Seismological and mineralogical constraints on the inner core fabric

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Abstract. Under the assumption of lattice preferred orientation of iron hcp crystals, the seismic anisotropy of the inner core is related to single crystal elastic properties by a fabric model. This model is able to explain a new seismological constraint: the constant behaviour of the ratio k of two anisotropy coefficients, despite radial and lateral variations of the anisotropy level in the inner core. The relevance of the theoretical calculations of iron single crystal elastic properties at inner core conditions are tested by a comparison between seismic estimates and computed values of this ratio k. Taking into account the error bar of the seismic estimate, iron hcp structures presenting fast and slow c axis could fit the data equally well.

1. Introduction

The seismological picture of the inner core has been improved during the past five years, exhibiting new complexities. At short length scales, the presence of kilometric scale scatterers is suggested by different studies [*Cormier et al.*, 1998; *Vidale and Earle*, 2000], and at large wavelengths radial and lateral variations of the inner core anisotropy have been specified [*Tanaka and Hamaguchi*, 1997; *Creager*, 1999; *Garcia and Souriau*, 2000, 2001; *Niu and Wen*, 2001]. Even if some studies have stressed the possibility of contamination by deep mantle structures [*Bréger et al.*, 1999], the coherency of the large scale inner core seismological structure obtained from different data sets with different investigation methods suggest that these effects are small. During the same time period, the theoretical determinations of iron properties at inner core conditions has greatly improved [*Stixrude and Cohen*, 1995; *Laio et al.*, 2000; *Steinle-Neumann et al.*, 2001]. Until now, the seismologically inferred inner core anisotropy and the single crystal elastic constants of iron have been compared by considering only the anisotropy level. In this study, another inner core anisotropy parameter is introduced which is related to single crystal iron elastic properties through an inner core fabric model.

First, the inner core large wavelength seismological properties are reviewed. Then, a fabric model is proposed to explain the seismological observations, and inner core anisotropy parameters are related to the theoretical elastic constants of iron at inner core conditions by using this model. In conclusion, the limitations of the model and the consequences for the inner core dynamics are discussed.

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2. Seismological observations

At large wavelengths,the seismological structure of the inner core, as seen by body waves, presents a property of transverse isotropy with a fast axis oriented along the spin axis of the Earth (see Creager 2000 for a review). Some complexities appear in the upper part of the inner core, in the top 100 km beneath the inner core boundary (ICB), where the P-wave velocity presents an hemispheric heterogeneity pattern and a low anisotropy level [*Niu and Wen*, 2001; *Ouzounis and Creager*, 2001; *Garcia*, in press]. Because this upper part is probably not anisotropic, it will be excluded of our analysis of the inner core anisotropy. However, in the rest of the inner core, the body wave data are properly explained by a model of cylindrical anisotropy with a fast axis along the spin axis of the Earth's, and radial and lateral variations of the anisotropy level [*Garcia and Souriau*, 2000, 2001]. In such an anisotropic model, the P-wave velocity perturbation is expressed as a function of the angle ξ between the PKPdf ray at its turning point and the Earth's spin axis as

$$\frac{\delta V(r,\xi)}{V_0(r)} = a(r,\varphi) + \epsilon(r,\varphi)cos^2\xi + \gamma(r,\varphi)sin^2 2\xi \quad (1)$$

in which $V_0(r)\approx V(r,\xi=90°)$ is the P-wave velocity of the reference Earth's model, $a(r,\varphi)$, $\epsilon(r,\varphi)$ and $\gamma(r,\varphi)$ are the parameters describing the anisotropy as a function of radius r and longitude φ. These three independant parameters characterize completely the velocity perturbation curve, and could be related to the elastic coefficients of the anisotropic media in the Love notation [*Babuska and Cara*, 1991; *Mensch and Rasolofosaon*, 1997]:

- $\gamma = \frac{4L+2F-A-C}{8C}$;
- $\epsilon = \frac{C-A}{2C} = \frac{V(\xi=0°)-V(\xi=90°)}{V_0}$ is the anisotropy level and indicates the amplitude of the curve,
- a is the offset of the curve, correcting for differences between V_0 and $V(\xi=90°)$.

