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The viscosity of liquid iron at the physical conditions of the Earth's core

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It is thought that the Earth's outer core consists mainly of liquid iron and that the convection of this metallic liquid gives rise to the Earth's magnetic field. A full understanding of this convection is hampered, however, by uncertainty regarding the viscosity of the outer core. Viscosity estimates from various sources span no less than 12 orders of magnitude[1,2], and it seems unlikely that this uncertainty will be substantially reduced by experimental measurements in the near future. Here we present dynamical first-principles simulations of liquid iron which indicate that the viscosity of iron at core temperatures and pressures is at the low end of the range of previous estimates—roughly 10 times that of typical liquid metals at ambient pressure. This estimate supports the approximation commonly made in magnetohydrodynamic models that the outer core is an inviscid fluid[3–5] undergoing small-scale circulation and turbulent convection[6], rather than large-scale global circulation.

In first-principles calculations, the system of interest is represented as a collection of atomic nuclei and electrons, and the total energy and the forces on all the nuclei are obtained by solving Schrödinger's equation to determine the electronic ground state. The calculations are based on density functional theory[7], with the electronic exchange-correlation energy treated using either the local-density approximation or the more sophisticated generalized-gradient approximation. First-principles calculations on a large variety of materials, including transition metals, have been shown to give accurate predictions of both static and dynamic quantities (see, for example, ref. 8). There have already been extensive first-principles calculations on crystalline iron over the pressure range from zero up to Earth's-core values[9,10], and it has been shown that the generalized-gradient approximation reproduces the density of the hexagonal close-packed (h.c.p.) structure (the likely stable structure at high pressure[11]) over the whole high-pressure range within ~6%; at ambient pressure the volume is overestimated slightly more (by ~9%). The equilibrium density and magnetic properties of the body-centred cubic (b.c.c.) structure of iron at ambient pressure are also accurately described.

To study a liquid with these methods, we must perform first-principles molecular dynamics. Car and Parrinello first showed how to do this by integrating Newton's equation of motion for the nuclei, with the forces calculated from the first-principles ground state[12]. The first-principles molecular dynamics technique that they pioneered uses the pseudopotential approach, in which only the valence electrons are explicitly represented, with the orbitals expanded in a plane-wave basis. Techniques of this kind have been widely used for studying liquid metals (see, for example, refs 8, 13, 14), and their accuracy in predicting both structural and dynamic properties is well established.

Our first-principles molecular dynamics simulations are based on ultrasoft pseudopotentials[15] of the Vanderbilt type[16], which allow a significant reduction in the computational effort with no loss of accuracy (the accuracy of the pseudopotentials will be demonstrated below). Electronic exchange-correlation is treated using the generalized-gradient approximation of Perdew *et al.*[17]. In achieving good accuracy for high-pressure iron, the choice of orbitals to be treated as valence orbitals is crucial. At ambient pressure, reasonable accuracy can be obtained by treating all atomic states up to and including 3*p* as core states, but this is not satisfactory here because the 3*p* states respond significantly at high pressures. By contrast, inclusion of 3*s* states in the atomic core gives insignificant errors, provided that nonlinear core corrections[18] are included.

We have probed the accuracy of our pseudopotential calculations using a range of tests on solid iron, with 3*p* states and above included in the valence set. Our calculated values of the atomic volume and bulk modulus of the b.c.c. and h.c.p. phases of iron, and the magnetic moment of the b.c.c. phase at ambient pressure, are compared in Table 1 with experimental values[19,20] and all-electron calculations[9]. The close agreement with the all-electron results indicates that the errors incurred by the pseudopotential approximation are very small, and the agreement with experiment confirms the accuracy of the generalized-gradient approximation. We tested the reliability of our calculations at high pressures by comparing our calculated pressure as a function of volume for the h.c.p. phase against experimental measurements[11] and previous all-electron predictions[9,10]. We find that the discrepancy between our predicted pressures and the measured values is <3% over the range 50–300 GPa, which covers most of the pressure range of the outer core. We have also used calculations of enthalpy as a function of pressure for the b.c.c. and h.c.p. phases of iron to predict the transition pressure between the two structures; our calculated value of ~10 GPa agrees with experimental values[21] in the range 10–15 GPa and with the value of ~11 GPa given by all-electron linearized augmented planewave[9] and linearized muffin-tin orbital[10] calculations. Finally, we have compared our calculated zone-boundary phonon frequencies for the highly compressed f.c.c. phase with the all-electron results of Söderlind *et al.*[10]. The discrepancies of <3% for all frequencies confirm again the accuracy of our pseudopotential methods.

