Viscoelasticity of Planetary Interiors from Seismic to Convective Timescales

Uli Faul

EAPS
Massachusetts Institute of Technology
Dalton et al. 2006

Kustowski et al. 2006

Attenuation

Shear Velocity

100 km depth
Today: fundamentals of defects, flow laws

Friday: flow laws (cont.), transient creep, seismic properties & applications
cross-polarized light image of a peridotite

peridotite xenolith
Ionic bonding

CsCl - simple cubic

NaCl - face centered cubic
Olivine structure looking down on (001) plane.

- Tetrahedrally coordinated Si, octahedrally coordinated M sites.
- Si-O bonds shortest and strongest.
- Large spacing of (010) planes and close spacing of (100) planes.
Olivine structure looking down on (100) plane. Oxygen in (100) planes near hexagonal close-packed arrangement.
Anisotropy due to crystal structure

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>unit cell dim. (Å)</td>
<td>4.78</td>
<td>10.25</td>
<td>6.3</td>
</tr>
<tr>
<td>V</td>
<td>9.89</td>
<td>7.72</td>
<td>8.43</td>
</tr>
<tr>
<td>V</td>
<td>4.89</td>
<td>4.42</td>
<td>4.87</td>
</tr>
</tbody>
</table>

$V_s(\text{max}) = 5.53 \text{ km/s}$
Elastic behavior: Solids

 Unique equilibrium position of atoms in crystal lattice displacement from that position requires force: elastic moduli
  e.g. $\sigma = E \varepsilon$
  $E$ Young’s modulus (tensile deformation, linear strain)
  $K$ bulk modulus (uniform compression)
  $G$ shear modulus (rigidity, shear deformation)
  Elastic moduli are of orders 10s of GPa
Finite T: thermal energy of atoms results in vibrations of atoms about equilibrium positions. This energy must be supplied as specific heat to raise the temperature.

Low T: vibrational amplitudes will be very small and approximately symmetric (sinusoidal) about the equilibrium positions (left).

High T: large asymmetric (i.e. non-sinusoidal or anharmonic) vibrations will be excited corresponding to states higher in the well (right).

Asymmetry of the vibration is such that the bond length averaged over one cycle of vibration is now greater than the equilibrium spacing.

This temperature-dependent increase in average bond length is thermal expansion.
Thermodynamics (Fundamental state functions)

Internal energy $U$: Energy content of a system, the sum of the potential energy stored in interatomic bonding (electrostatic energy) plus the kinetic energy of atomic vibrations.

Temperature

In the Earth need to account for pressure:

Enthalpy: $H = U + PV$
Entropy $S$: measure of the state of disorder in a system.

Example: Configurational entropy:
Entropy is at a maximum for $XB = XA$
Deformation:
stress = modulus x strain

\[ \sigma = E \varepsilon \]
(Hooke’s law)

\[ E \sim 10 \text{ GPa} = 10^{10}\text{Pa} \text{ (ice)}, \]
\[ \varepsilon \sim 1 \]

flow of ice due to gravity:
\[ P = \text{density x } g \times \text{thickness} \]
\[ = 1000 \text{ kg/m}^3 \times 10 \text{ m/s}^2 \times 1000 \text{ m} = 10^7 \text{ Pa} \]
moduli of rock-forming minerals of order of 100 GPa
convective stresses $\sim 0.1$ MPa
Defects!
(point defects)

Frenkel

Schottky
defects can also be impurity atoms
Thermodynamically why do we have defects?

Creation of point defect requires energy:
local distortion of lattice + imperfect satisfaction of bonding
enthalpy H increases.

But: point defect increases disorder in an otherwise perfect crystal:
entropy S increases.

(S is associated with the number of ways to distribute defects within the crystal structure.)

For small defect concentrations entropy increase is greater than enthalpy increase, for larger defect concentrations enthalpy increase dominates:

Minimum in Gibbs free energy at some finite concentration of point defects!
Transmission electron microscope image of screw dislocations in olivine
Lattice planes in a cubic crystal

Insert an extra half plane

Edge dislocation
edge dislocation: Burgers vector perpendicular to dislocation line l
TEM lattice-fringe images with electron beam parallel to dislocation line.
screw dislocation: Burgers vector parallel to dislocation line $l$
dislocations: mixed character
Strain due to dislocation creep

Movement in a glide plane

edge  (a)  screw  (b)
stress (strain) field surrounding dislocations
Dislocation geometry is controlled by crystal lattice

Dislocations move on glide planes

slip plane

Peierls potential

(Poirier, 1985, Ranalli, 1995)
Generation of dislocations: Frank-Read sources
(dislocation multiplication due to stress/strain)
Obstacles to dislocation motion

subgrain boundary

0.2μm
Climb by diffusion of a row of atoms from the extra half plane. Screw dislocations have no extra half plane and cannot climb.
<table>
<thead>
<tr>
<th></th>
<th>Temperature</th>
<th>Shear Stress</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Dislocations</strong></td>
<td>• Not produced by,</td>
<td>Sensitive to and interact with</td>
</tr>
<tr>
<td></td>
<td>• Annealed by,</td>
<td></td>
</tr>
<tr>
<td><strong>Point Defects</strong></td>
<td>Dependent</td>
<td>Do not interact</td>
</tr>
</tbody>
</table>
From dislocations to grain boundaries
Arrays of dislocations: subgrain boundaries
subgrain boundaries in quartz

undulose extinction in quartz
Construct grain boundaries from arrays of dislocations

Low angle tilt boundary
Misorientation angle:
\[ \theta = 2 \tan \left( \frac{b}{2h} \right) \approx \frac{b}{h} \]
Grain boundaries

Why look at grain boundaries?
1. GB as crystalline defect present in all rocks.
2. GB affect
   • diffusion
   • deformation
   • seismic properties
   • electrical conductivity....

