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MAGNETIC SUSCEPTIBILITY OF HCP IRON AND SEISMIC ANISOTROPY OF THE EARTH'S CORE

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The seismic anisotropy of the Earth was proposed to be due to a preferred orientation of HCP iron crystals that constitutes the dominating element in the core. The suggested mechanism involves the anisotropy of the magnetic susceptibility χ of HCP iron, and it is argued that if χ is sufficiently anisotropic, a preferential orientation of the HCP crystals may occur. We have calculated ab initio χ and the anisotropy energy of HCP iron for pressures and temperatures corresponding to the Earth's inner core conditions. Our calculations demonstrate that χ is smaller when the field is along the c-axis of HCP iron. Hence, a toroidal magnetic field is shown to orient HCP Fe with c-axis along the north–south direction, and combined with the data on elastic constants this explains the seismic anisotropy.

It has been suggested [1], as an alternative to contending mechanisms of seismic anisotropy in the Earth's core [2–4], that this anisotropy results from the preferred orientation in an aggregate of magnetically anisotropic iron crystals. Such a mechanism assumes that magnetic field, generated in the outer core, aligns iron crystals in the inner core, provided the crystals possess HCP structure and an anisotropic magnetic susceptibility, χ. Although there is little doubt that the inner core consists of HCP Fe, the validity of the proposed mechanism is much dependent on the unknown anisotropy of χ in HCP Fe. Also, the assumed anisotropy of χ may have a pronounced effect on geometry of the geomagnetic field (called the far sided effect [5,6]) and the dynamics of the core.

Ab initio calculations [2,7–10] and experimental studies [11,12] have confirmed the stability of the HCP ground state of iron at high pressures. The calculations, however, have not provided a value of χ and its anisotropy for the inner core. The experimental study of magnetic properties of iron, compressed in a diamond anvil cell up to 17 GPa at temperatures about 260°C (i.e. far below the Earth's core conditions), suggests [13] that HCP Fe is paramagnetic with χ ranging from 0.15 to 0.001 (in SI units), but little information may be drawn from this study whether or not the magnetic explanation for the seismic anisotropy is correct. First principles calculations have shown a reliability in calculating the susceptibility of metals [14,15] and an avenue to verify the magnetic model is to study χ of HCP Fe theoretically at the Earth's core conditions, which is the purpose of the present investigation.

Our calculations are performed using a full-potential linear muffin-tin orbital method (FPLMTO) [16] within the local spin density approximation. The details of the method are given elsewhere [9,15,16], and here we touch upon only the principal features of the present implementation. Only HCP structure and volume are input parameters to the calculations, and the corresponding pressures are taken from molecular dynamic simulations [10]. All relativistic effects, including spin-orbit coupling, were included in the calculations. Under the Earth's core pressure the conduction electrons are pushed closer to the nuclei with a consequent increase of the kinetic energy. Therefore, the relativistic effects can be of considerable significance even for «light» elements, like Fe. The effect of an external magnetic field, $\mathbf{B}$, was taken into account self-consistently by means of the Zeeman operator, $\mathbf{B}(2\mathbf{s} + \mathbf{l})$ ($\mathbf{s}$ is the spin operator and $\mathbf{l}$ the orbital angular momentum operator), which has been incorporated in the Hamiltonian for calculations of field-induced spin and orbital magnetic moments [14,15]. The integration over the Brillouin zone was performed using the special points sampling and with Fermi-Dirac distribution corresponding to a number of temperatures up to the estimated Earth's inner core temperature of 6000 K. The basis set included the $3s$ and $3p$ orbitals as well as the $4s$, $4p$, and $3d$ orbitals within a single, fully hybridizing, energy panel. The calculated total energies and magnetic moments were well converged with respect to all parameters involved, such as k-space sampling and basis set truncation. The components of magnetic susceptibility, $\chi_{\|}$ and $\chi_{\perp}$, were derived from the magnetic moments obtained in an external field of 10 T, applied parallel and perpendicular to the [0001] direction, respectively. By this way the corresponding volume magnetization can be evaluated, and the ratio between the magnetization and the field strength is the paramagnetic susceptibility. In the relevant range of magnetic fields, the calculated χ appeared to be field independent. The diamagnetic contributions coming from core and conduction electrons are usually assumed to be negligible for transition metals, in comparison to the large paramagnetic contribution to χ. Although the diamagnetism of conduction electrons could contribute to the total anisotropy at low temperatures, this contribution was found to decrease rapidly at elevated temperatures [17,18].