Our first-principles molecular dynamics simulations of molten iron use essentially the same approximations as our calculations on the solid phases, and we expect to achieve similar accuracy. (For present purposes, the 3*p* states are not included explicitly, but their effect is correctly reproduced by a pairwise additive potential.) We performed simulations at thermodynamic states corresponding roughly to the core–mantle boundary (CMB) and the boundary between the molten outer core and the solid inner core (ICB). The temperature T in the Earth's core is uncertain: estimates of T at the ICB range from 4,000 to 8,000 K and at the CMB from 3,000 to

Table 1 Calculated and experimental properties of iron

Phase property	All electron (ref. 9)	Pseudopotential (this work)	Expt (refs 19, 20)
b.c.c. V_0 (Å^3)	11.4	11.55	11.80
b.c.c. K (GPa)	189	176	162–176
b.c.c. μ (μ_B per atom)	2.17	2.25	2.12
h.c.p. V_0 (Å^3)	10.2	10.4	11.2
h.c.p. K (GPa)	291	290	208

Comparison of present pseudopotential calculations with all-electron calculations and experimental values for atomic volume V_0, bulk modulus K and magnetic moment μ of b.c.c. and h.c.p. iron.

4,500 K (ref. 22). The pressure in the core is accurately known (330 GPa at the ICB)[22]. Initially we assumed that the core lies on an adiabat whose temperature at the ICB pressure is 6,000 K. Using the data compiled by Anderson and Ahrens[23] for the equation of state of liquid iron, we then find that the density ρ at the ICB state is $1.33 \times 10^4\,\mathrm{kg\,m^{-3}}$, and that T and ρ at the CMB state are 4,300 K and $1.07 \times 10^4\,\mathrm{kg\,m^{-3}}$, respectively. In order to allow for the uncertainty in T, simulations at these two states were supplemented by a further simulation at the CMB value of ρ but at the lower temperature of 3,500 K. The simulations used a periodically repeated 64-atom system (for possible system-size effects, see below), and Brillouin-zone sampling was performed at the Γ-point only. All three simulation runs had a duration of $\sim$2 ps after equilibration. They showed good stability, with total energy drift corresponding to temperature changes of only a few tens of degrees per picosecond.

An important check on the realism of our simulations can be made by comparing the calculated pressure of the liquid with the Anderson and Ahrens data[23]. As shown by the results in Table 2, the calculated and experimental pressures differ by $<$10% for the ICB state and even less for the CMB state. Our simulations show that the structure of high-pressure molten iron, as described by the radial distribution function $g(r)$, is close packed, with a coordination number of slightly over 12. (Detailed $g(r)$ results will be reported elsewhere[24].) This means that the liquid structure closely resembles that of the h.c.p. crystal.

We obtain an estimate for the shear viscosity η of molten iron from our simulations by using its connection with the self-diffusion coefficient D. (The direct calculation of η from first-principles simulations is theoretically possible, but has not yet been achieved for any liquid, because of the very long simulations needed to obtain useful statistical accuracy.) We calculate D via the Einstein relation:

$$\langle \Delta r(t)^2 \rangle \rightarrow B + 6Dt \qquad (1)$$

where B is a constant. Equation (1) tells us that the mean square distance $\langle \Delta r(t)^2 \rangle$ travelled by any atom in time t becomes linear in t at long times. In all our simulations, we find that $\langle \Delta r(t)^2 \rangle$ settles down to a linear dependence on t in $<$0.5 ps, so that values for D are straightforward to extract. Our values of D at the CMB and ICB states (Table 2) are of the same order as the diffusion coefficients of typical liquid metals at ambient pressure[25].

We now obtain the viscosity via the Stokes–Einstein equation:

$$D\eta = k_B T/2\pi a \qquad (2)$$

This equation from the theory of brownian motion gives an exact relation between the diffusion coefficient D of a brownian particle of diameter a and the viscosity η of the surrounding liquid (k_B is the Boltzmann constant). It is often applied also to the diffusion of atoms in liquids, in which case the relation is only approximate. However, its empirical accuracy when applied to the diffusion of atoms is very good. If a is taken to be the nearest-neighbour distance in the solid, then predictions of η using measured values of D agree with experimental data to within 40% for a wide range of liquid metals. Simulation studies on the hard-sphere liquid[26] demonstrate that the accuracy of the Stokes–Einstein relation remains very good even at high pressures where the free volume becomes small. Taking a from our calculated pressure–volume relation for the h.c.p. solid, we obtain the η values for molten iron under Earth's-core conditions reported in Table 2. Our calculated viscosities are roughly ten times those of typical liquid metals at ambient pressure.

