Viscous Strength of HCP Iron at Conditions of Earth's Inner Core

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Introduction and research summary

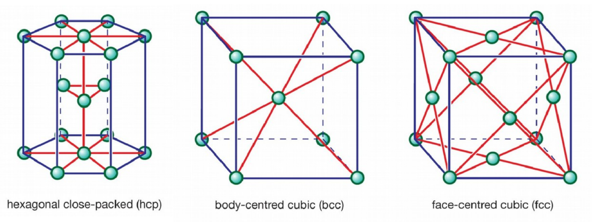
The mechanical properties of Earth's inner core are key for understanding its dynamics and evolution, *e.g.* viscous strength of the inner core (Yoshida et al. 1996; Karato 1999), the origin of its seismic anisotropy (Deuss 2014), inner core translation (Deguen *et al.* 2013) and its rotational dynamics (Buffett 1997; Aubert & Dumberry 2011). All of these issues rely on the viscosity of the inner core, which is barely constrained.

Here, we propose a theoretical mineral physics approach to infer the viscosity of hexagonal close packed (hcp) iron at inner core pressure (P) and temperature (T). High-T plastic deformation in metals is strongly rate-limited by atomic self-diffusion. So far, the self-diffusion properties of iron (alloys) from experiments rely on extrapolation to inner core pressures (Yunker and Van Orman 2007; Reaman *et al.* 2012). Here, we use a **density functional approach** to study vacancy diffusion in the hcp phase of iron and predict the corresponding self-diffusion coefficient at conditions of Earth's center.

Results are applied to microphysical models of intracrystalline plasticity to compute the rate-limiting creep behavior of hcp iron numerically. We show that dislocation creep is one of the likely mechanisms driving deformation of hcp iron at inner core conditions, which can lead to the formation of crystallographic preferred orientations (CPO). This suggests that plastic flow of hcp iron might contribute to crystal alignment and thus to the observed seismic anisotropy in the inner core. The associated viscosity is significantly lower than that of Earth's mantle, which rules out inner core translation – one of the main hypotheses to explain the hemispherical asymmetric anisotropy structure of the inner core – but allows for the occurrence of the seismically observed fluctuations in the rate of inner core differential rotation.

Atomistic Modeling

We consider the three polymorphs of iron:



and quantify lattice self-diffusion coefficient :

$$D_{sd} = Z_f \frac{Z_m}{6} f\, l^2 X_v \Gamma$$

Quantifying diffusion parameters:

- Intrinsic vacancy concentration

$$X_v = exp\left(\frac{\Delta S_f}{k_b}\right) exp\left(-\frac{\Delta H_f}{k_b T}\right) = exp\left(-\frac{\Delta G_f}{k_b T}\right)$$

- Atomic jump probability

$$\Gamma = \nu^* exp\left(-\frac{\Delta H_m}{k_b T}\right)$$

Electronic structure calculations

- Supercell approach: 107-128 atoms
- PWSCF: Quantum Espresso
- Exchange-correlation functional: GGA
- USPP: $3s^2 3p^6 3d^{6.5} 4s^1 4p^0$
- Fermi-Dirac smearing 0.002 Ry
- Monkhorst-Pack k-point sampling: 64 – 96
- spin polarization taken into account

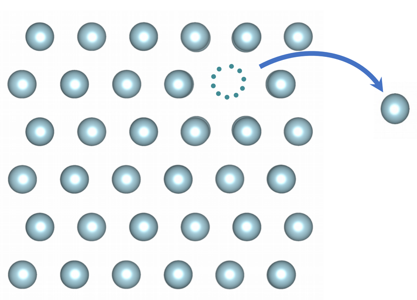
Defect energetics

Activation energy self-diffusion:

