Anisotropy and history of the Earth's inner core: forward models and input from mineralogy

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Earth's inner core



Illustration : Tkalčić, *Rev Geophys*. 2015

- 1220 km radius
- Crystallization of Fe-alloy due to Earth's cooling
- Pressure range: 330-365 GPa
- Temperature: ~6000 K
- Seismic anisotropy
 - North-South inner core Pwaves faster than equatorial paths
- Complex structure:
 - Outer inner core isotropic
 - Inner inner core anisotropic
 - Stronger anisotropy in western hemisphere
 - Super-rotation: 0.3-1.1°/y (?)

Inner core anisotropy



Illustration : Deuss, Annu. Rev. Earth Planet. Sci. 2015

Inner core anisotropy: measurement



Inner core anisotropy **Global models**



e.g. Karato 1993

e.g. Yoshida et al 1996

Implications



Models

Key questions for mineralogists

Crystal structure for inner-core Fe alloy (cubic or hexagonal)

Elasticity

Mechanisms for crystal alignment

- Crystallization
- Plastic deformation

Numerical model for polycrystal behavior

- Model for crystal alignment
- Elasticity at polycrystal scale

High P/T phase diagram for pure Fe



Stable phase of pure Fe at core conditions is *hcp*

But...

Impurities (light elements) may stabilize other phases such as fcc or bcc

Tateno et al, Science, 2010

Deformation Experiments on hcp-Fe (old work)

Collaboration

H.-R. Wenk (Berkeley), C.N. Tomé (Los Alamos), L. Miyagi (Utah), N. Nishiyama (Hamburg), Y. Wang (Chicago), and many others...

Plastic deformation at high pressure



- Controlled axial deformation
- Axial or lateral compression
- Deformation cycling possible
- Constant pressure
- P_{max} ~ 20 GPa T_{max} ~ 2000 K
- Samples: cylinders, ~mm diam.



- Un-controlled axial deformation
- Pressure increases with deformation
- $P_{max} \sim 300 \text{ GPa at } 300 \text{ K}$
- $P_{max} \sim 50$ GPa at 1500 K (resistive heating)
- Higher T with laser heating

In-situ measurements



Synchrotron x-ray diffraction



Experimental results



Macroscopic strain vs. time



Merkel *et al*, Modelling Simul. Mater. Sci. Eng. 2012





Microscopic vs. macroscopic strain



Interpretation of experimental results Polycrystal plasticity

Self-consistent polycrystal plasticity

- Iterative calculation
- Grain = ellipsoidal inclusion in homogeneous matrix

Parameters

- Sample phases
- Crystal structures
- Elasticity
- Plastic deformation mechanisms
- Deformation geometry

Approximations

- Elasto-plastic
- Visco-plastic
- Elasto-visco-plastic

Uses

- Interpretation of experimental data
- Modeling of polycrystal behavior

Codes : Los Alamos (EPSC, VPSC, EVPSC, C. Tomé, R. Lebensohn) Paris (VPSC, O. Castelnau), etc

Results for hcp-Fe

Plastic mechanisms for hcp-Fe

- 300 K, up to 200 GPa (DAC): basal slip + twinning dominant
- 17 GPa, up to 600 K (D-DIA): activity of pyramidal <c+a> increases less twinning
- 30 GPa, 2000 K (DAC) basal and pyramidal <c+a> slip
- Full self-consistent model of D-DIA experiments







slip



Wenk et al Nature, 2000 Merkel et al PEPI, 2004 Miyagi et al JAP, 2008 Merkel et al MSME, 2012

New Experiments Dynamic compression of of Fe Alloys

Collaboration

A. Gleason, C. Bolme (Los Alamos) W. Mao (Stanford)

Laser Compression



Ramp compression of iron to 273 GPa

Jue Wang,¹ Raymond F. Smith,² Jon H. Eggert,² Dave G. Braun,² Thomas R. Boehly,³ J. Reed Patterson,² Peter M. Celliers,² Raymond Jeanloz,⁴ Gilbert W. Collins,² and Thomas S. Duffy¹



X-ray free electron laser + laser compression In-situ plasticity studies







MEC beamline at LCLS/SLAC, Stanford

Preliminary Analysis

Peak shock pressure: \sim 140 GPa

T ~ 2000-3000 K

Diffraction pattern at multiple times: before, during, and after the shock







In-situ x-ray diffraction

Evidences for

- Phase transition to hcp
- Full hcp
 - Back-transformation to bcc







Inner Core Anisotropy Model

Inner core anisotropy Multi-scale forward model



Objectives

Literature

- Multiple models for inner formation, multiple choices for structure of inner core Fe-alloy, multiple sets of elastic moduli
- No integrated model of inner core anisotropy

This work

- Multiscale forward model:

core formation geodynamical model single crystal deformation and elasticity seismic measurement simulation

Objectives

- Can we even get 3% global IC anisotropy?
- Crystal structure, deformation, elasticity of IC Fe-alloy?
- What is driving inner core dynamics?

