Rheology II
Transport properties

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CIDER Summer Program: Flow In the Deep Earth
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The unreachable Earth
Mechanical properties of wadsleyite

\[ \dot{\varepsilon} = 10^{-5} \text{s}^{-1} \]
Mechanical properties of ringwoodite

\[ \dot{\varepsilon} = 10^{-5} \text{s}^{-1} \]

\[ \sigma \text{ (MPa)} \]

\[ T \text{ (K)} \]

Hustoft et al., 2013
Kavner et al., 2001
Meade and Jeanloz, 1990
Miyagi et al., 2014
Nishiyama et al., 2005
Mechanical properties of bridgmanite

\[ \sigma \text{ (MPa)} \]

\[ T \text{ (K)} \]

Merkel et al. 2003
Meade et al. 1990
Girard et al. 2015
Constitutive equations

\[ \dot{\varepsilon} \propto \sigma^n e^{-Q/kT} \]

Mackwell, 2008

Also need to take high-pressure into account:
\[ Q + PV \]
Extrapolating to natural timescales

\[ \dot{\varepsilon} \propto \sigma^n \cdot e^{-\frac{Q}{kT}} \]

Extrapolation to natural conditions
The University of Queensland pitch drop experiment (started 1927)

Here featuring, Professor John Mainstone (taken in 1990, two years after the seventh drop and 10 years before the eighth drop fell).

Professor John Mainstone died on 23 August 2013, aged 78, after having watched the experiment 52 years.

Bitumen $\eta = 2.3 \times 10^{11}$ Pa.s
What if….

\[ \dot{\varepsilon} = 10^{-16} \text{s}^{-1} \]

\[ \varepsilon = 10^{-6} = 0.0001\% \text{ in 4 centuries} \]

100 nm shortening for a 10 cm sample….
From crystals to mantle flow

Can we bridge scales?
Deforming crystals

transport of matter
**Diffusion creep**

- Nabarro (1948) - Herring (1950) creep

\[
\begin{align*}
C^+ &= C_0 \exp\left(\frac{\sigma b^3}{kT}\right) \\
C^- &= C_0 \exp\left(-\frac{\sigma b^3}{kT}\right)
\end{align*}
\]

\[
J = -D_v \nabla C \approx \alpha D_v \frac{C^+ - C^-}{d}
\]

\[
\dot{\varepsilon} = \alpha \frac{D_{sd} \sigma \Omega}{d^2 kT}
\]

\[
\sigma = \frac{d^2 kT}{\alpha D_{sd} \Omega} \dot{\varepsilon}
\]

**Newtonian**
Diffusion creep in the mantle

Glišovic et al. (2015)
Shearing crystals
Shearing crystals

Ringwoodite (20 GPa)
(110) plane

Easy shear path along the $\frac{1}{2}[-110]$ direction

Defines the **Burgers vector**

Ritterbex et al. (2015)
Slip systems

Ringwoodite (20 GPa)

Slip along $<110>$ in: {001} {110} {111}

Ritterbex et al. (2015)
We learnt: Slip systems

Plasticity of crystals - Schmid & Boas (1950)

\(<uvw>\{hkl}\>

Uchic et al. 2004
We don’t understand: stresses

\( \tau_{\text{max}}/\mu = 0.2-0.3 \)

Two to four orders of magnitude too large

Need for defects: dislocations
The Volterra defects

Vito Volterra (1860-1940)

Crystal defects: dislocations

Egon Orowan
Sir Geoffrey Ingram Taylor
Michael Polanyi

1934
Dislocations duality

Near field: atomistic

Far field: elastic

\[ \sigma = \frac{\mu b}{2\pi r} f(\theta) \]

Long-range interactions
Dislocations respond to stress

External loading $\sigma$

Peach & Koehler (1950) force $\mathbf{F} = \bar{\mathbf{\sigma}} \cdot \mathbf{b} \times \mathbf{L}$

velocity $\mathbf{v}$
From dislocations to plasticity: the toolbox

- 3D dislocation dynamics
- 2.5 D dislocation dynamics
- Orowan equation

\[ \dot{\varepsilon} = \rho \, b \, v \]

\( \dot{\varepsilon} \) = Strain rate
\( \rho \) = Dislocation density
\( b \) = Burgers vector modulus
\( v \) = Dislocation velocity

MgO
J. Amodeo et al.