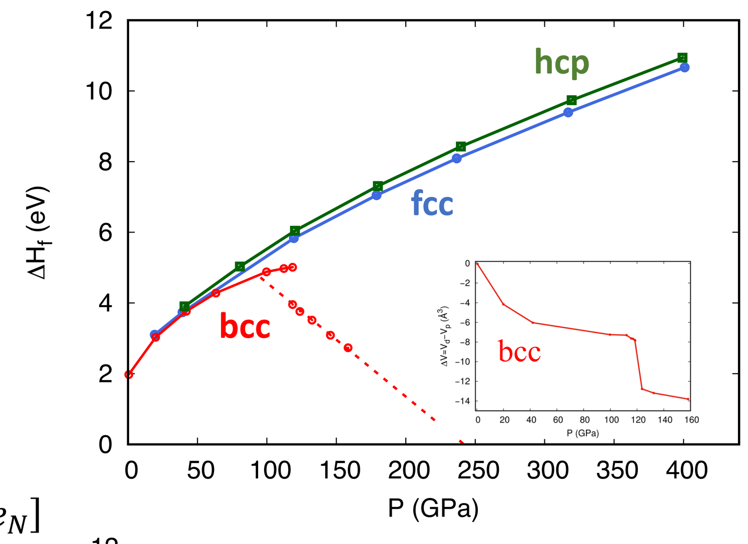
$$\Delta H_{sd} = \Delta H_f + \Delta H_m = \Delta E + P\Omega$$

$$D_{sd} = D_0 exp\left(-\frac{\Delta H_f + \Delta H_m}{k_b T}\right)$$

- **vacancy formation** (concentration)

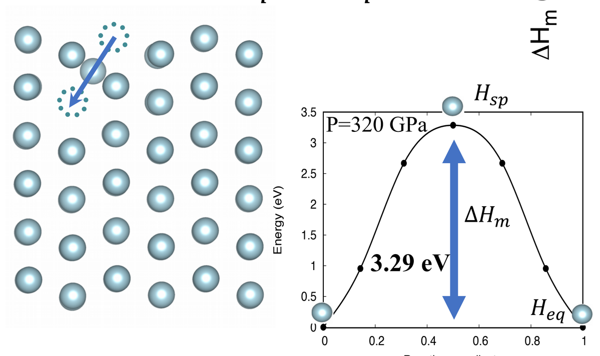


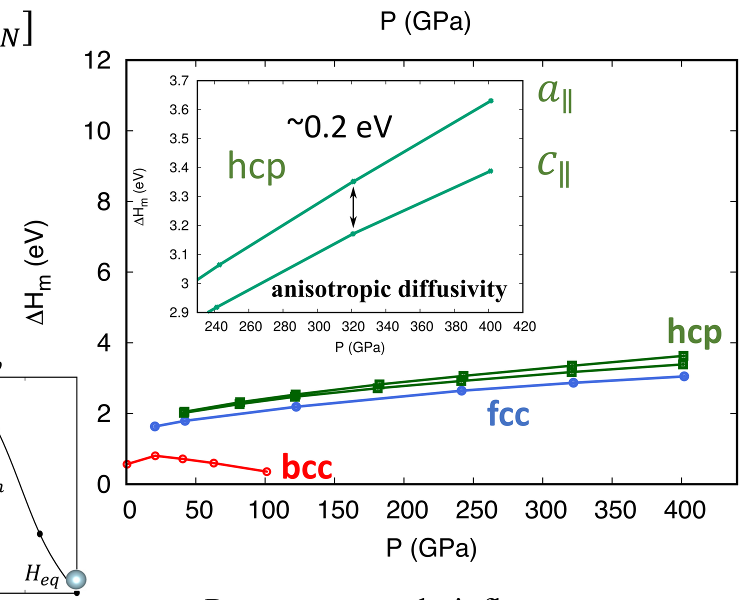
$$\Delta H_f = H[Fe_{N-1}] - \frac{N-1}{N} H[Fe_N]$$



- **vacancy migration** (diffusivity)

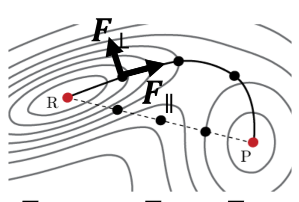
$$\Delta H_m = H_{sp} - H_{eq}$$





CI-NEB method

CI-NEB method (Henkelman et al. 2000) is used to find minimum energy paths and the corresponding energy barriers of vacancy migration



$$F_{NEB} = F_\perp + F_\parallel$$

- Pressure strongly influences formation enthalpy of all iron polymorphs.
- fcc and hcp iron show similar trends in defect energetics.
- bcc structure becomes mechanically unstable at pressures > 120 GPa.

