ORIGINAL PAPER

Y. Zhang · G. Guo · G. Nie

A molecular dynamics study of bulk and shear viscosity of liquid iron using embedded-atom potential

Abstract Molecular dynamics simulations employing a many-body embedding potential model have been conducted to calculate both bulk and shear viscosity of pure liquid iron at the Earth's outer core conditions. Liquid iron shear viscosity thus obtained is in the order of 10^{-2} Pa · s and is in close agreement with previous estimates. In contrast, liquid iron bulk viscosity is in the order of 10^{-3} to 10^{-4} Pa · s and is much smaller than previous estimates. Consequently, the ratio of bulk to shear viscosity is close to 0.1. This value disagrees with both the common speculation that bulk and shear viscosities are equal at ambient pressure, and the previous inference that bulk viscosity of liquid iron is much larger than shear viscosity at outer core conditions. Potential implications of present data are also briefly given for the dynamic state of the outer core.

Introduction

The Earth's outer core is believed to be in liquid state and to consist principally of iron with some light alloying elements. Its bulk and shear viscosity properties are two key parameters in our establishment of geodynamo models (e.g. Glatzmaier and Roberts 1995; Kuang and Bloxham 1997), and in the interpretation of geodetic and seismological data, such as those from studies of the damping of whole Earth torsional and radial mode oscillations (Anderson 1980). Principally, determination of bulk and shear viscosity of pure liquid iron at outer core

Y. Zhang (✉) · G. Guo
Institute of Geology and Geophysics,
Chinese Academy of Sciences,
PO Box 9825, Beijing 100029, China
e-mail: zhangyg@igcas.igcas.ac.cn

G. Nie
Institute of Geology,
Chinese Seismology Bureau,
Beijing 100029, China

conditions will help us to infer the dynamic state of the outer core if influences from alloying elements are negligible or known.

At present, shear viscosity of liquid iron at outer core conditions has been studied extensively using different liquid metal theories and many data have been accumulated (see Table 4 of Secco 1995 for summary and references), giving shear viscosity in the order of 10^{-3} to 10 Pa · s. More recently, De Wijs et al. (1998) gave liquid iron shear viscosity of $1.2 \sim 1.5 \times 10^{-2}$ Pa · s at the outer core conditions, and Stixrude et al. (1998) obtained a value of $5 (\pm 3) \times 10^{-3}$ Pa · s for that at the bottom of the outer core. Both studies use first-principles molecular dynamics and Sutherland-Einstein equation. (Here, the use of the name Sutherland-Einstein is according to Iida and Guthrie 1988, where they used the name Stokes-Einstein to denote the equation $D = K_B T/6\pi\mu r$ and Sutherland-Einstein to represent $D = K_B T/4\pi\mu r$. In these two formulae, D denotes the self-diffusion coefficient, μ the shear viscosity, K_B the Boltzmann constant, r the radius of the diffusing particle, and T the temperature. The former equation is often used in studies of magmatic melts. For our case and those of De Wijs et al. (1998) and Stixrude et al. (1998), the latter equation is more appropriate as it concerns with diffusion of particle of size equal to those of the medium. To distinguish the two equations, the name Sutherland-Einstein was used throughout present study.)

In contrast to the studies of shear viscosity, relatively little attention has been given to the studies of bulk viscosity. The bulk viscosity of liquid iron has not been measured experimentally due to the very high quality factor, Q, of liquid iron and is assumed frequently to be similar to its shear viscosity value at ambient pressure (e.g. Nasch and Manghnani 1994). Anderson (1980) inferred that bulk viscosity of liquid iron at outer core conditions is about $10 \sim 1000$ Pa · s based on the two-state theory and consideration of temperature and pressure effect on bulk modulus and relaxation time.

In the present study, we conducted molecular dynamics simulations to calculate both bulk and shear

viscosity of pure liquid iron. In the next section, we first present the two methods used for the calculation of liquid iron viscosity and then the potential model employed for molecular dynamics simulations. In the third section, we first demonstrate the applicability of the Sutton-Chen type of many-body embedding potential in the description of liquid iron properties, then show that both Sutherland-Einstein and Green-Kubo equations are applicable to the study of viscosity of liquid iron, and finally present and compare our results with previous investigations and discuss briefly potential implications of our data. To our knowledge, this is the first time that the bulk viscosity of liquid iron is obtained at outer core conditions using molecular dynamics.