Olivine
Boioli et al. (2015)
Dislocation velocities: can we measure?

New approach based on nanomechanical testing of olivine in the TEM
Nanomechanical testing in the TEM
The Push-to-Pull device (Hysitron®)

Collaboration with H. Idrissi Antwerpen, Belgium & C. Bollinger, Bayreuth, Germany
Nanomechanical testing in the TEM
Nanomechanical testing in the TEM
Nanomechanical testing in the TEM
Dislocation velocities: can we calculate?
Dislocation core modeling

Perovskite MgSiO$_3$: orthorhombic: 20 atoms / unit cell

LAMMPS molecular statics
30 000 atoms

Antoine Kraych’s PhD
[100] screw dislocation in bridgmanite at 30GPa

Density of Burgers vector in (010) planes (30GPa)

Dislocation position along [001] (Å)
Dislocation gallery

Bridgmanite

[100](010)

[010](100)
Dislocation gallery

1/2<111>{101}

Wadsleyite

Stacking fault

½ [111](101)
Wadsleyite
Dislocation gallery

Ringwoodite
Dislocation gallery

Post-perovskite

[100](010)
• We know: the « crystallography of defects »

• We don’t know: their « dynamics »

Questions:
• Do dislocations move easily when stress is applied?
• What is their velocity?
• How does it depend on stress? temperature?
Lattice friction: the brutal force

Peierls stress
Lattice friction

[100](010) in bridgmanite at 30 GPa
The "Nudged Elastic Band" (NEB) method
→ energy barrier

Kraych et al. EPSL in revision
Dislocations: how they move

(a) [100](010)

(b) [010](100)

Kraych et al. EPSL in revision
Wadsleyite: Peierls stresses

[100](010) \[\dot{\varepsilon} = 10^{-5} \text{s}^{-1}\]

\[\frac{1}{2} [111](101)\]

\[\sigma \text{ (MPa)}\]

\[T \text{ (K)}\]

Nishihara et al., 2008
Kawazoe et al., 2013
Kawazoe et al., 2010
Hustoft et al., 2013
Farla et al., 2015
Ringwoodite: Peierls stresses

\[ \frac{1}{2}<110>|{111} | \quad \epsilon = 10^{-5} \text{s}^{-1} \]

\[ \frac{1}{2}<110>|{110} \]

- Hustoft et al., 2013
- Kavner et al., 2001
- Meade and Jeanloz, 1990
- Miyagi et al., 2014
- Nishiyama et al., 2005
Lattice friction in MgSiO$_3$ Perovskite

2 easiest slip systems:
- [100](010)
- [010](100)
Lattice friction in MgSiO₃: from bridgmanite to post-perovskite
• We know: the intrinsic resistance that the crystal opposes to dislocation motion: the Peierls stress

• We don’t know: how temperature helps to overcome this lattice friction
Modeling dislocation mobility

Core structure, Peierls Potential

Stress assisted thermal activation: \((\tau, T)\)

Kink pair mechanism:

Modeling rare events:

Wadsleyite; 1700K, 1 GPa: 100ps
MgSiO$_3$ perovskite: kink pair mechanism

Transient state theory

$$v = a' \cdot \frac{L}{w^*(\tau)} \cdot \frac{v_D b}{w^*(\tau)} \cdot \exp\left(-\frac{\Delta H^*(\tau)}{kT}\right)$$
Dislocation velocities

PV $T=2000 \text{ K} \ P=30 \text{ GPa}$

Rwd $T=1800 \text{ K} \ P=20 \text{ GPa}$

OI $T=1600 \text{ K} \ P=0 \text{ GPa}$

Glide velocity (m/s)

Resolved shear stress $\tau$ (MPa)
From dislocations to plasticity: a practical example