Lattice dynamics

Direct force constant method

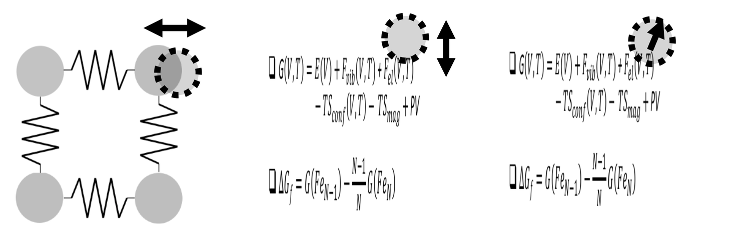
- Phonon dispersion $\nu(q,P)$

Effect of temperature and entropy

- Thermal expansion (EoS)
- Gibbs formation energy ΔG_f
- Effective jump frequency ν^*

Vineyard theorem $\nu^* = \prod_{i=1}^{3N-3} \nu_i^e \Big/ \prod_{j=1}^{3N-4} \nu_j^s$

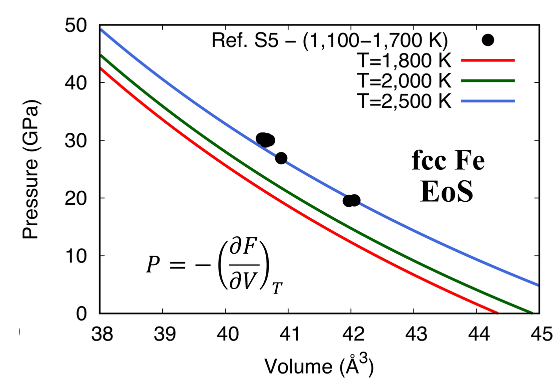
Quasi-harmonic approximation:



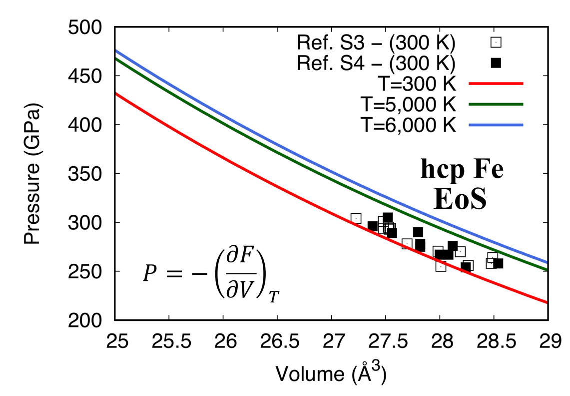
$$F_{vib}(V,T) = \frac{1}{2}\sum_{q,i} h\nu_{q,i} + k_b T \sum_{q,i} \ln\left(1 - \exp\left(-\frac{h\nu_{q,i}}{k_b T}\right)\right)$$

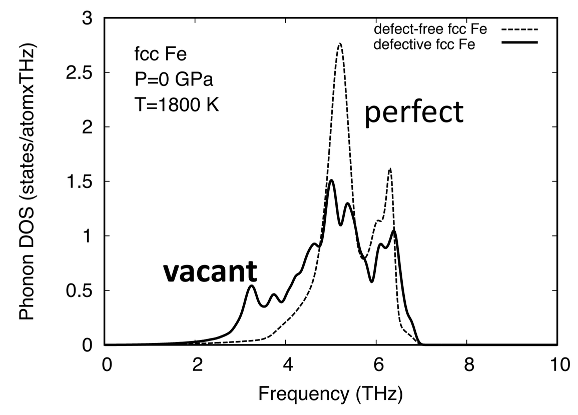
- $G(V,T) = E(V) + F_{vib}(V,T) + F_{el}(V,T) - TS_{conf}(V,T) - TS_{mag} + PV$
- $\Delta G_f = G(Fe_{N-1}) - \frac{N-1}{N} G(Fe_N)$