Method

There are two methods available, when using molecular dynamics, to obtain shear viscosity (hereafter as η_s) of a liquid. The first is an indirect method. It consists of using the Einstein relation, $\langle[r(t)-r(0)]^2\rangle = 6\ Dt$, to obtain the self-diffusion coefficient D at first, and then using Sutherland-Einstein equation of the form, $\eta_s = K_B T/2\pi Da$, to obtain finally η_s. In the former formula, $r(t)$ and $r(0)$ are the atomic positions at time t and zero, and $\langle[r(t)-r(0)]^2\rangle$ is the so-called mean square displacement. In the latter formula, K_B is the Boltzmann constant, a is called size parameter of the diffusing atom and was taken in present study as the first-neighbor distance (the position of the first peak in the pair correlation function).

The second method for obtaining η_s is the direct application of the Green-Kubo equation:

$$\eta_s = \frac{V}{K_B T}\int_0^\infty \mathrm{d}t\langle P_{\alpha\beta}(t)P_{\alpha\beta}(0)\rangle$$

where V is the volume of the simulation cell, $P_{\alpha\beta}$ is the off-diagonal ($\alpha \neq \beta$) element of the stress tensor with α and β as Cartesian components representing the x-, y- or z-axis. The procedure consists mainly of the integration of shear stress auto-correlation function (hereafter as SSACF) in the angular brackets.

Calculation of bulk viscosity (hereafter as η_v) is similar, the only need is to replace in the above formula $\langle P_{\alpha\beta}(t)P_{\alpha\beta}(0)\rangle$ by $\langle \delta P(t)\delta P(0)\rangle$, where $\delta P(t) = P(t)-\langle P(t)\rangle$ with $P(t)$ as the instantaneous pressure of the simulated system at time t and $\langle P(t)\rangle$ as the average pressure for the whole simulation period (Allen and Tildesley 1987).

The most essential assumption in a molecular dynamics study is that the employed potential model can represent the real interactions between atoms. In present study, we used the Sutton-Chen type of potential, in the following form (Sutton and Chen 1990):

$$E = \varepsilon\left[\frac{1}{2}\sum_i\sum_{i\neq j}\left(\frac{a}{r_{ij}}\right)^n - c\sum_i\sqrt{\rho_i}\right]$$

The first term on the right hand side is the pairwise interatomic potential and the second term is the many-body embedding potential for consideration of the bonding by de-localized electrons in metals with ρ_i defined as:

$$\rho_i = \sum_{j\neq i}\left(\frac{a}{r_{ij}}\right)^m$$

where r_{ij} is the distance between atom i and j. The parameters ε, a, c, n, m were obtained from fitting experimental data on hexagonal close packed (hcp) and face centered cubic (fcc) irons (Mao et al. 1990; Andrault et al. 1997; Jephcoat et al. 1986; Zarestky and Stassis 1987; Singh et al. 1998). The best set of parameters we obtained are as follows: $\varepsilon = 0.052899$ eV, $a = 3.0$ Å, $c = 11.906667$, $n = 9.0$, $m = 6.0$ with a cutoff distance of 9.5 Å.

Compared with first-principles molecular dynamics, the use of empirical potential in the simulation is more efficient in terms of computer time and thus allows longer simulation time and systems with relatively larger number of particles to be studied. These are important because calculation of viscosity using the Green-Kubo formulation requires very long simulation time to achieve better statistics, and potentially influencing factors, such as system size effect need to be eliminated. Due to the relatively slow speed, these are difficult to be performed using first-principles molecular dynamics. For this reason, only the indirect method applying the Sutherland-Einstein equation has been used in first-principles molecular dynamics with relatively small particle numbers in the simulated system (e.g. De Wijs et al. 1998 used 64 atoms in their system). To consider the system size effect in our case, a series of trial experiments using 256, 512, and 1024 particles in the simulated system were done and showed that particle number greater than 512 is enough for obtaining consistent results for both self-diffusivity and viscosity. All our simulations were done with 1024 iron atoms. Other simulation conditions were as follows: all simulations were done in microcanonical ensemble, i.e. particle number, volume, and total energy of the simulated system are kept constant during simulation. Cubic periodic boundary conditions were applied to the simulation cells. Each time step lasted 0.5 fs (femtosecond), total simulation time was equal to 50 ps (picosecond) with the first 2.5 ps for scaling temperature to the desired value and the second 2.5 ps for equilibration. Stress data accumulated for the subsequent 45 ps were used for the calculation and integration of correlation functions. The positions of center of mass of Fe atoms from the last 10 ps were collected for mean square displacement calculations.