Orowan equation  \[ \dot{\varepsilon} = \rho b v(\tau, T) \]

\[ v(\tau, T) = v_0 \exp \left( \frac{-\Delta H^*(\tau)}{kT} \right) \]

\[ \Delta H^*(\tau) = 2H_k \left( 1 - \left( \frac{\tau}{\tau_p} \right)^p \right)^q \]

\[ \tau = \tau_p \left( 1 - \left( \frac{T}{H_k} \right)^{1/q} \right)^{1/p} \]

\[ C = \frac{k}{2} \ln \left( \frac{\nu_D a' b^2}{2w^*} \sqrt{\rho} \frac{\dot{\varepsilon}}{\dot{\varepsilon}} \right) \]

The strain rate is here
Dislocation Glide in Ringwoodite (20 GPa)

![Graph showing dislocation glide in Ringwoodite with multiple data points and labels.]

- Kavner et al., 2001
- Hustoft et al., 2013
- Miyagi et al., 2014
- Nishiyama et al., 2005
- Meade and Jeanloz, 1990

**Engineering stress (GPa)**

- $2 \times $CRSS
- $1/2<110>\{111\}$
- $1/2<110>\{110\}$

**Time (K)**

- $\dot{\epsilon} = 10^{-5} \text{ s}^{-1}$

Ritterbex et al. (2015) PEPI
Dislocation Glide in Wadsleyite (15 GPa)

Hustoft et al., 2013
Kawazoe et al., 2010
Kawazoe et al., 2013
Nishihara et al., 2008
Farla et al., 2015

\[ \dot{\epsilon} = 10^{-5} \text{s}^{-1} \]
$\text{MgSiO}_3$ perovskite (30 GPa)

$P = 30 \text{ GPa} ; \dot{\varepsilon} = 10^{-5} \text{ s}^{-1} ; \rho = 10^{13} \text{ m}^{-2}$

- Meade et al. 1990
- Merkel et al. 2003
- Girard et al. 2016

![Graph showing engineering stress vs. temperature for MgO with different crystallographic orientations.](Kraych et al. EPSL submitted – Results on MgO from Amodeo et al. Phil. Mag. 2012)
• We know: the intracrystalline flow properties of major high pressure minerals

![Image](image.png)

Courtesy J. Girard

• We don’t know the mechanical properties of the « rock »
From the grain to the aggregate

Collaboration with O. Castelnau & K. Derrien
ENSAM, Paris

- Visco Plastic Self Consistent modelling
- Finite Elements modelling

Building an aggregate

Equivalent strain
From the grain to the aggregate

work in progress!

Collaboration with O. Castelnau & K. Derrien
ENSAM, Paris

Nishihara et al., 2008
Kawazoe et al., 2013
Kawazoe et al., 2010
Hustoft et al., 2013
Farla et al., 2015
This study
• We can model (and we agree with) mechanical data obtained in laboratory conditions

• But we can do the same at mantle strain-rates (no extrapolation !)
Dislocation Glide in Wadsleyite (15 GPa)

\[ \frac{1}{2}<111>\{101\} \text{ screw} \]

\[ [100](010) \text{ screw} \]

\[ \dot{\varepsilon} = 10^{-16} \text{s}^{-1} \]

Ritterbex et al. Am. Mineralogist in press
Dislocation Glide in Ringwoodite (20 GPa)

\[ \dot{\varepsilon} = 10^{-16} \text{s}^{-1} \]

- \( \frac{1}{2} <110> \{111\} \)
- \( \frac{1}{2} <110> \{110\} \)

Lower Transition Zone

Ritterbex et al. (2015) PEPI
MgSiO$_3$ perovskite (30 GPa)

\[ \dot{\varepsilon} = 10^{-16} \text{s}^{-1}; \quad \rho = 10^8 \text{ m}^{-2} \]

\[ P = 30 \text{ GPa} \]

Kraych et al. EPSL submitted – Results on MgO from Amodeo et al. Phil. Mag. 2012
MgSiO$_3$ perovskite (60 GPa)

**Results** on MgO from Amodeo et al. Phil. Mag. 2012
MgSiO$_3$ post-perovskite (120 GPa)

\[ E = 10^{14} \text{ s}^{-1} \]
\[ \rho = 10^8 \text{ m}^{-2} \]

A. Goryaeva in prep
Which mechanism?

Glide is extremely difficult!