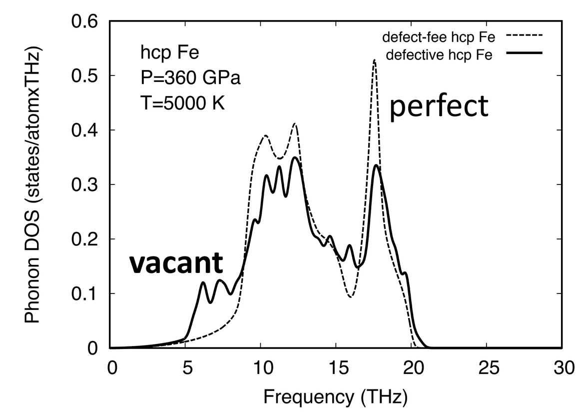
Benchmark



Inner core conditions







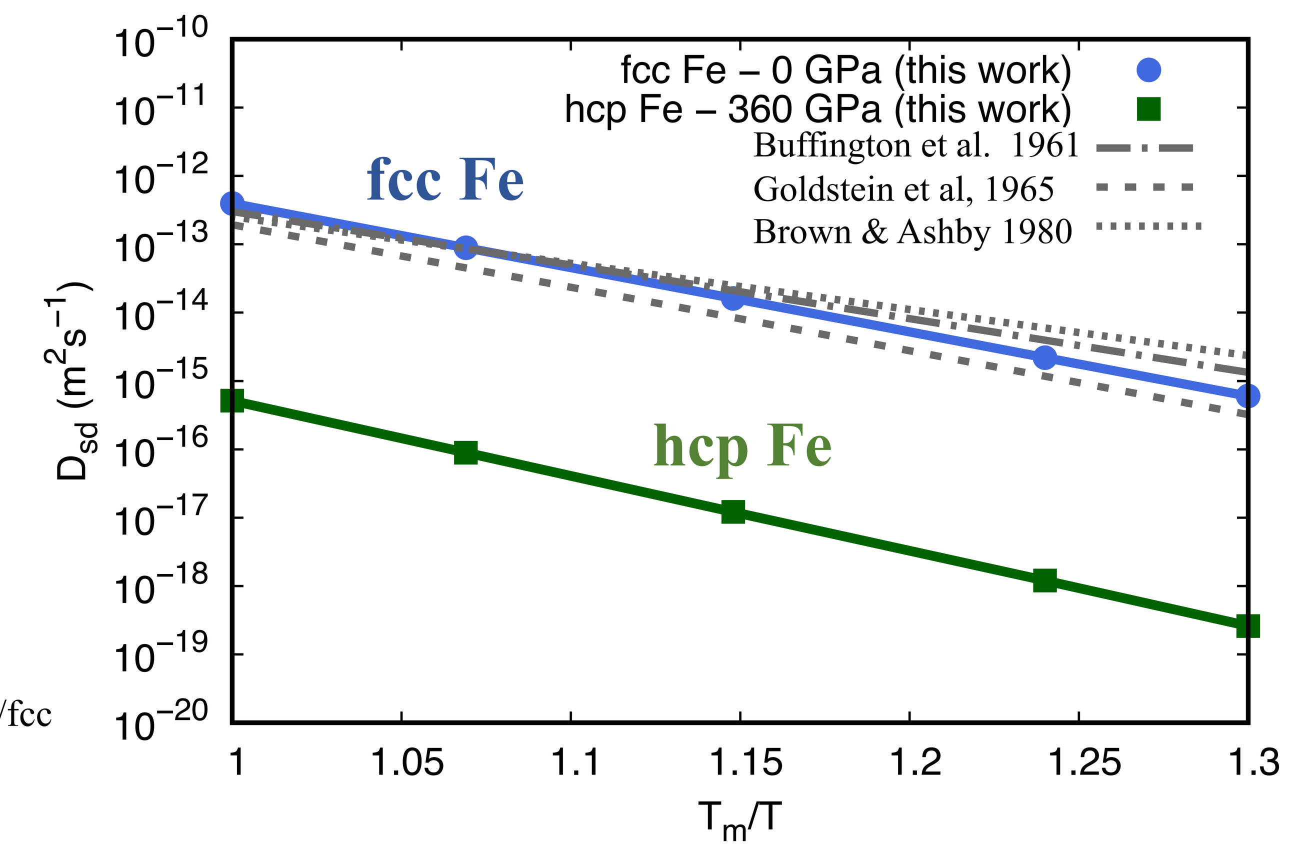
Lattice self-diffusion

$$D_{sd} = Z_f \frac{Z_m}{6} f\, l^2 \nu^* exp\left(\frac{\Delta S_f}{k_b}\right) exp\left(-\frac{\Delta H_f + \Delta H_m}{k_b T}\right)$$