Results and discussion

We first tested the reliability of our potential. For that purpose, we compared pressure-temperature-volume properties of liquid iron predicted using our potential at the Earth's outer core conditions with previous estimates. At inner core boundary (ICB), the PREM model (Dziewonski and Anderson, 1981), Belonoshko and Ahuja (1997) and Anderson and Ahrens (1994) gave a density of 12.17, 12.49, and 13.31 g/cm^3, respectively. Our potential model gave a density of 12.51 g/cm^3 if the temperature at ICB is assumed to be 6000 K, which is very close to previous investigations. Comparison at core mantle boundary (CMB) is similar. We gave a density of 10.37 g/cm^3 at 4000 K, comparable with previous works which are 9.9 (Dziewonski and Anderson 1981), and 10.46 (Belonoshko and Ahuja 1997), and 10.86 (Anderson and Ahrens 1994) g/cm^3. Our potential model also gave a prediction of isentropic bulk modulus similar to the PREM model (Fig. 1).

It is well known that Sutton-Chen or similar types of potential model are very capable in the description of fcc type solid metals, but encounter difficulty in the description of hcp type solid metals. To overcome the difficulty, different alternatives of the potential have been given, most of them are through adding an angular term into the potential model (Baskes and Johnson 1994), using more complicated mathematical forms (Ackland et al. 1995), or combining different potential

types (Belonoshko and Ahuja 1997). Figure 1, together with above density comparisons, demonstrates that the relatively simple form of Sutton-Chen potential is good enough for the description of liquid iron properties at very high temperatures and pressures.

Now we look at the applicability of the aforementioned two methods for the calculation of liquid iron viscosity. For the direct method, determination of the final viscosities (both η_s and η_v) depends decisively on the accuracy of correlation functions. It is a common experience in the practical application of Green-Kubo equation that relatively large errors exist in correlation functions even with very long simulation time (e.g. Allen and Tildesley 1987). Statistics cannot be improved significantly by extending further the total simulation time. The situation is further complicated by the possible existence of long time tails (Levesque et al. 1973) as we do not know its behavior very clearly. As for the indirect method, applicability of Sutherland-Einstein equation to the system under study depends on our ability to calculate the self-diffusion coefficient accurately at the temperature and pressure conditions of investigation and our choice of the size parameter.

We will show, in the following, that η_s calculated using both the direct and the indirect methods agree very closely, indicating that both methods are applicable to the study of liquid iron viscosity at very high temperatures and pressures.

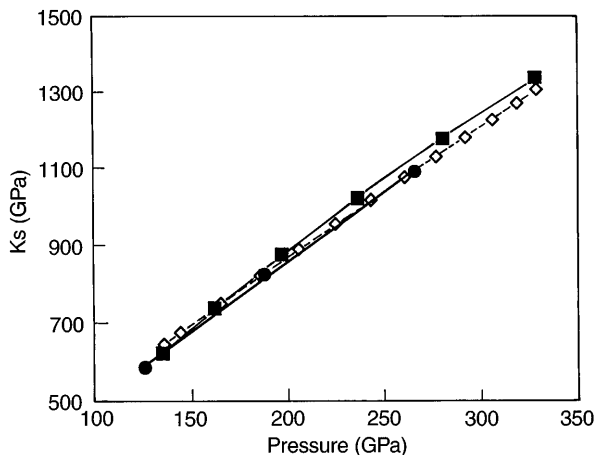For liquid iron, its SSACF reaches zero very quickly, typically in a time scale of 0.2 to 1.0 ps and then starts to fluctuate evenly along the horizontal axis (Fig. 2). If there exists any long time tail (Levesque et al. 1973), it must be much smaller than the fluctuations. Otherwise a trend in the fluctuations would be seen. So in the present study, instead of integrating the SSACF in the whole time span and thus including large errors and small long time tail if it does exist, we stopped the integration of SSACF when SSACF first reaches zero. This removes large errors and the small long time tail in the SSACF all together. It may be argued that the neglect of the long time tail in our treatment of SSACF would cause large error in the final result of viscosity, but the close agreement between data calculated using the Sutherland-Einstein and those using the Green-Kubo formulae (Fig. 3) demonstrates that this treatment is valid. The average absolute difference between viscosities using the two methods is 7% with the largest difference of 24%. This gives us also an idea about uncertainties of η_s data obtained in present study.