The velocity perturbation could also be parametrized using the ratio $k=\frac{\epsilon}{\gamma}$. Figure 1 gives a graphic interpretation of the various parameters, and k could be related to the shape of the curve.

With such an anisotropic model, an hemispherical pattern appears in the 100-400 km depth range below the ICB as could be seen in figure 2. However, the isotropic average of the anisotropic velocity perturbation ($(\frac{\delta V}{V_0})_{iso} = a+\frac{\epsilon}{3}+\frac{8}{15}\gamma$) does not vary laterally [*Creager*, 1999; *Garcia and Souriau*, 2000, 2001]. This important observation indicates that there are probably not large chemical or thermal heterogeneities in the inner core, and favours a homogeneous inner core mineralogical structure. As seen on figure 3.a, another important feature of this model is that the ratio $k=\frac{\epsilon}{\gamma}$ shows little variations in the inner core below 100 km depth. Moreover, the comparison between previously determined values of the ratio k (figure 3.b and Table 1) shows that this ratio is in the range -2 ± 1 despite the different data sets, parametrizations and results of these inner core studies. The coherency between these different estimates of the ratio k increases as the radius decreases. All these observations suggest that the inner core anisotropy has the same caracteristics in the whole inner core, below 100 km beneath the ICB. The almost constant behaviour of the parameters $(\frac{\delta v}{v_0})_{iso}$ and k in the inner core indicates that the inner core anisotropy and its variations could be parametrized by one parameter ($\epsilon(r,\varphi)$) instead of three.

3. Fabric interpretation

In this part, two simple models of inner core fabric are proposed, and the seismic P-wave anisotropy is compared to the anisotropy predicted by the fabric model and theoretical determinations of iron elastic constants at the inner core conditions. If the inner core anisotropy is due to the lattice preferred orientation (LPO) of crystals, the seismological observations indicate that the mineralogical structure is the same over all the inner core, and that the fabric is a one parameter function allowing variations of the anisotropy level, but keeping the ratio k constant. In this study, only hexagonaly close packed (hcp) single crystals will be considered because the iron hcp phase is the most stable at inner core conditions [*Vočadlo et al.*, 1999, 2000]. Two inner core fabrics are proposed depending on the elastic constants of inner core single crystals. These fabrics are defined by their orientation distribution functions (ODF) in the Euler space [*Bunge and Esling*, 1982; *Mainprice et al.*, 2000]. If the iron hcp single crystals present a fast c axis [*Stixrude and Cohen*, 1995], a fabric defined by a proportion α of the crystals with their c axis exactly aligned along the spin axis of the Earth, and the rest oriented at random, could simulate the observed anisotropy. The ODF of such a fabric is defined by $f_c(\mathbf{g}) = (1-\alpha)+2\alpha\frac{\delta(\phi)}{sin\phi}$, in which $\mathbf{g}$ is the orientation in the Euler space, ϕ is the second Euler angle between the single crystal c axis and the spin axis of the Earth, and $\delta(\phi)$ is the Dirac function. Such a model is very simplistic because the inner core ODF is certainly not discontinuous, but the introduction of the parameter α allows us to easily quantify the degree of crystal alignement. Similarly, if the iron hcp single crystals present a slow c axis [*Steinle-Neumann et al.*, 2001], a fabric defined by a proportion α of the crystals with their c axis perpendicular to the spin axis of the Earth, and the rest oriented at random, could simulate the observed anisotropy. The ODF of such a fabric is defined by $f_a(\mathbf{g}) = (1-\alpha)+2\alpha\delta(\frac{\pi}{2}-\phi)$. The **"Voigt average"** of the inner core elastic coefficients could be calculated from the single crystal elastic coefficients assuming the fabric is governed by these ODF, following the formula [*Mainprice et al.*, 2000]:

$$< c_{ijkl} >= \int c_{ijkl}(\mathbf{g})f(\mathbf{g})d\mathbf{g} \qquad (2)$$

with, $c_{ijkl}(\mathbf{g}) = g_{ip}g_{jq}g_{kr}g_{lt}c_{pqrt}(\mathbf{g0})$, $< c_{ijkl} >$ and c_{ijkl} being the components of the inner core and single crystal stiffness tensor, $\mathbf{g}$ and $\mathbf{g0}$ the directions in the inner core and crystal co-ordinates, g_{ij} the components of the rotation matrices, and $f(\mathbf{g})$ the ODF characterizing the fabric. The results of this integration are summarized in Table 2 for the two fabrics considered here. For a given single crystal elastic structure, the coefficients ϵ and γ depend only on the degree of crystal alignement α, and the ratio $k = \frac{\epsilon}{\gamma}$ does not depend on the parameter α. So, the whole inner core anisotropic structure could be explained by the same fabric by only varying radially and laterally the degree of crystal alignement α. The seismological parameters ϵ, γ and k are calculated from the fabric model and theoretical calculations of iron hcp elastic coefficients. They are presented in Table 3 for three different studies. The degree of crystal alignement α is allowed to vary in our model to fit the seismological estimate of the anisotropy level ϵ. For example *Stixrude and Cohen* [1995] model requires $\alpha = 1$ to fit the seismological observations in the center of the inner core, whereas *Steinle-Neumann et al.* [2001] model requires $\alpha = 0.35$. Since the ratio k is fixed by only the single crystal elastic properties, it could be used to infer the relevance of the theoretical calculations. The calculated values of the ratio k are closer to the seismological observations for *Steinle-Neumann et al.* [2001] and *Stixrude and Cohen* [1995] models than in *Laio et al.* [2000] model. However, this comparison must be taken with caution because the effects of light elements in the inner core are poorly known, the fabric model is probably not unique, and the various theoretical computations are performed at different temperature and pressure conditions. Moreover, taking into account the error bars of the seismological estimate of the ratio k, we could not discriminate between fast or slow c axis models.

4. Conclusion and discussion

Under the hypothesis of LPO of hcp inner core crystals, a simple fabric model is proposed to relate theoretical calculations of iron hcp elastic coefficients to the seismic anisotropy of the inner core. Even if the fabric model is probably not unique, it is able to explain all the seismological observations, and particularly the constant behaviour of the seismological parameter $k = \frac{\epsilon}{\gamma}$ despite the radial and lateral variations of the anisotropy level. The theoretical calculations of the single crystal properties are used in the fabric model, and a comparison is made between observed and modelled values of the ratio k. Unfortunately, this comparison does not allow to discriminate between iron hcp models presenting fast or slow c axis. However, most of the mechanisms proposed to create the inner core anisotropy present strong North-South [*Romanowicz et al.*, 1996] or equator to pole [*Yoshida et al.*, 1996; *Karato*, 1999; *Buffett and Wenk*, 2001] flow fields, that induce a strong polar shearing in the center of the inner core. So, if the primary slip system is basal [*Poirier and Price*, 1999; *Wenk et al.*, 2000], the crystals have their c axis preferentially oriented perpendicular to spin axis of the Earth and a single crystal slow c axis is favoured. Asymmetric boundary conditions could create lateral variations of the degree of crystal alignement, and explain the hemispheric variation of the anisotropy level observed in the 100-400 km depth range in the inner core.