Parameters	hcp iron (P = 360 GPa, T = 5,000 K)	fcc iron (P = 0 GPa, T = 1,800 K)
ΔH_f (eV)	10.3	1.97
ΔH_m (eV)	3.21	1.41
ΔS_f (k_b)	3.26	7.35
ν^* (THz)	21.3	7.34
f	0.78146	0.78146

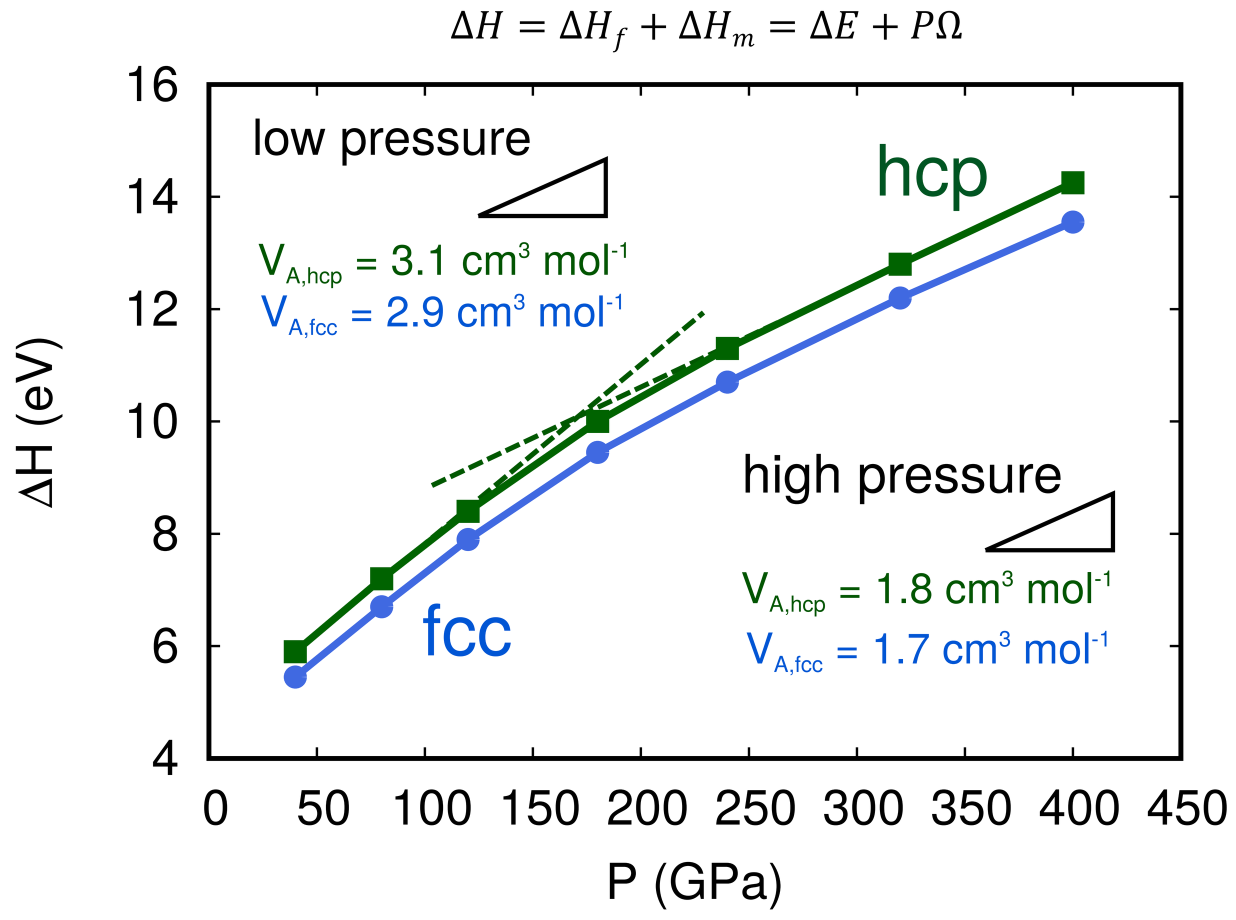
- Typical diffusivity of hcp iron at inner core P,T conditions: $10^{-17} - 10^{-16}$ m^{2}s^{-1}
- Activation volume $V_a = \partial H/\partial P$ for vacancy diffusion in hcp/fcc iron decrease with increasing pressure
- Pressure has an intrinsic effect on atomic diffusivity in iron

