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Shape preferred orientation of iron grains compatible with Earth's uppermost inner core hemisphericity

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ABSTRACT

Constraining the possible patterns of iron fabrics in the Earth's Uppermost Inner Core (UIC) is key to unravel the mechanisms controlling its growth and dynamics. In the framework of crystalline micro-structures composed of ellipsoidal, aligned grains, we discuss possible textural models of UIC compatible with observations of *P*-wave attenuation and velocity dispersion. Using recent results from multiple scattering theory in textured heterogeneous materials, we compute the *P*-wave phase velocity and scattering attenuation as a function of grain volume, shape, and orientation wrt to the propagation direction of seismic *P*-waves. Assuming no variations of the grain volume between the Eastern and Western hemisphere, we show that two families of texture are compatible with the degree-one structure of the inner core as revealed by the positive correlation between seismic velocity and attenuation. (1) Strong flattening of grains parallel to the Inner Core Boundary in the Western hemisphere and weak anisometry in the Eastern hemisphere. (2) Strong radial elongation of grains in the Western hemisphere and again weak anisometry in the Eastern hemisphere. Both textures can quantitatively explain the seismic data in a limited range of grain volumes. Furthermore, the velocity and attenuation anisotropy locally observed under Africa demands that the grains be locally elongated in the direction of Earth's meridians. Our study demonstrates that the hemispherical seismic structure of UIC can be entirely explained by changes in the shape and orientation of grains, thereby offering an alternative to changes in grain volumes. In the future, our theoretical toolbox could be used to systematically test the compatibility of textures predicted by geodynamical models with seismic observations.

1. Introduction

From the analysis of differential travel times of *PKP* phases, Tanaka and Hamaguchi (1997) detected for the first time the hemispherical seismic structure of the Earth's inner core with polar rays faster in the western hemisphere than in the eastern hemisphere. Other evidences of this hemispherical structure have been later described in many other studies (for a review, see Souriau and Calvet, 2015 and Tkalčić, 2015). In particular, Niu and Wen (2001) observed that $PKiKP$–$PKIKP$ travel times differential residuals in the 130°–141° epicentral distance range, which sample the first 100 km of the inner core, are systematically larger by about 0.8 s in the quasi-Eastern (qE) hemisphere (40°E–180°E) than in the quasi-Western (qW) hemisphere (180°W–40°E). Later, Wen and Niu (2002) found that the P-wave quality factor is about 250 in the qE hemisphere and 600 in the qW hemisphere. They also observed a positive correlation between velocity and attenuation, i.e. high (resp. low) velocities are correlated with high (resp. low) attenuations. When exploring the Uppermost Inner Core (UIC) at a more local scale, however, this general picture should be nuanced. For instance, Attanayake et al. (2014) and Iritani et al. (2014) have shown that the Central Pacific region, which has been previously considered as a part of the qW hemisphere, is rather characterized by low velocity and strong attenuation.

The first 100 km of the inner core are mostly isotropic, but anisotropy in velocity and attenuation has been observed locally under Africa (qW hemisphere) with the direction of high (resp. low) attenuation corresponding to high (resp. low) velocity (Yu and Wen, 2006). At larger depth, the inner core is anisotropic with a qW hemisphere more anisotropic than the eastern one (Tanaka and Hamaguchi, 1997). Observations of $PKiKP$ coda have also confirmed the widespread presence of small-scale heterogeneities in the UIC (Vidale and Earle, 2000; Koper et al., 2004). Leyton and Koper (2007) suggested an hemispherical distribution of these scatterers as $PKiKP$ codas are stronger in the qW hemisphere than in the qE one. Although observations of $PKiKP$ coda are

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still too sparse to draw firm conclusions about the hemispherical distribution of scatterers, it is very likely that small-scale heterogeneities play a key role in PKIKP wave attenuation and its correlation with the velocity structure.

In view of the numerous observations of heterogeneity in UIC, it appears natural to re-examine – in a scattering framework – the textural interpretation of its degree-one velocity and attenuation structure. Indeed, a variety of geodynamical models have been proposed in the literature to explain this particular feature. Both the localization of the areas of melting/freezing and the resulting textures are the subject of a long-standing debate in the seismological literature. The presence of fluid inclusions in the inner core has often been invoked to explain, through viscoelastic processes, $PKIKP$ attenuation (Singh et al., 2000). The different seismic properties of the qW and qE hemispheres may thus reflect spatial variations in the melt distribution (fluid content and porosity) (Wen and Niu, 2002; Cao and Romanowicz, 2004; Gubbins et al., 2011; Pejić et al., 2017). This attractive model may nevertheless run into difficulties in explaining other key observations. In particular, large (i.e. kilometric) pockets of melt or fluids would have to be present in the UIC to explain the observed scattering (Vidale and Earle, 2000). Such large volumes of melts, in turn, seem difficult to reconcile with geodynamical models of the mushy zone (Deguen et al., 2007). Furthermore, Calvet and Margerin (2008) have shown that mineralogical models of iron, when properly converted to seismic models, leave little room for the presence of fluids.