In assessing the reliability of our calculations, we note first that our simulations were necessarily done on a rather small system. System size errors in calculated transport coefficients have been exhaustively studied for simple systems such as the Lennard–Jones and hard-sphere liquids. (These are highly relevant, because the present simulations demonstrate that high-pressure liquid iron closely resembles these liquids.) In such systems, the calculated D depends only weakly on the system size, and the simulation data of ref. 27 indicate that D calculated with 64 atoms will underestimate the true value by $\sim$20%. This means that our η values obtained from the Stokes–Einstein relation are probably too high by $\sim$20%. We have already noted that the Stokes–Einstein relation itself should be good to 40% or better, so the technical error in our η values should be no worse than 60%. Turning now to uncertainties about the temperature T in the core, we note from Table 2 that the CMB value of η increases by $\sim$25% as T goes from 4,300 to 3,500 K. Assuming an Arrhenius temperature dependence, this means that if T at the CMB were as low as 3,000 K, η would be 1.8×10^{-2} Pa s. Taking all these uncertainties together, we believe that the overall error is unlikely to be worse than a factor of three.

We also note that the Earth's core does not consist of pure iron, but contains light impurities (carbon, oxygen, silicon or sulphur) at a total concentration of up to 10%. The effect of these impurities on the viscosity under Earth's-core conditions is not known, but they seem very unlikely to affect it substantially, given their low concentration. (The influence of dissolved sulphur on the viscosity of liquid iron at much higher concentrations has been studied in ref. 28.)

Our overall conclusion is that the shear viscosity of liquid iron in the Earth's core is $\sim 1.5 \times 10^{-2}$ Pa s, with an uncertainty of a factor of three. This is at the low end of the range of previous estimates, though it is similar to values suggested by some earlier work (see, for example, ref. 1). It is very much lower than apparent viscosity values deduced from geodetic and seismic measurements, but it is recognized that because of their timescale the latter may be influenced by dissipative processed other than shear viscosity[2,29]. A low viscosity has important implications for the geodynamic description of the outer core. The nonlinear equations of magnetohydrodynamics cannot be solved exactly, and simplified linear approximations are often used. Depending on these approximations, contributions to the forces acting on the fluid in the outer core, such as Coriolis, Lorentz and viscous, may be treated as small or negligible. The relative importance of the viscous and Coriolis forces is characterized by the Ekman number given by $\mathrm{Ek} = \eta/(\rho\Omega L^2)$, where ρ is the fluid density, Ω is the Earth's rotational velocity, and L is the fluid thickness. With $\eta = 0.015$ Pa s, $\rho = 1.06 \times 10^4\,\mathrm{kg\,m^{-3}}$, $\Omega = 7.3 \times 10^5\,\mathrm{rad\,s^{-1}}$ and $L = 2{,}000$ km, this gives $\mathrm{Ek} = 4 \times 10^{-15}$, indicating that viscous forces are indeed negligible when compared with the Coriolis force. This supports models based on the assumption that the viscosity of the core is negligible[3–5], and favours a picture in which the core is in a state of small-circulation turbulent convection, in contrast to models having a viscosity of $\sim 10^7$ Pa s which imply a coherent pattern on a much larger scale, comparable with the core radius[6,30]. □

Table 2 Calculated and experimental properties of iron at Earth's-core conditions

	T (K)	ρ ($10^4\,\mathrm{kg\,m^{-3}}$)	p_{exp} (GPa)	p_{calc} (GPa)	D ($10^{-8}\,\mathrm{m^2\,s^{-1}}$)	η (10^{-2} Pa s)
ICB	6,000	1.33	330	358	0.5	1.3
CMB	4,300	1.07	135	132	0.4	1.2
CMB	3,500	1.07		125	0.3	1.5

Shown are the calculated and experimental pressures p_{calc} and p_{exp}, and calculated diffusion coefficient D and viscosity η of molten iron at thermodynamic states corresponding to the inner-core boundary (ICB) and the core–mantle boundary (CMB). Values of temperature T and density ρ are explained in the text.