In order to verify the accuracy of our method, we compared experimental and theoretical χ of transition metals that form in the HCP crystal structure at ambient conditions. The experimental anisotropy [17], $\Delta\chi = \chi_{\|} - \chi_{\perp}$, is reproduced for all studied elements, namely, the calculated $\Delta\chi$ is positive in Ti, Zr, and Hf (group IVA), but $\Delta\chi$ is negative in Ru and Os (group VIIIA). As is seen in Table 1, the absolute values of $\Delta\chi$ are also in agreement with experiment, with allowance made for the observed [17] strong temperature dependence of $\Delta\chi$.

The results of our calculations show that Fe does not spontaneously order magnetically at conditions of the Earth's core, and a small magnetic moment develops only in the presence of a magnetic field. The field-induced moments were calcu

Table 1

Anisotropy of the magnetic susceptibility, $\Delta\chi = \chi_{\|} - \chi_{\perp}$, of HCP transition metals (in SI volume units)*

Metal	$\Delta\chi\cdot10^6$	
	theory	experiment [17]
Ti	4.8	6
Zr	5.5	10
Hf	5.2	9
Fe	–5.2	–
Ru	–4.6	–5
Os	–3.4	–4

*The experimental data and our calculations for Ti, Zr, Hf, Ru, and Os correspond to ambient pressure and T = 1000 K. The calculated anisotropy of HCP Fe, corresponds to the Earth′s inner core conditions (P = 350 GPa, T = 6000 K).

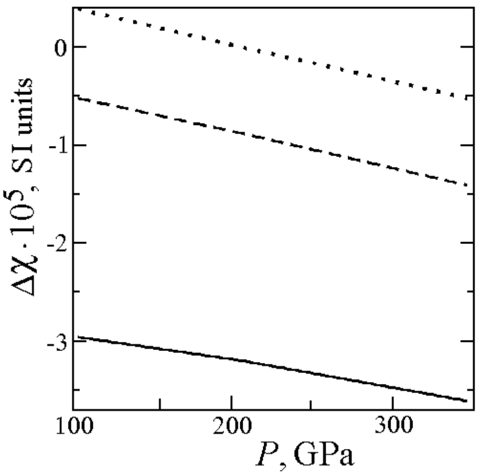

Fig. 1. Pressure dependence of the magnetic susceptibility anisotropy of HCP iron. The solid, dashed, and dotted lines correspond to the temperatures 0, 3000, and 6000 K, respectively