Diffusion coefficients as a function of homologous temperature



Activation volume V_a for vacancy diffusion

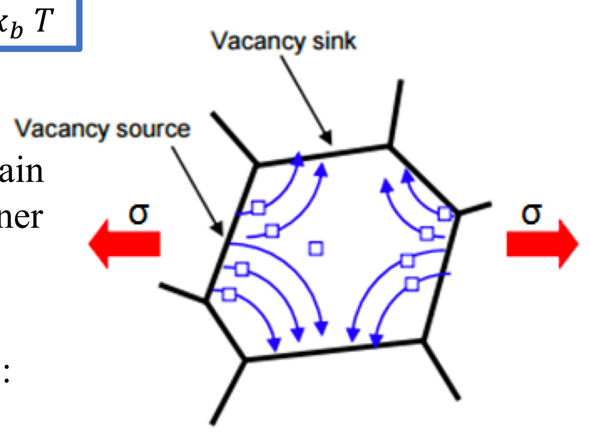
$$\Delta H = \Delta H_f + \Delta H_m = \Delta E + P\Omega$$



Diffusion creep versus Dislocation creep

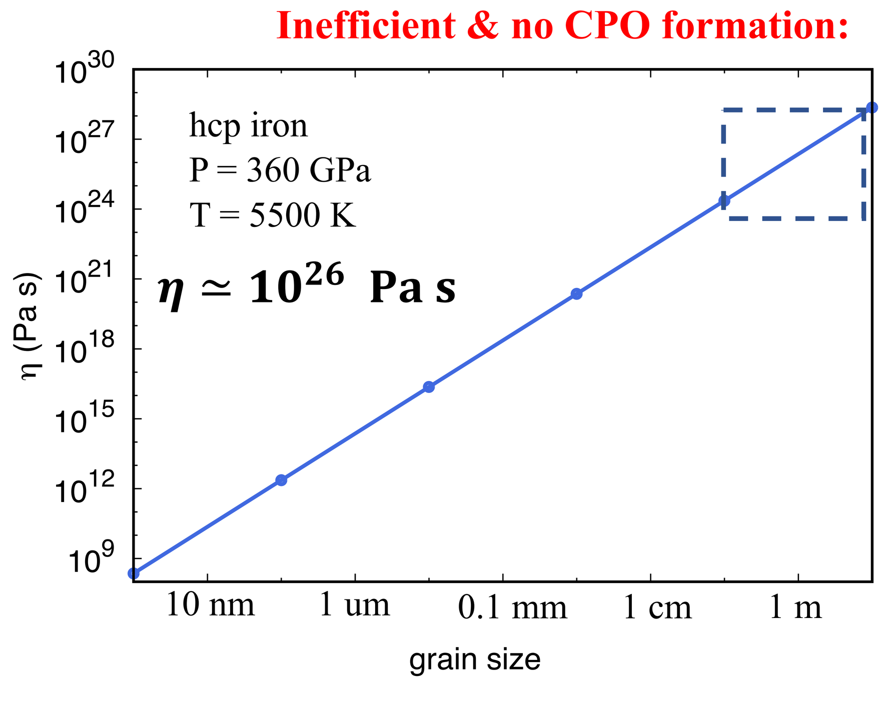
Diffusion creep — Nabarro 1948 & Herring 1950

$$\dot{\varepsilon}_{NH} = \frac{\tau}{\eta} = \frac{16}{3} \frac{D_{sd}\, \tau\, V_a}{gs^2\, k_b\, T}$$



- Bergman (1998) arguments that grain size (gs) in the inner core is ~[m]
- Yamazaki et al. (2017) suggest gs: ~[m] to [km]