Dislocation creep

Diffusion creep?
• We understand, model, quantify dislocation glide

• But creep in the mantle would involve glide and climb!
What is climb?

- Point defects (vacancies) diffuse toward the dislocations
- They are absorbed (or emitted)

The dislocation moves away from its glide plane

\[ v_{climb} = \frac{2\pi D_{Si}^{sd}}{\ln \frac{R}{r_c} b} \left( \exp \left( \frac{\tau \Omega}{kT} \right) - 1 \right) \]
Interplay between glide and climb [100] dislocations

Olivine Ratio $v_g / v_c$
Interplay between glide and climb
[100] dislocations

\[ \rho_0 = 1.4 \times 10^{12} \text{m}^{-2} \]
\[ T = 1600 \text{ K} \]
\[ \sigma = 40 \text{ MPa} \]

Graph showing the interplay between glide and climb over time.

Initial configuration vs Glide only

Boioli et al. Phys Rev B 2015
Interplay between glide and climb [100] dislocations

\[ \rho_0 = 1.4 \times 10^{12} \text{m}^{-2} \]
\[ T = 1600 \text{K} \]
\[ \sigma = 40 \text{MPa} \]

Uniaxial tension
Single slip + climb

Initial configuration
Glide only
Glide + Climb
Interplay between glide and climb

[100] dislocations

At steady state: nearly constant dislocation density

Plastic strain is mostly produced by glide

Boioli et al. Phys Rev B 2015
Activation enthalpy

![Graph showing activation enthalpy for glide, creep, and diffusion processes under varying pressures and temperatures.](image)

<table>
<thead>
<tr>
<th></th>
<th>glide</th>
<th>creep</th>
<th>diffusion</th>
</tr>
</thead>
<tbody>
<tr>
<td>(eV)</td>
<td>5.7</td>
<td>4.7</td>
<td>4.25</td>
</tr>
</tbody>
</table>

Stress exponent

Boioli et al. Phys Rev B 2015
Olivine rheology at low temperature [001] glide

Boioli et al. EPSL 2015
Creep in the lower mantle

(A) Olivine

Ratio $v_g / v_c$

(B) Ringwoodite $10^{-10}$ $10^{-6}$ $10^{-2}$ $10^{2}$ $10^{5}$

(C) Bridgmanite $10^{-20}$ $10^{-10}$ $10^{0}$ $10^{8}$

$T$ (K)

$\sigma$ (MPa)
Introducing pure climb creep

- Strain is produced by dislocation *climb*
- Dislocations act as sources and sinks of point defects (vacancies)
- Dislocations exchange vacancies
- The characteristic diffusion length is determined by the dislocation density
Modelling pure climb creep

(A)  

(B)  

\[ T = 1900 \text{ K} \]
\[ P = 24 \text{ GPa} \]
\[ \sigma = 40 \text{ MPa} \]
\[ \dot{\varepsilon}_{\text{xx}} (\%) = 10^{-5} \]

(C)  

(D)  

\[ \sigma_x (\text{MPa}) \]
\[ y (\mu m) \]
\[ c_x (\text{MPa}) \]
\[ y (\mu m) \]
Modelling pure climb creep in bridgmanite

T = 1900 K; P = 24 GPa; \( X_v = 10^{-5} \)

Strain rate \( \text{strain rate (s}^{-1}) \)

\[ \text{CLIMB } \rho_0 = 10^{12} \text{ m}^{-2} \]

\[ \text{CLIMB } \rho_0 = 10^{8} \text{ m}^{-2} \]

\[ \text{N-H } d = 0.1 \text{ mm} \]

\[ \text{N-H } d = 10 \text{ mm} \]

\[ \text{COBLE } d = 0.1 \text{ mm} \]

\[ \text{COBLE } d = 10 \text{ mm} \]
Pure climb creep:
A very important mechanism for planetary interiors rheology