Figure 4 illustrates the typical shapes of time correlation functions $\langle \delta P(t) \delta P(0) \rangle$. They are different from those of SSACF in that they decrease rapidly at first, and then return back and decay slowly to a point where they start to fluctuate evenly along the horizontal axis. The second peak is large at higher density, but becomes smaller and tends to disappear as density decreases. Although it is the first time that the appearance of a second peak in time correlation function $\langle \delta P(t) \delta P(0) \rangle$ was observed, a similar phenomenon was observed in SSACF by Daivis and Evans (1995) in their study of shear viscosity of liquid butane, and in dynamical structure factor $S(k,\omega)$ expressed by the real part of the Fourier-Laplace transform of the longitudinal current correlation function (Levesque et al. 1973). As shown by Levesque et al. (1973), the second peak is enhanced at small wave vector, k and gradually disappears at high wave vector.

The locations of the point where $\langle \delta P(t) \delta P(0) \rangle$ starts to fluctuate evenly along the horizontal axis were typi-
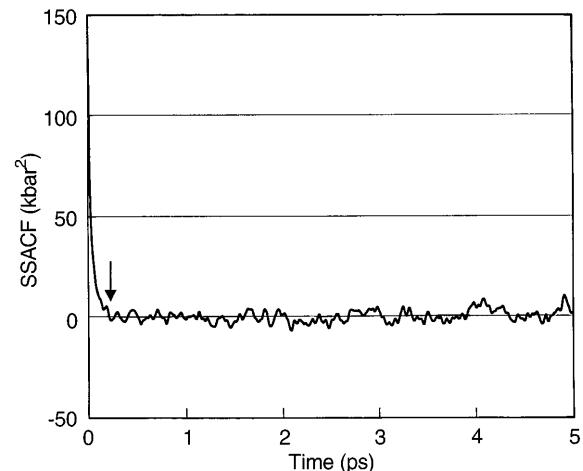

Fig. 1 Comparison of isentropic bulk modulus of the present study with that of PREM (Dziewonski and Anderson 1981). For our calculation, $Ks = K_T(1 + \gamma \alpha T)$ was used. The Grüneisen parameter γ, thermal expansion α, and temperature profile in the outer core were according to Stacey (1992). The *dashed line with open diamonds* denotes the PREM model. *Thin line with solid squares* and *thick line with solid circles* were calculated using isothermal bulk modulus K_{6000} and K_{5000}, respectively. The coincidence of these two lines indicates dK_T/dT is close to zero. Our calculated Ks also show a very slight downward curvature, which results in a decrease of dKs/dP with pressure. These features are also similar to the PREM model. The largest difference of our prediction with PREM is 2.5%. The similarity of Ks of liquid iron with that of the outer core has also been shown by Anderson and Ahrens (1994)

