dislocation increase during growth
  (2) 3D modeling for off-axis crystals



Extra slide : Schmid law

T = 2300 K



→ phi = pi/4

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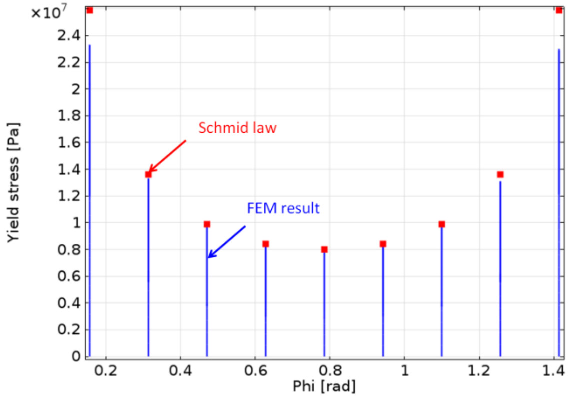
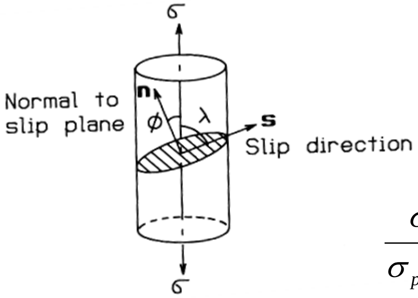




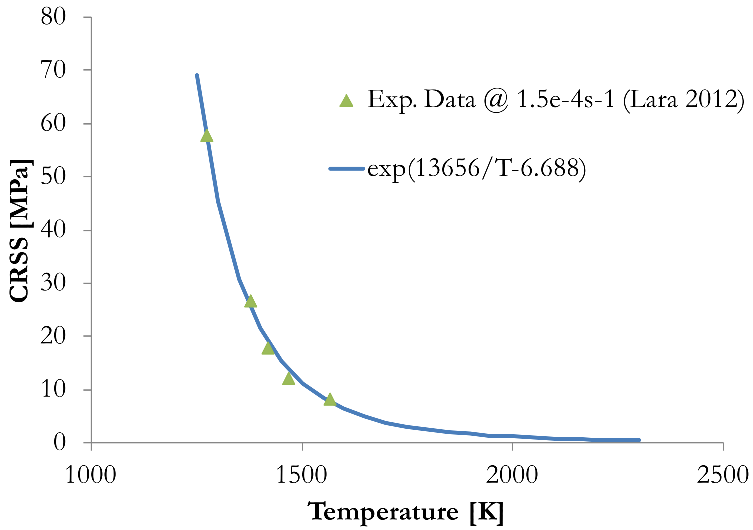
Schmid law

$$\tau = \sigma \cos\phi \cos\lambda$$

↓

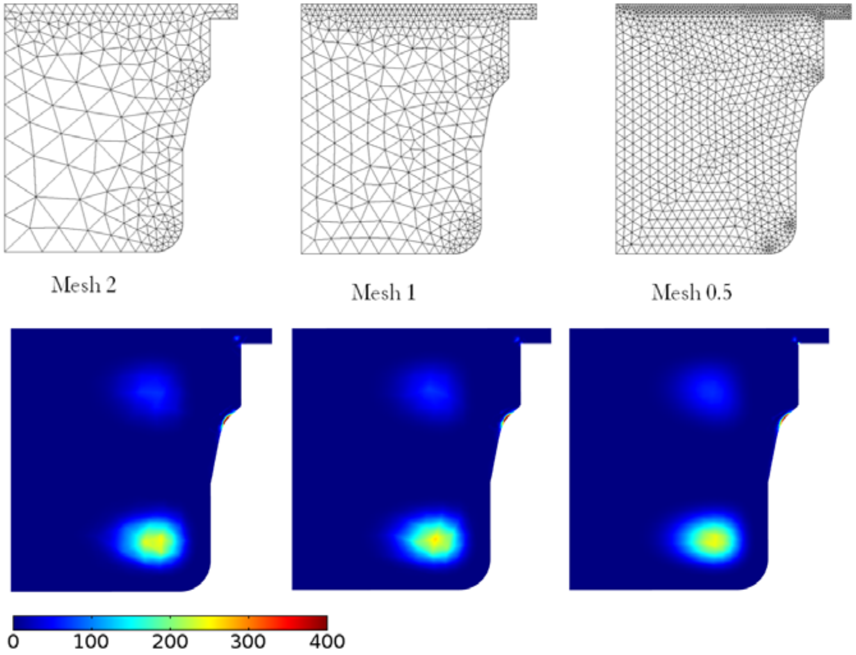
$$\frac{\sigma_{phi}}{\sigma_{phi=\pi/4}} = \frac{1}{2\cos(phi)\cos(\pi/2 - phi)}$$

