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Letter to the Editors

The crystal structure of iron in the Earth's inner core

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SUMMARY

Seismic *P*-waves travelling in a N–S direction through the inner core of the Earth are slightly faster than those travelling in the equatorial plane, and these results have been interpreted in terms of an anisotropic inner core with cylindrical symmetry aligned with the Earth's axis of rotation. In this letter it is shown that this interpretation places an important constraint on the crystal structure of the inner core, and in particular is inconsistent with a cubic crystal structure (BCC or FCC). These results therefore provide further evidence for the stability of the HCP phase of iron under the Earth's core conditions.

Key words: Earth's core, iron, *P*-waves.

The solid inner core and liquid outer core of the Earth are composed mainly of iron (Stevenson 1981), with the hexagonal close-packed (HCP), face-centred cubic (FCC) and body-centred cubic (BCC) phases having been suggested as the phase of iron present in the inner core (Jephcoat & Olson 1987; Ross, Young & Grover 1990). Evidence for an anisotropic inner core comes from the traveltime residuals of the *PKIKP* phase obtained between 170° and 180° which show an axisymmetric pattern of degree 2 with an amplitude of about 2 s (Morelli, Dziewonski & Woodhouse 1986). Morelli *et al.* (1986) found that this could not be explained by a physically realistic radial distribution of (isotropic) heterogeneity and proposed that the inner core is anisotropic with cylindrical symmetry aligned with the Earth's axis of rotation. Similar conclusions were made by Shearer, Toy & Orcutt (1988). In support of this interpretation, Giardini, Li & Woodhouse (1987) have argued, from observations of splitting in free oscillation spectra of the Earth, that a cylindrically anisotropic inner core is the most natural explanation of the anomalously large splitting of modes penetrating deeply into the core. Jeanloz & Wenk (1988) have suggested convection in the inner core as a possible mechanism for producing anisotropy in the inner core.

If anisotropy is considered as a perturbation from the isotropic state, the *P*-wave velocity can be written in the form

$$v_P = v_{eq}(1 + \epsilon \cos^2 \chi + \sigma \cos^2 \chi \sin^2 \chi) \quad (1)$$

where v_{eq} is the velocity of *P*-waves travelling in the equatorial plane and χ is the angle between the propagation direction and the N–S axis (Morelli *et al.* 1986). ϵ and σ were assumed by Morelli *et al.* (1986) to taper off with depth as $(r/R_{IC})^2$ where R_{IC} is the radius of the inner core and r is the distance from the centre. With this assumption, the parameters ϵ and σ attain their maximum values at the top of the inner core where they are given by $\epsilon = 0.032$, $\sigma = -0.064$.

A possible cause of this anisotropy is the alignment of anisotropic crystallites within the core (Morelli *et al.* 1986). The orientation of a crystallite with respect to a set of reference axes $Ox_1x_2x_3$ may be described in general by three Euler angles ψ, θ and ϕ. The orientation distribution of crystallites may then be specified by the crystallite orientation distribution function $W(\xi, \psi, \phi)$ where $\xi = \cos\theta$ (Roe 1965). $W(\xi, \psi, \phi)\, d\xi\, d\psi\, d\phi$ gives the fraction of crystallites between ξ and $\xi + d\xi$, ψ and $\psi + d\psi$ and ϕ and $\phi + d\phi$. The measured velocity anisotropy can be used to obtain the coefficients W_{lmn} of a series expansion of the crystallite orientation distribution function in generalized Legendre functions. Assuming that the crystal structure of iron in the inner core is HCP, this is consistent with an alignment of *c*-axes along the Earth's axis of rotation (Sayers 1989). The purpose of this letter is to examine if the observed anisotropy of the inner core could be consistent with a cubic crystal structure. It is assumed following Morelli *et al.* (1986) and Shearer *et al.* (1988) that the inner core is cylindrically anisotropic with symmetry axis aligned along the Earth's axis of rotation. A set of reference axes $Ox_1x_2x_3$ fixed in the core is chosen with Ox_3 aligned N–S and Ox_1 and Ox_2 lying in the equatorial plane. For axial symmetry, the three elastic wave velocities for propagation at an angle χ to the symmetry axis have been given by