Single crystal: Fe structures



Core formation model Preferrential growth at the equator



component of seismic

anisotropy

Yoshida et al, 1996

Extensions



Preferential growth Random crystallization Yoshida *et al*, 1996



Preferential growth Crystallization textures Yoshida et al, 1996 + Bergman *et al*, 1997





Preferential growth with chemical stratification Deguen *et al*, 2009

Virtual inner core



Lincot et al, Geophys. Res. Lett. 2015

Virtual inner core: seismic response



Procedure

- Choose random ray path
- Calculate velocity at each point along the ray
- Slowness: $\langle s \rangle = 1/\langle V_{\rho} \rangle$
- Seismic residual $\delta t/t = (\langle s \rangle s_0)/s_0$

Repeat 300 000 times...

Plot results as seismologists do

- Residual vs.
 - Angle to rotation axis (ξ)
 - Depth of the ray (a)

Lincot et al, C.R. Geosc. 2014

Virtual inner core seismic response Cubic-Fe



Virtual inner core seismic response hcp-Fe



Core formation models

Core formation model Deformation based on flow in core-formation model Additions: stratification, crystallization textures Elastic moduli from the literature



Lincot et al, C.R. Geosc. 2014

Extension of the work

- Difficult to get ~3% global seismic anisotropy
- Room for improvement:
 - Geodynamics :
 - locked (difficult to produce more deformation with a quadrupolar flow)
 - Choice of plastic mechanism
 - Multiple choices for hcp-Fe
 - Elasticity :
 - hcp-Fe : large panel of single crystal anisotropy
 - cubic-Fe : only a few models published
- Solution
 - Test multiple slip systems for hcp-Fe
 - Monte-Carlo search for elastic moduli: test all possible sets of elastic moduli for the inner core Fe-alloy

Results: cubic-Fe



Results: cubic-Fe



Cubic structure for Fe?



Lincot et al, GRL 2015

Global anisotropy results: hcp-Fe

Hcp-Fe

- Preferential growth at equator with chemical stratification
- Dominant pyramidal slip

45

5000 sets of elastic moduli tested

Lincot *et al*,

2016

Geophys. Res. Lett.



Hcp elastic anisotropy parameters



Hcp elastic anisotropy parameters



Hcp elastic anisotropy parameters



Effect of dominant slip system



Effect of inner-core formation model



Dominant pyramidal <c+a>

Global anisotropy results: hcp-Fe

Hcp-Fe

Preferential growth at equator with chemical stratification

Dominant pyramidal slip

Squares: Vocadlo et al, 2009 Diamond: Sha and Cohen, 2010 Triangles: Martotell *et al*, 2013

Lincot *et al*, *Geophys. Res. Lett*. 2016

Equatorial Growth+Stratification



Finally...



Lincot *et al*, *Geophys. Res. Lett*. 2016

Take home messages

Not so straightforward to build inner core model with 3% global anisotropy:

- Simple core formation model
 Ex: preferential growth at equator + extensions
- Structure for Fe alloy Impossible with cubic structure Possible with hcp
- Dominant deformation by pyramidal slip Most efficient at aligning c-axes
- ~ 20% elastic anisotropy in the single crystal (depends on the core formation model)
- Details of inner-core history Can not discriminate at this point



Future works

Seismology

- Add new data points (e.g. virtual path from ambient noise)
- Publish actual residuals, with entry and exit points for the used paths
- Mineral physics
 - HP/HT phase diagrams of Fe-alloys
 - Effect of HT on plastic deformation mechanisms
 - Confirm crystallization mechanisms

Modeling

- Build virtual inner cores with full-field, direct models of seismic travel times
- Constrain inner-core history based on seismic measurements and input from mineral physics