Fig. 2 Shear stress auto-correlation function (SSACF) at 10.18 g/cm^3, 5041 K, and 135 GPa. The *arrow* marks the point where we stopped the integration of SSACF
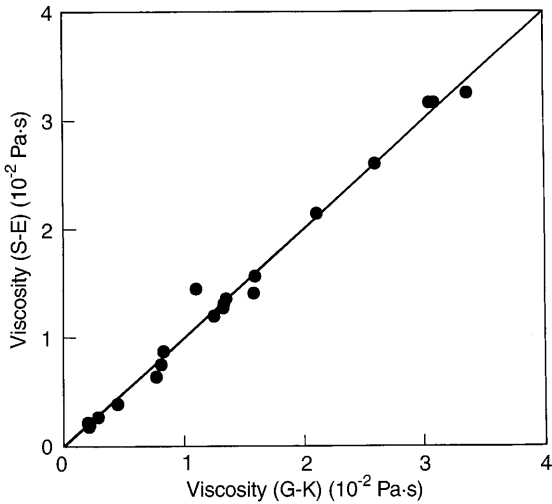
Fig. 3 Comparison of shear viscosity calculated using the Green-Kubo formula (*horizontal axis*) with that using the Sutherland-Einstein equation (*vertical axis*). The straight line has the slope of 1

cally at 0.2 to 1.0 ps, similar to those of our SSACF. We stopped integration of the time correlation function $\langle \delta P(t)\delta P(0)\rangle$ at that point, as we had similarly done for SSACF.
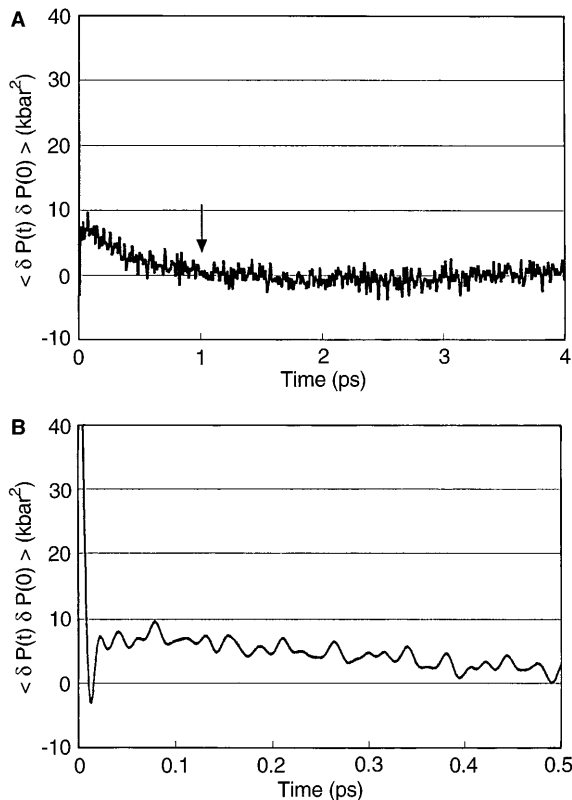

Fig. 4A, B Time correlation function $\langle \delta P(t)\delta P(0)\rangle$ at 12.51 g/cm^3, 5955 K, and 329 GPa. **B** is an enlarged view of **A** in the horizontal axis. The *arrow* in **A** marks the point where we stopped the integration of $\langle \delta P(t)\delta P(0)\rangle$

We are less certain about the possible errors involved in the calculated η_v as a comparative method similar to that for η_s is not available. Integrating the correlation functions with different time spans resulted in a η_v difference of 40% in the largest case. Uncertainties obtained by repeating simulation runs at exactly the same starting conditions were about 15%.

Some of our simulation results at conditions relevant to the Earth's outer core are listed in Table 1. As the estimation of thermal state in the outer core spans in a large range (Duffy and Hemley 1995), we conducted MD simulation at different temperature conditions for CMB and ICB. Differences of 34% for η_s and of 53% for η_v are created if the temperature at CMB is changed from 4000 K to 5000 K. These differences were calculated using viscosity data obtained from the Green-Kubo equation.

From Table 1 we can see, first of all, that η_s of liquid iron at Earth's outer core conditions are in the order of 10^{-2} Pa · s. These values are in very close agreement with earlier estimates using different liquid metals theories, such as Gans (1972) ($3.7 \times 10^{-3} \sim 1.85 \times 10^{-2}$ Pa · s), Poirier (1988) ($3 \times 10^{-3} \sim 6 \times 10^{-3}$ Pa · s), and Svendsen et al. (1989) ($9 \times 10^{-3} \sim 1.4 \times 10^{-2}$ Pa · s), and for more recent ones, with those using first-principles molecular dynamics simulations (De Wijs et al. 1998; Stixrude et al. 1998). In addition, the close agreement of shear viscosity between present study and that of De Wijs et al. (1998) employing ultrasoft pseudopotentials indicates that calculations of shear viscosity of liquid iron using molecular dynamics are independent of the details of employed potential models. However, our results are somewhat different from that of Anderson (1980), which gives a liquid iron shear viscosity of $1 \sim 10$ Pa · s at the Earth's outer core conditions.