Musgrave (1970). The P-wave velocity is given by

$$\rho v_P^2 = C_{44} + \{h\cos^2\chi + a\sin^2\chi + [(h\cos^2\chi + a\sin^2\chi)^2 - 4(ah - d^2)\cos^2\chi\sin^2\chi]^{1/2}\}/2. \quad (2)$$

Here $a = C_{11} - C_{44}$, $d = C_{13} + C_{44}$ and $h = C_{33} - C_{44}$. C_{ij} is the elastic stiffness tensor of the inner core in the Voigt (two-index) notation with non-zero components $C_{11} = C_{22}$, C_{33}, C_{12}, $C_{13} = C_{23}$, $C_{44} = C_{55}$ and $C_{66} = (C_{11} - C_{12})/2$ for the assumed axial symmetry with symmetry axis along Ox_3. It is convenient to write the fourth-order elastic stiffness tensor of the inner core in the form

$$C_{ijkl} = C^0_{ijkl} + \Delta_{ijkl}$$

where Δ_{ijkl} is the difference between C_{ijkl} and the elastic stiffness tensor C^0_{ijkl} the inner core would have if the crystallites had no preferential orientation. C^0_{ijkl} is given by

$$C^0_{ijkl} = \lambda\,\delta_{ij}\,\delta_{kl} + \mu(\delta_{ik}\,\delta_{jl} + \delta_{il}\,\delta_{jk})$$

where δ_{ij} is the Kronecker delta and λ and μ are the second-order elastic constants in the absence of crystallite alignment. For cubic crystals λ and μ are given in the Voigt approximation by

$$\lambda = (c_{11} + 4c_{12} - 2c_{44})/5,$$
$$\mu = (c_{11} - c_{12} + 3c_{44})/5.$$

For small anisotropy, equation (2) reduces to

$$[v_P(\chi) - v_P(0)]/v_P(0) = [4(\Delta_{11} - \Delta_{33})(1 - \cos 2\chi) - (\Delta_{11} + \Delta_{33} - 2\Delta_{13} - 4\Delta_{44}) \times (1 - \cos 4\chi)]/16(\lambda + 2\mu), \quad (3)$$

where $\rho v_P^2(0) = \lambda + 2\mu + \Delta_{33}$. The elastic constants C_{ij} of an axially symmetric aggregate of cubic crystallites can be written in terms of the single crystal elastic constants c_{ij} and the coefficients W_{lmn}. For axial material symmetry and cubic crystallites, the non-zero W_{lmn} are all real and are restricted to $m = n = 0$ and even values of l. The combinations of the Δ_{ij} giving the angular dependence of the P-wave velocity are

$$\Delta_{11} - \Delta_{33} = -4\sqrt{2}\,\pi^2 c W_{400}/7,$$
$$\Delta_{11} + \Delta_{33} - 2\Delta_{13} - 4\Delta_{44} = 4\sqrt{2}\,\pi^2 c W_{400},$$

where the single crystal anisotropy factor c for cubic crystals is given by

$$c = c_{11} - c_{12} - 2c_{44}.$$

It is seen that the coefficients of the $\cos 2\chi$ and $\cos 4\chi$ terms in equation (3) are not independent, the assumption of a cubic crystal structure giving

$$v_P(\chi) = A + B\cos 2\chi + C\cos 4\chi$$

with $C/B = 7/4$. Comparing with equation (1), $A = v_{eq}(1 + \epsilon/2 - \sigma/8)$, $B = v_{eq}\epsilon/2$ and $C = -v_{eq}\sigma/8$ (Shearer *et al.* 1988) and therefore $C/B = -\sigma/4\epsilon = 0.5$ for the values $\epsilon = 0.032$, $\sigma = -0.064$ given by Morelli *et al.* (1986). Shearer *et al.* (1988) found a better fit could be obtained by assuming uniform anisotropy throughout the inner core, rather than an assumption that ϵ and σ vary as $(r/R_{IC})^2$. With this assumption $B = 0.054\ \mathrm{km\,s^{-1}}$, $C = 0.024\ \mathrm{km\,s^{-1}}$ and hence $C/B = 0.44$. The values of C/B obtained by Morelli *et al.* and Shearer *et al.* are therefore inconsistent with an assumption of cubic crystallographic structure for iron under the conditions obtained in the inner core. These results therefore add further support to the conclusion that under the conditions of the inner core, iron takes the HCP form (Anderson 1986).

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