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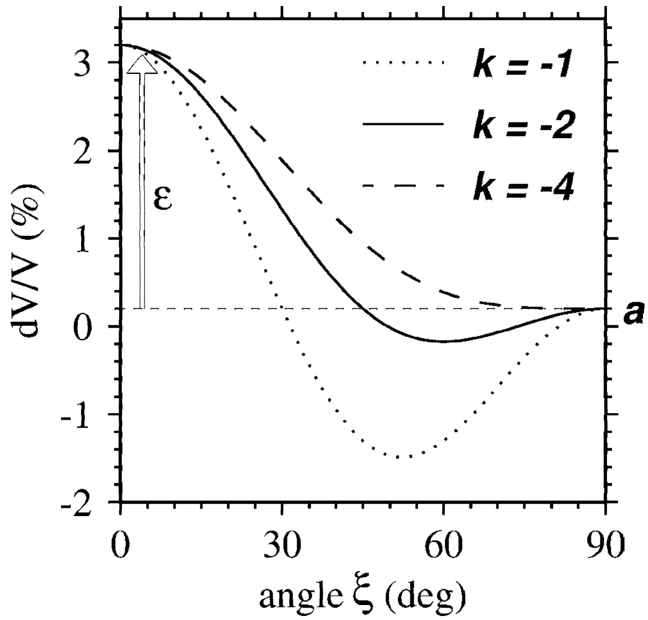

Figure 1. Graphic interpretation of the various parameters involves in the equation (1), with $\epsilon = 3\%$, $a = 0.2\%$ and $k = \frac{\epsilon}{\gamma}$.

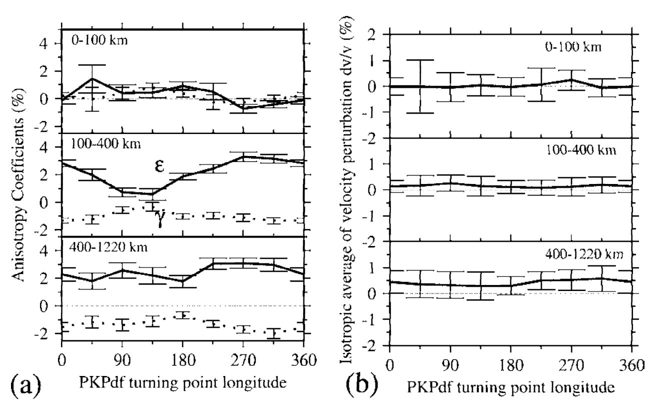

Figure 2. Inner core anisotropy model. (a) parameters $\epsilon(r,\varphi)$ (full line) and $\gamma(r,\varphi)$ (dotted line) (in %) of the relationship $\frac{\delta v(r,\xi)}{v_0} = a(r,\varphi) + \epsilon(r,\varphi)cos^2\xi + \gamma(r,\varphi)sin^2 2\xi$ describing the inner core anisotropy, represented as a function of the position of a 90° wide moving window applied to PKPdf turning point longitude (in degrees) for the three layers: 0-100 km (top), 100-400 km (middle) and 400-1220 km depths (bottom) below the inner core boundary. (b) isotropic average of the velocity perturbation with respect to model ak135 $(\frac{\delta v}{v_0})_{iso}$ (in %).

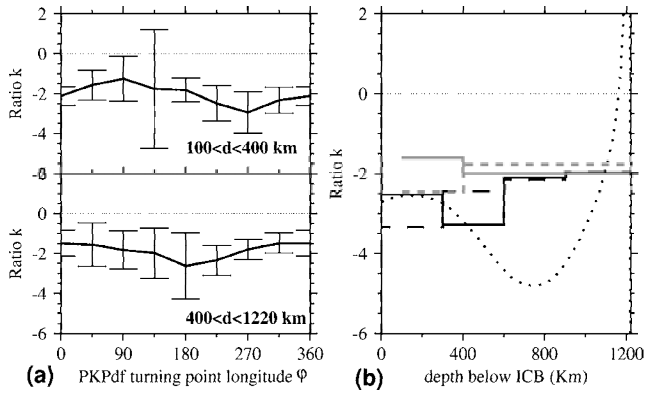

Figure 3. Ratio $k = \frac{\epsilon}{\gamma}$ for different inner core models. (a) $k(r,\varphi)$ for the inner core model by Garcia and Souriau (2000), where d is the depth below the ICB. (b) $k(r)$ for the inner core models by McSweeney et al. (1997) (dotted line), Su and Dziewonski (1995) ICA4A (dashed line) and ICA4B (full line), and Garcia and Souriau (2000) for East (grey line) and West (grey dashed line) hemispheric averages.