Ekman's number, Ek $= \eta/(d\Omega L^2)$ is frequently invoked to characterize the relative importance of viscous and Coriolis forces in the outer core (e.g. Gans 1972; Poirier 1988; De Wijs et al. 1998). In the formula, η is the shear viscosity, d the fluid density, Ω the Earth's rotational angular velocity (7.3×10^{-5} rad · s^{-1}), and L the fluid thickness (2000 km). Putting our data into the formula, we obtained Ek $= 1.25 \times 10^{-2}$(Pa · s)/ $[10.37(\text{g} \cdot \text{m}^{-3}) \times 7.3 \times 10^{-5}(\text{rad} \cdot \text{s}^{-1}) \times (2000 \text{ km})^2] = 4 \times 10^{-15}$. Thus, our data support the general consensus that viscous force is negligible in magnetohydrodynamic modeling of the outer core and that the Earth's outer core is in its instability field undergoing small-scale circulation and turbulent convection instead of large-scale global circulation (Gans 1972; Poirier 1988; De Wijs et al. 1998).

In the case of bulk viscosity, liquid iron bulk viscosity at outer core conditions is in the order of 10^{-3} to 10^{-4} Pa · s from the present study. This is in large contrast with the previous estimate of 10–1000 Pa · s based on the two-state theory (Anderson 1980). Bulk viscosity of liquid iron is closely related to the damping of radial modes of the Earth's free oscillation, especially the

Table 1 Transport properties of liquid iron at the Earth's outer core conditions. (D self-diffusion coefficient, a the size parameter in the Sutherland-Einstein equation, η_s(S-E) shear viscosity calculated using the Sutherland-Einstein equation, η_s(G-K) shear viscosity calculated using the Green-Kubo equation, η_v bulk viscosity; † values after ± represent root mean square fluctuations during simulation)

Density (g/cm^3)	Temperature (K)	Pressure (GPa)	D (10^{-9} m^2/s)	a (Å)	η_s(S-E) (10^{-2} Pa · s)	η_s(G-K) (10^{-2} Pa · s)	η_v (10^{-2} Pa · s)
12.18	8016 ± 103†	329.5 ± 0.8	5.37	2.075	1.58	1.40	0.14
12.51	5955 ± 115	328.5 ± 0.9	1.87	2.075	3.37	3.25	0.32
10.37	3970 ± 74	135.2 ± 0.5	3.20	2.175	1.25	1.20	0.12
10.18	5041 ± 90	135.3 ± 0.6	6.15	2.175	0.83	0.87	0.057

fundamental mode, $_oS_o$ (Anderson 1980). Our bulk viscosity data imply a very high quality factor, Q for $_oS_o$ in the outer core if influence from alloying elements in the outer core is ignored. However, recent experimental study by Nasch et al. (1997) on the Fe-5%Ni-10%S system has shown that sulfur not only increases effectively the viscosity of the system, but also has a differential effect on the relative values of bulk and shear viscosity, making bulk viscosity the major component of the dynamic longitudinal viscosity. If this phenomenon persists to the outer core's temperature and pressure conditions, the quality factor, Q will be reduced accordingly through mechanisms, such as concentration fluctuations (Flinn et al. 1974; Anderson 1980; Nasch et al. 1997). At present we are conducting molecular dynamics simulations on the system Fe-Ni to account for the possible effects of the addition of nickel on the shear and especially on the bulk viscosity of liquid iron.

As for the relative values of bulk and shear viscosity, it is commonly assumed that at ambient pressure, bulk and shear viscosities are similar (Anderson 1980; Nasch and Manghnani 1994). Anderson (1980) gave a value of 10–100 for bulk to shear viscosity ratio, η_v/η_s at outer core conditions. Our data disagree with these earlier estimates. The average value of η_v/η_s obtained in the present study is 0.12 ± 0.07 using the whole set of our data, which is much smaller than previous estimates. Furthermore, we observed that η_v/η_s is relatively stable with temperature and pressure changes, indicating that temperature and pressure have similar effect on bulk and shear viscosity. As noted earlier, if the influence from alloying elements is considered, this ratio may possibly increase according to previous investigations (Flinn et al. 1974; Anderson 1980; Nasch et al. 1997).