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Reproductive cessation in female mammals

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In female mammals, fertility declines abruptly at an advanced age. The human menopause is one example, but reproductive cessation has also been documented in non-human primates, rodents, whales, dogs, rabbits, elephants and domestic livestock[1–3]. The human menopause has been considered an evolutionary adaptation[4–7], assuming that elderly women avoid the increasing complications of continued childbirth to better nurture their current children and grandchildren. But an abrupt reproductive decline might be only a non-adaptive by-product of life-history patterns. Because so many individuals die from starvation, disease and predation, detrimental genetic traits can persist (or even be favoured) as long as their deleterious effects are delayed until an advanced age is reached, and, for a given pattern of mortality, there should be an age by which selection would be too weak to prevent the onset of reproductive senescence[4,5,8]. We provide a systematic test of these alternatives using field data from two species in which grandmothers frequently engage in kin-directed behaviour. Both species show abrupt age-specific changes in reproductive performance that are characteristic of menopause. But elderly females do not suffer increased mortality costs of reproduction, nor do post-reproductive females enhance the fitness of grandchildren or older children. Instead, reproductive cessation appears to result from senescence.

Age-specific rates of mortality and maternity are broadly similar in olive baboons and African lions (Fig. 1). In baboons, female mortality reaches a minimum between 4 and 5 years of age and then accelerates; no female has survived beyond 27 years of age (Fig. 1a). But the maternity rate remains constant until 21 years of age, when it decreases (Fig. 1c). In female lions, mortality reaches a minimum between 3 and 4 years and then rapidly accelerates; no lioness has survived beyond 17 years of age (Fig. 1b). Lion maternity rates remain relatively constant before decreasing at 14 years of age (Fig. 1d).

Infant survival declines rapidly when female baboons reach 21 years (Fig. 2a), which is the age at which pregnancies are more likely to end in miscarriage (Fig. 2b). Baboons also show striking changes in menstrual cycles with advancing age. The length of the cycle remains constant until about 23 years of age (Fig. 3a), when cycles also become more irregular (Fig. 3b). Fertility decreases at 23 years of age and essentially ceases at 24 (Fig. 3c). Because of low fertility, elderly females experience a peak number of cycles during their 24th year (comparable to the period of 'adolescent sterility'), but cycling diminishes thereafter until ceasing altogether (Fig. 3d). Constant cycling is known to lower the age of menopause in women[9], and one female baboon stopped cycling at 20 years and remained acyclic until her death aged 26. She had shown unusually low fertility throughout life and experienced 127 menstrual cycles by her 20th birthday, whereas all other 20-year-old females averaged only 50 cycles (range 35–98, $n = 23$).

Less detailed data are available on the precise reproductive performance of ageing female lions (see Methods). The survival of lion cubs remains constant with maternal age (Fig. 2c), but litter size declines markedly at 14 years (Fig. 2d). Falling litter size cannot account for the overall decline in maternity rates between prime- and old-aged females (Fig. 1d), so elderly lions must also experience a reduction in cycling and/or fertility.

Are these declines adaptive? Baboons and lions are good candidates for an 'adaptive menopause' because both species engage in a high degree of kin-directed cooperative behaviour. Typical of cercopithecine monkeys, baboon mothers help to determine their daughters' dominance rank, and they also groom and intervene on behalf of their descendent kin[10]. Female lions participate in joint territorial defence[11–13] and, when raising cubs communally, nurse their daughters' cubs as often as their own[14].

The adaptive menopause hypotheses assume that post-reproductive females actively enhance the fitness of their prior offspring[4–6]. This benefit would be lost by her death in the 'risky childbirth' hypothesis[4] or by the intensive demands of infant care in the 'opportunity costs' hypothesis[7]. However, neither the survival of grandchildren nor the reproductive performance of adult daughters is improved in the predicted manner (Fig. 4). Lion cubs only show higher survival when their grandmothers are reproductively active: elderly female lions only engage in allomothering while tending their own cubs[14]. The typical interbirth interval is two years in both species and, whereas infant survival is highly dependent on maternal survival (Fig. 5), juvenile survival is unaffected by either the mother's survival or her subsequent reproduction (Fig. 5). Thus mothers do not invest in subsequent offspring until their prior brood has been successfully 'fledged' and continued reproduction inflicts no opportunity costs.

In both species, breeding females showed similar survival to non-