Table 1. Anisotropy coefficients for inner core models parametrised with a uniform cylindrical anisotropy oriented along the spin axis of the Earth.

References	ϵ (in%)	γ (in%)	$k = \frac{\epsilon}{\gamma}$
Morelli et al. 1986	3.2	-1.6	-2.0
Shearer et al. 1988	0.98	-0.43	-2.25
Shearer and Toy 1991	0.61	-0.13	-4.25
Creager 1992	3.92	-1.39	-2.82
Song and Helmberger 1993	3.02	-1.36	-2.22

Table 2. Elastic properties of the inner core (Love notation) as a function of the hcp single crystal elastic properties (C_{ij} matrix notation) for the two fabrics. Coefficients $\bar{\lambda}$ and $\bar{\mu}$ are the isotropic Lamé parameters obtained for a random fabric, α is the degree of crystal alignement.

	$f_c(\mathbf{g})$	$f_a(\mathbf{g})$
A $=< c_{1111} >=$	$(1-\alpha)(\bar{\lambda}+2\bar{\mu})+\alpha C_{11}$	$(1-\alpha)(\bar{\lambda}+2\bar{\mu})+\frac{\alpha}{8}(3C_{11}+3C_{33}+2C_{13}+4C_{44})$
C $=< c_{3333} >=$	$(1-\alpha)(\bar{\lambda}+2\bar{\mu})+\alpha C_{33}$	$(1-\alpha)(\bar{\lambda}+2\bar{\mu})+\alpha C_{11}$
F $=< c_{3311} >=$	$(1-\alpha)\bar{\lambda}+\alpha C_{13}$	$(1-\alpha)\bar{\lambda}+\frac{\alpha}{2}(C_{11}+C_{13}-2C_{66})$
L $=< c_{1313} >=$	$(1-\alpha)\bar{\mu}+\alpha C_{44}$	$(1-\alpha)\bar{\mu}+\frac{\alpha}{2}(C_{44}+C_{66})$
N $=< c_{1212} >=$	$(1-\alpha)\bar{\mu}+\alpha C_{66}$	$(1-\alpha)\bar{\mu}+\frac{\alpha}{8}(C_{11}+C_{33})$
$\epsilon =$	$\alpha\frac{C_{33}-C_{11}}{2C}$	$\alpha\frac{5C_{11}-3C_{33}-2C_{13}-4C_{44}}{16C}$
$\gamma =$	$\alpha\frac{4C_{44}+2C_{13}-C_{11}-C_{33}}{8C}$	$\alpha\frac{6C_{13}+12C_{44}-3C_{11}-3C_{33}}{64C}$
$k = \frac{\epsilon}{\gamma}$	$4\frac{C_{33}-C_{11}}{4C_{44}+2C_{13}-C_{11}-C_{33}}$	$4\frac{5C_{11}-3C_{33}-2C_{13}-4C_{44}}{6C_{13}+12C_{44}-3C_{11}-3C_{33}}$

Table 3. Inner core anisotropy coefficients calculated from the fabric model (ODF $f_c(\mathbf{g})$ and $f_a(\mathbf{g})$) and the iron single crystal elastic properties extracted from theoretical caculations.

References	Temp. (in °K)	Press. (in GPa)	ODF	ϵ (in %) for $\alpha = 1$	α to fit ϵ at Earth's center	$k = \frac{\epsilon}{\gamma}$
Stixrude and Cohen 1995	0 K	240 GPa	$f_c(\mathbf{g})$	3.0	1	-1.17
Laio et al. 2000	0 K	210 GPa	$f_c(\mathbf{g})$	6.7	0.45	-17.92
Steinle-Neumann et al. 2001	5700 K adiabatic	330 GPa	$f_a(\mathbf{g})$	8.6	0.35	-3.10