Inefficient & no CPO formation:

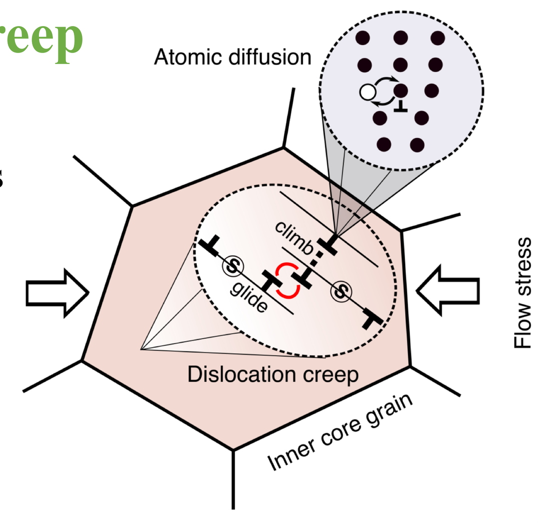


Dislocation creep — Weertman, 1955/1957

Recovery of dipole interactions

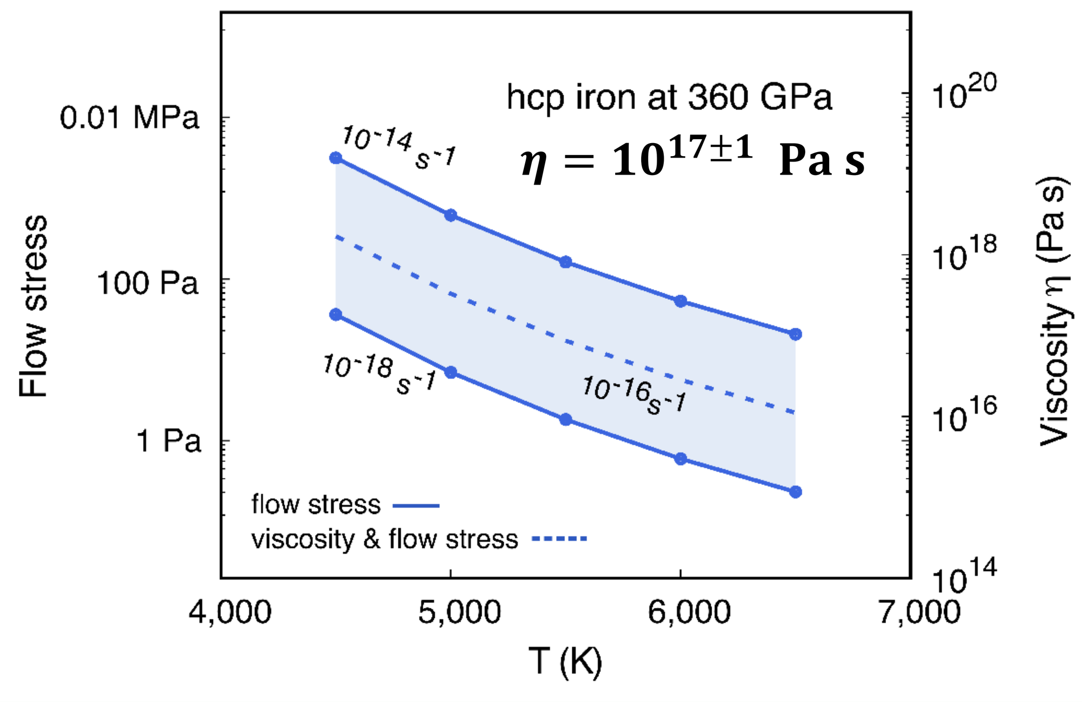
- $\dot{\varepsilon} = \rho b v = \rho b \frac{L}{d} v_{climb}$
- $v_{climb} = C_0 \frac{D_{sd}}{b}\left[\exp\left(\frac{\sigma V_a}{k_b T}\right) - 1\right]$
- $L = \rho_t^{-1/2} = (\sigma/\alpha\mu b)^{-1}$

$$\dot{\varepsilon}_W = A(\sigma) \frac{D_{sd}\mu b}{k_b T}\left(\frac{\sigma}{\mu}\right)^3$$