lated for a number of volumes, corresponding to pressures from 20 to 350 GPa where the HCP phase is stable [2,8,10], and the c/a axial ratio is taken equal to 1.59 [8,9]. The spin contribution to χ appeared to be somewhat less than the orbital contribution ($\chi_{\text{spin}} = 0.7\chi_{\text{orb}}$ at pressures about 300 GPa). The averaged value of the susceptibility of HCP Fe, $\langle\chi\rangle = (\chi_{\|} + 2\chi_{\perp})/3$, is found to be ranging from $3\cdot10^{-4}$ (P = 350 GPa) to $5\cdot10^{-4}$ SI units (P = 20 GPa), which is consistent with the experimental estimations of χ under lower pressures [13] (P = 17 GPa). As can be expected, the anisotropy of χ in HCP Fe comes from the orbital contribution. The calculated pressure and temperature dependence of $\Delta\chi$ of HCP Fe is presented in Fig. 1. As is clear from this figure, $\Delta\chi$ is less than 0 at pressures above 200 GPa, i.e. the susceptibility is the largest when the field is perpendicular to the c-axis. Thus, our calculations give $\Delta\chi$ that is of opposite sign to what Karato assumed [1]. The exact pressure at the Earth's core is somewhat uncertain, but as Fig. 1 shows, $\Delta\chi$ does not change sign and is not substantially modified at pressures higher than 200 GPa. Our results in Fig. 1 would seem to show that the model of a strong toroidal field is inapplicable for explaining the seismic anisotropy of the Earth's core. However, it was recently pointed out [4] that the anisotropy of the elastic constants is of opposite sign to what Karato assumed. Therefore, if the correct value of the anisotropy of χ is accounted for, then the c-axis of HCP iron would be parallel to the north–south direction, subject to the condition that the toroidal field is stronger than the poloidal field. It should be noted that the magnitude of $\Delta\chi$ is ten times smaller than what Karato assumed, and one may argue that the anisotropy is not sufficiently strong to orient the HCP iron grains. In order to critically evaluate this we quote the result of [1], based on energetic grounds, that the criterion for the magnetic effect to be operational is that the ratio β of magnetic anisotropy energy to thermal energy is larger than one, which can be expressed as [1,19]:

$$\beta = (1/2)\mu_0|\Delta\chi| VH^2/k_BT > 1, \quad (1)$$

where μ_0 is magnetic permeability of vacuum, V is the volume of iron grains, H is the strength of the magnetic field, k_B is the Boltzmann constant, and T is the temperature. In Fig. 2, we plot a phase diagram, with the diameter of iron in

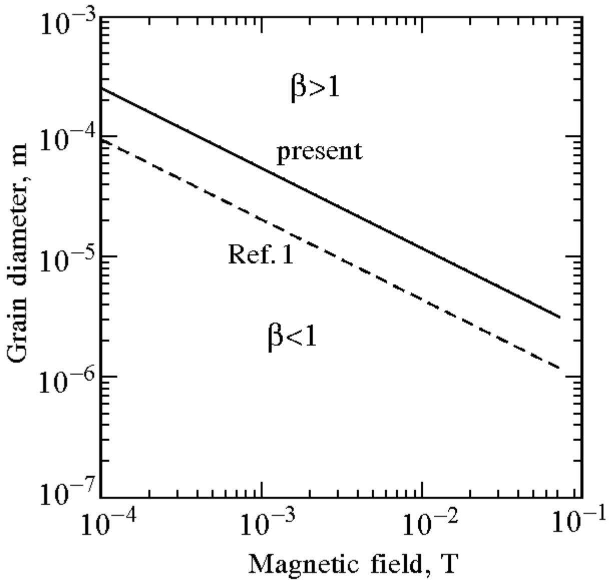

Fig. 2. Phase diagram for the ratio β between magnetic anisotropy energy and thermal energy as function of grain diameter and magnetic field. The solid line represents the $\beta = 1$ borderline evaluated in the present work, whereas the corresponding dashed line is taken from Ref. [1]

in the Earth's inner core and the magnetic field of the Earth's core as critical parameters. In the region where β is larger than one, the magnetically driven preferential orientation is expected. In Fig. 2, we also show the results of Karato. Note that although the presently calculated value of $\Delta\chi$ is smaller than the value assumed in [1], this gives little difference in the estimated grain size that is sufficient for the preferential orientation. The reason is that according to Eq. (1), for a chosen $\beta > 1$ the grain diameter is proportional to $\Delta\chi^{-1/3}$. In the region of relevant fields between 10^{-3} and 10^{-2} T, grains with a diameter larger than $5\cdot10^{-5}$ m have enough anisotropy energy to orient in the north–south direction. It has been suggested that the grains of the Earth's core have diameters substantially larger than this [1], and our analysis hence shows that, together with the recent data of anisotropy of the elastic constants in HCP iron, the present calculations of $\Delta\chi$ demonstrate that the magnetic anisotropy model can explain the seismological experiments.

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