A few facts:

• Strain is produced by dislocation *climb*

• Strain is not produced by shear: no crystal preferred orientations

• No grain size dependence

• Controlled by diffusion, but rheology *may not* be linear
• Diffusion creep ✓
• Dislocation creep ✓
• Pure climb creep ✓

• What about grain boundaries?
Toward a more general elastic field theory

Collaboration with C. Fressengeas & V. Taupin, Metz

Displacement field: \( \vec{u} \)

Total distortion tensor: \( \overline{U} = \text{grad} \ \vec{u} \)

Cauchy stress: \( \sigma = C : \varepsilon \)

Equilibrium condition \( \text{div} \ \overline{\sigma} = 0 \)

Energy: \( E_{\text{Cauchy}} = \frac{1}{2} \sigma_{ij} \varepsilon_{ij} \)

Rotation vector: \( \vec{\omega} = -\frac{1}{2} \omega : \overline{X} \)

Curvature tensor: \( \overline{\kappa} = \text{grad} \ \vec{\omega} \)

Couple stress tensor: \( \overline{M} = A : \overline{\kappa} \)

Equilibrium condition \( \text{div} \ \overline{M} = 0 \)

Energy: \( E_{\text{couple}} = \frac{1}{2} M_{ij} \kappa_{ij} \)
Toward a more general elasto-plastic field theory

Compatibility equations: \[ \text{curl } \overline{U} = 0 \quad \text{curl } \overline{\kappa} = 0 \]

Incompatible elasto-plasticity:

Nye's dislocation density tensor:
\[ \overline{\alpha} = \text{curl } \overline{U}_e = -\text{curl } \overline{U}_p \]

Disclination density tensor:
\[ \overline{\theta} = \text{curl } \overline{\kappa}_e = -\text{curl } \overline{\kappa}_p \]

Burgers vector: closure defect obtained by integrating the incompatible elastic distortions along a circuit \( C \)
\[ \mathbf{b} = \int_C \overline{U}_e \cdot d\mathbf{r} = \int_S \overline{\alpha} \cdot \mathbf{n} dS \]

Frank vector: closure defect obtained by integrating the incompatible elastic curvature along a circuit \( C \)
\[ \overline{\Omega} = \int_C \overline{\kappa}_e \cdot d\mathbf{r} = \int_S \overline{\theta} \cdot \mathbf{n} dS \]
Toward a more general elasto-plastic field theory

\[ \text{curl } \kappa = 0 \]

Disclination density tensor:

\[ \tilde{\theta} = \text{curl } \kappa_e = -\text{curl } \kappa_p \]

Frank vector: closure defect obtained by integrating the incompatible elastic curvature along a circuit \( C \)

\[ \bar{\Omega} = \int_C \kappa_e \cdot dr = \int_S \bar{\theta} \cdot n \, dS \]

You remember?
Disclinations were recently evidenced in metals, here Al.

Beausir & Fressengeas (2013)
Dislocation and disclinations analysis by EBSD

OOM – naturally deformed mylonitic harzburgite from the Oman ophiolite (Sumail massif)

T0548
Experimentally deformed at 1200°C

Cordier et al. Nature 2014
Grain boundary modeling based on disclinations

Grain boundary

Atomistic configuration

Displacement
Dislocation density
Rotation
Disclination density
Dislocation/Disclination continuous modeling

Sun et al. IJP 2016
Grain boundary modeling based on disclinations

Forsterite: (011)/[100] tilt grain boundary with misorientation 60.80° (coll S. Jahn)
Grain boundary modeling based on disclinations

Forsterite: (011)/[100] tilt grain boundary with misorientation 60.80° (coll S. Jahn)

Sun et al. Phil Mag 2016
Forsterite: (011)/[100] tilt grain boundary with misorientation 60.80° (coll S. Jahn)
Shear–coupled boundary migration
Final stop: Thank you!

Visit our website:

www.rheoman.eu

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Multiscale Modeling of the Rheology of the Mantle (RheoMan)