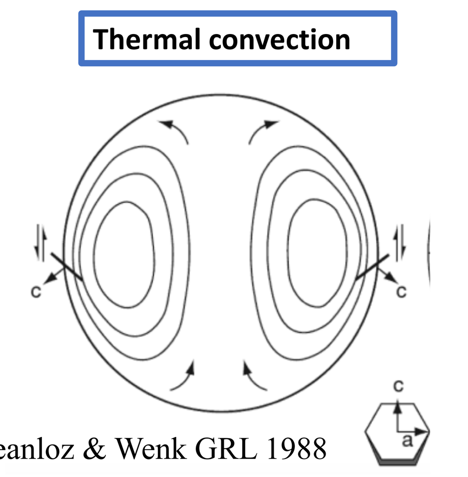
basal glide : < $\bar{1}2\bar{1}0$ > {0001}
(Nishihara et al. *EPSL* 2018)

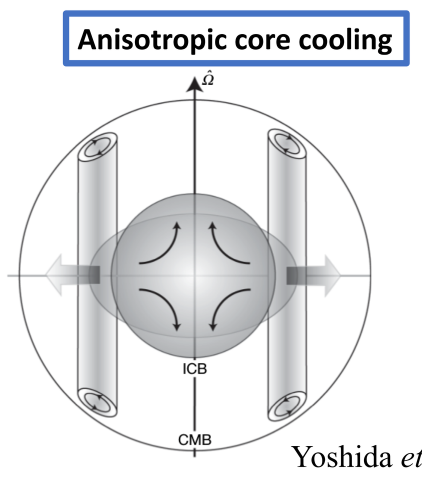
Most efficient mechanism :

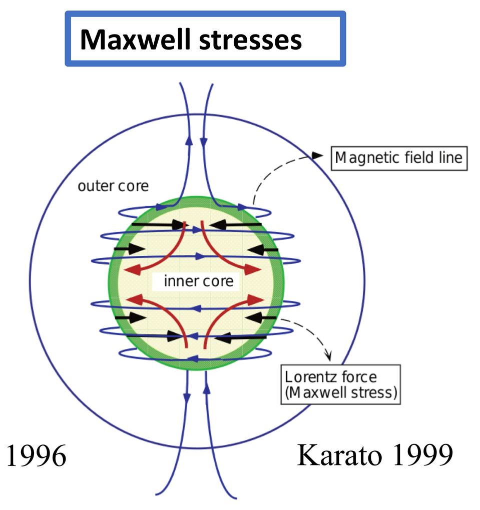


Models of inner core convection

Inner Core Plasticity







- $\dot{\boldsymbol{\varepsilon}} = \boldsymbol{u}/\boldsymbol{a} \simeq\ 10^{-17}$ s^{-1}
- $\boldsymbol{\sigma} = \boldsymbol{B^2}/\boldsymbol{\mu_0} \sim \mathbf{1} - \mathbf{100}$ **Pa**

In good agreement with recovery-controlled dislocation creep

- Plastic deformation of the inner core might contribute to the observed seismic anisotropy
- Low IC viscosity is consistent with the observation of J-waves: readily deforming IC (Tkalčić & Pham *Science* 2018)
- Small oscillations in inner core rotation: 0.1 – 1 degree/yr (Tkalčić et al., *Nat. Geo.* 2013)

Gravitational coupling Mantle – Inner core:
→ $\boldsymbol{\Gamma\tau} \lesssim \mathbf{2{\times}10^{20}}$ N m yr (Dumberry & Mound GJI 2010)
→ $\tau = 1 - 6$ yr → Buffett, Nat. 1997: $\boldsymbol{\eta} = \mathbf{0.5 - 3{\times}10^{17}}$ Pa s

Theoretical viscosity in agreement with observations of small inner core differential rotation.

- Observations of variations in the length of a day (Dumberry & Mound 2010) can be explained by the gravitational coupling between the mantle and inner core ($\eta = 10^{17\pm1}$ Pa s).
- The estimated viscosity is too low for inner core translation. (Deguen *et al. Geophys. J. Int.* 2013; Lasbleis & Deguin *PEPI* 2015)