Alternatively, modeling the relation between velocity and attenuation through scattering opens the possibility to explain the UIC hemispherical pattern in terms of spatial variations of iron fabrics (Wen and Niu, 2002; Cormier, 2007; Monnereau et al., 2010). While the exact proportion of scattering vs absorption in the attenuation process is not yet precisely known, the fact that the former plays a very significant role is documented by waveform analysis and observations of the coda of $PKiKP$ (Vidale and Earle, 2000; Leyton and Koper, 2007). In this study, we *assume* that scattering is the dominant mechanism for seismic attenuation and propose an iron fabric interpretation of the UIC hemisphericity.

Solidification texturing controlled by outer core flow and heat flux extraction at the Inner Core Boundary (ICB) and convection within the inner core are the most popular mechanisms to explain seismic heterogeneities and anisotropy in the inner core (see Lasbleis and Deguen, 2015, for a recent review). But they result in contradictory fabric interpretations of the UIC hemispherical structure. Modeling thermochemical convection in the outer core, Aubert et al. (2008) have shown that a long-term cyclonic circulation beneath Asia may cause faster freezing in the qE hemisphere than in the qW one resulting in the velocity and attenuation degree-one structure. They argued that a well-textured aggregate with radially elongated grains may develop in the slow freezing hemisphere (qW) while a rather untextured iron aggregate may develop in the fast freezing hemisphere (qE). Monnereau et al. (2010) and Alboussiere et al. (2010) proposed that the hemispherical heterogeneity of the inner core results on the convectional translation of materials from the crystallizing qW hemisphere to the melting qE hemisphere. Monnereau et al. (2010) demonstrated that a degree-one distribution of the grain size, with larger spheroidal grains in the qE hemisphere, may induce larger P-wave velocity and attenuation in the qE hemisphere than in the qW one. Next, in order to also explain the hemispherical pattern in anisotropy described by Tanaka and Hamaguchi (1997), Bergman et al. (2010) proposed a variant of the translation model with a dendritic crystallization in the western hemisphere. As recrystallization processes during annealing erase the initial texture acquired in the qW hemisphere, translation would entail de-texturing from west to east, accompanied by a change of the grain shape – from radially elongated grains in the qW hemisphere to equi-axed grains in the qE one. In sharp contrast, Cormier (2007) advocated the opposite textural scenario (i.e. de-texturing from east to west) from waveform modeling of $PKIKP$ and $PKiKP$ waves. He proposed that heterogeneities are radially elongated in the qE hemisphere while they may be flattened and horizontally oriented (Cormier, 2007) or equi-axed (Cormier et al., 2011) in the qW hemisphere.

This non-exhaustive review illustrates the current debate on the inner core textures compatible with seismic observations. This controversy does not find its origin in the data: while seismic models differ in the details, most authors agree on the gross features of UIC as summarized above. Part of the problem certainly stems from relations put forward in the literature between UIC fabrics and seismic observables, that have not always been supported by solid quantitative analysis. Hence, the present study represents an effort at bridging the gap between micro-structural and seismic models of UIC. Furthermore, translation dynamics which has proven so effective in explaining IC hemisphericity, implies a large contrast of grain size between the qE and qW hemispheres. Because recent estimates of iron conductivity (Pozzo et al., 2014) compromise the viability of internally-driven core convection, it appears necessary to reconsider textural interpretation focusing on grain shape rather than grain volume.

In Section 2, we develop a multiple scattering model for seismic waves in anisometric media (i.e. with a preferential shape orientation, SPO) which has recently received support from ab-initio wave equation simulations (Van Pamel et al., 2017). We calculate the velocity and attenuation anisotropies of iron crystal aggregates as a function of the volume, aspect ratio and elastic properties of the grains (Calvet and Margerin, 2016). In Section 3, considering the dominant degree-one structure of UIC, and neglecting local anisotropy in the qW hemisphere, we describe the characteristics of iron textures which verify simultaneously larger P-wave velocity and attenuation in the qE hemisphere than in the qW hemisphere. Section 4 critically examines various textural models of UIC previously proposed in the literature.

2. Multiple scattering theory

In this section, we develop a multiple scattering model for seismic waves propagating in polycrystalline aggregates with oriented ellipsoidal grains (SPO) with no preferential orientation of the crystallographic axes (LPO). Including a LPO in our model is theoretically possible but requires methodological developments that go beyond the scope of this study. The LPO would probably lower the effective material heterogeneity with respect to a material with random crystallographic axes. This in turn would lower the overall attenuation and limit the wave speed renormalization (i.e. the velocity shift in the random medium wrt to the Voigt average). However, because estimates of anisotropy of individual grain vary largely in the literature, it may be considered as a free parameter that can be adjusted to match the seismic observations. To further simplify the analysis, we consider iron crystal aggregates with elongated or flattened grains (Fig. 1). The ellipsoidal shape of the grain is represented by a spatial correlation function of the form:

$$\eta(x, y, z) = \exp\left(-\sqrt{\frac{x^2}{a_x^2} + \frac{y^2}{a_y^2} + \frac{z^2}{a_z^2}}\right) \qquad (1)$$

where (a_x, a_y, a_z) are the ellipsoid radii in the global cartesian (x, y, z) coordinate system (Margerin, 2006; Yang et al., 2011). This correlation function properly describes the variable shape and linear dimensions of grains in polycrystals (Stanke, 1986). We introduce a cylindrical symmetry by letting $a_x = a_y$. The aspect ratio of the grain is defined as $R_0 = a_z/a_x$. We also introduce the radius a_r of an equiaxed grain whose effective volume is equal to the one of