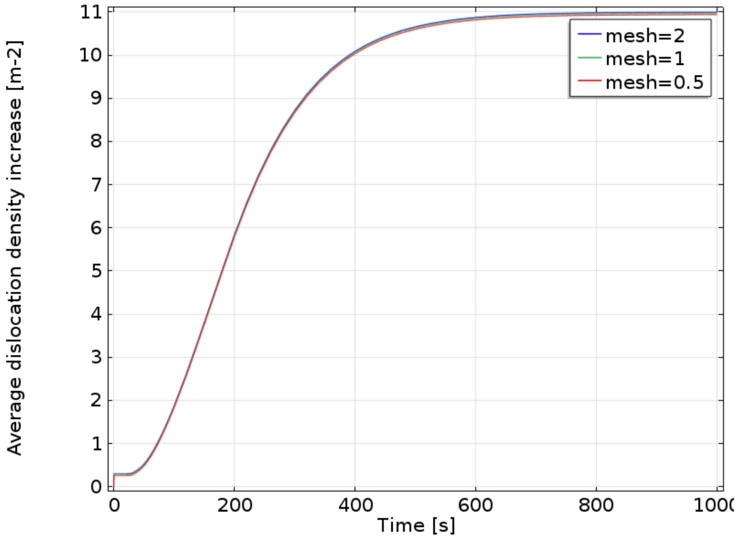
- Extra slide : CRSS decrease with T



CRSS ~ 0.5 MPa @ 2300 K

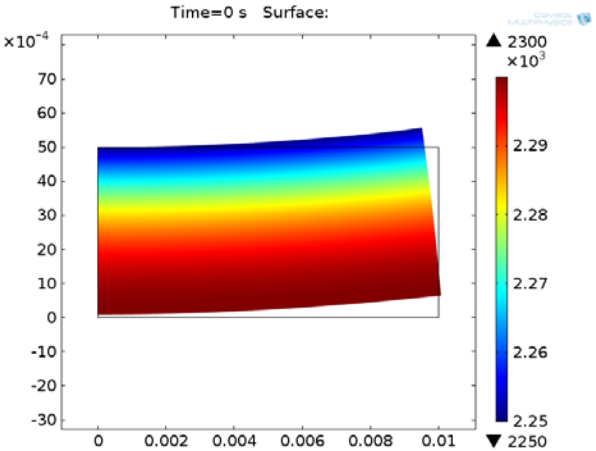
- Extra slide : mesh convergence

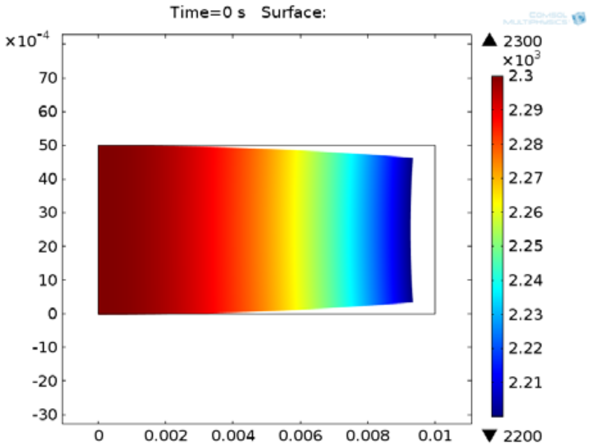




- Cylindrical crystal

Radial cooling vs axial cooling

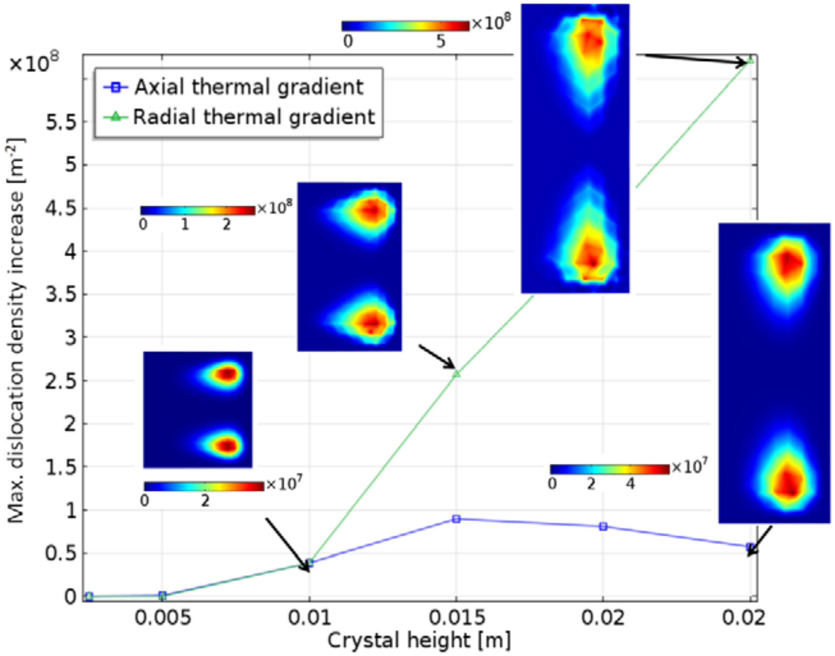




Axisymetric model ; imposed quadratic thermal fields

- Cylindrical crystal

Effect of crystal height



Axisymetric model ; cylindric crystal ; imposed quadratic thermal fields