GB: 2-D lattice defect that introduces a change in lattice orientation

Lattice misorientation given by $\theta$
Boundary type as a function of relative orientation of neighboring grains

Tilt boundary
rotation axis is parallel to
boundary plane
misorientation generated by
inserting edge dislocations

Twist boundary
rotation axis is
perpendicular to boundary
plane
misorientation generated
by 2 sets of screw
dislocations
Read-Shockley dislocation model for grain boundary energy $\gamma$

$$\gamma_s = \gamma_0 \theta (C - \ln \theta)$$

where the relative rotation $\theta = b/d$, with $b$ Burgers Vector $d$ dislocation spacing
$$\gamma_0 = \frac{Gb}{4\pi(1-\nu)}$$

with $G$ shear modulus and $\nu$ Poisson’s ratio,
$$C = 1 + \ln(b/2\pi r_0)$$

with $r_0$ radius of the dislocation core
Definitions

Subgrain boundaries: Dislocation cores non-overlapping, boundary consists of a (more or less ordered) array of dislocations.

High angle grain boundaries: Dislocations can no longer be identified, boundary structure and properties independent of misorientation angle.
Dependence of relative grain boundary energy on misorientation for NiO
Visualization of types of grain boundaries

\[
\cos \frac{\theta}{2} = \frac{\gamma_{ss}}{2\gamma_{sl}}
\]

\(\gamma_{ss}\) = solid - solid surface energy

\(\gamma_{sl}\) = solid - liquid surface energy
- the vast majority of grain boundaries are general, high angle grain boundaries
Grain boundaries: melt-free polycrystalline olivine

TEM

D

D

1 μm

Jackson et al., 2002

defects: grain boundaries, dislocations
High resolution image of olivine grain boundaries

(010) lattice fringes in olivine

Faul et al., 2004
Grain boundaries in olivine: no evidence for dislocations, no steps, about 1 nm wide
For comparison: Steps on high angle grain boundary of titanate-perovskite (SrTiO$_3$)

Webb et al., 1999
Grain boundary analysis by TEM

~ 1 nm

elongate beam position

100 nm
TEM EDS spectroscopy peak/background ratios of trace elements in olivine

Grain boundary composition distinct from grain interior, correlates with grain interior composition
elements with low concentrations in the olivine grains are indicative of the statistical profiles measured from five grain boundaries. The negative compositional values of trace analysis for elements in the vicinity of the grain boundaries. The profile is the sum of the Ca concentration (molar occupancy of octahedral M sites), in Ca-doped MgO (ref. 15).

represents the concentration if the solute were confined entirely to the grain-boundary plane. This concentration may, in fact, rep-

Figure 2

Hiraga et al., 2004
Deformation - flow laws

‘first principles‘ derivations - physical model

constitutive equations relating strain rate to stress

Poirier, Creep of Crystals, 1985
Vacancies

Atoms

Pure shear deformation of a single crystal: Nabarro- Herring creep

Compressive stress at face B reduces the number of vacancies. Tensile stress at face A increases the number of vacancies.
differential stress -> concentration gradients -> diffusion

congestion gradient ~ grain size (face A - face B)
diffusion ~ diffusivity (atom species, crystal structure), temperature

flow law (constitutive equation, strain rate \( \dot{\varepsilon} \) as a function of stress \( \sigma \)):

\[
\frac{d\varepsilon}{dt} = \dot{\varepsilon} = A \sigma \ d^{-2} \ \text{exp}[-(E+PV^*)/RT]
\]

A constant (experimentally determined), \( d \) grain size,
\( E \) activation energy, \( V^* \) activation volume

\[
\frac{d\varepsilon}{dt} = A \ D_{sd} \ \Omega \ \sigma/kTd^2
\]
Diffusion is rate controlling:
slowest species along its fastest path

Temperature [°C]

Log (D [m²/s])

Dohmen & Milke, 2010
flow law for grain boundary diffusion

\[ \dot{\varepsilon} = A \sigma d^{-3} \exp\left[-\frac{(E+PV^*)}{RT}\right] \]

but \( A, E, V^* \) are also specific to diffusion mechanism

Faul and Jackson, 2007

H&K (03), melt-free, \( d = 4.5 \mu m, 1200^\circ C \)
Fit parameters

(a) $n = 1.37$

(b) $p = 3$

(c) $E = 484 \text{ kJ/mol}$
But: “Pure” diffusion creep would lead to shape change of grains:

Observation: Grains remain equiaxed after deformation
Diffusionally accommodated grain boundary sliding (diffusion creep)

Macroscopic shape change without grain shape change
Dislocation creep
(Weertman creep)

glide velocity: \( v \sim b v_0 \exp(-E/kT) \)
(b Burgers vector)

but dislocations get 'stuck' (entangled): edge dislocations have to 'climb' out of their glide plane, climb is rate limiting. Climb is a diffusive process.

\[
\dot{\varepsilon} = A \sigma^n \exp[-(E+PV^*)/RT]
\]

dislocation density \( \sim \) stress: strain rate depends on stress\(^n\)
dislocations are intracrystalline, no grain size dependence
Deformation Mechanism Map

Olivine, 1250°C, 0.4 GPa
Electron backscatter diffraction map