As for the application of present results to the real Earth, it is generally recognized that large discrepancy exists between molecular viscosity calculated using different liquid metal theories and molecular dynamics simulations and other viscosity (modified or eddy) estimated from geophysical observations, including the most recent one by Smylie (1999). Several mechanisms have been put forward to explain this discrepancy, such as the dynamic effects proposed by Lumb and Aldridge (1991) and those pointed out by Secco (1995). The presence of other loss mechanisms in the long observation period for some methods, the difficulty in accounting for all sources of loss (scattering, attenuation outside the core), and the potentially large influence from alloying elements (e.g. sulfur and nickel) are apparently the possible reasons for creating the discrepancy. Clearly more data are needed to finally reconcile the large difference between the theoretical calculations and the real Earth observations.

Conclusions

Molecular dynamics simulations employing an embedded-atom potential model have been conducted in the present study to obtain both bulk and shear viscosity of pure liquid iron at the Earth's outer core physical conditions. We have shown in present study:

(1) Sutton-Chen type of potential is well suited for the description of static and dynamic properties of liquid iron;
(2) Both Green-Kubo and Sutherland-Einstein equations are applicable to obtain viscosity of liquid iron;
(3) The shear viscosity of liquid iron at the outer core's temperature and pressure conditions is in the order of 10^{-2} Pa · s and is in very close agreement with previous studies;
(4) The bulk viscosity of liquid iron at the Earth's outer core conditions is in the order of 10^{-3} to 10^{-4} Pa · s and is much smaller than previous estimates;
(5) The average ratio of bulk to shear viscosity is 0.12 ± 0.07 and agrees neither with the general speculation that bulk and shear viscosities are similar at ambient pressures, nor with the inference that bulk viscosity is much higher than shear viscosity at outer core conditions.

References

Ackland GJ, Wooding SJ, Bacon DJ (1995) Defect, surface and displacement-threshold properties of zirconium simulated with a many-body potential. Philos Mag 71(3):553–565
Allen MP, Tildesley DJ (1987) Computer simulation of liquids. Clarendon, Oxford

Anderson DL (1980) Bulk attenuation in the Earth and viscosity of the core. Nature 285:204–220

Anderson WW, Ahrens TJ (1994) An equation of state for liquid iron and implications for the Earth's core. J Geophys Res 99:4273–4284

Andrault D, Fiquet G, Kunz M, Viscocekas F, Hausermann D (1997) The orthorhombic structure of iron: an in situ study at high-temperature and high-pressure. Science 278:831–834

Baskes MI, Johnson RA (1994) Modified embedded atom potentials for HCP metals. Modelling Simul Mater Sci Eng 2:147–163

Belonoshko AB, Ahuja R (1997) Embedded-atom molecular dynamic study of iron melting. Phys Earth Planet Inter 102:171–184

Daivis PJ, Evans DJ (1995) Transport coefficients of liquid butane near the boiling point by equilibrium molecular dynamics. J Chem Phys 103(10):4261–4265

DeWijs GA, Kresse G, Vočadlo L, Dobson D, Alfè D, Gillan MJ, Price GD (1998) The viscosity of liquid iron at the physical conditions of the Earth's core. Nature 392:805–807

Duffy TS, Hemley RJ (1995) Some like it hot: the temperature structure of the Earth. Rev Geophys Supplement: 5–9

Dziewonski AM, Anderson DL (1981) Preliminary reference Earth model. Phys Earth Planet Inter 25:297–356

Flinn JM, Gupta PK, Litovitz TA (1974) Mechanism of volume viscosity in the liquid metal system lead-bismuth. J Chem Phys 60(11):4390–4395

Gans RF (1972) Viscosity of the Earth's core. J Geophys Res 77(2):360–366

Glatzmaier GA, Roberts PH (1995) A three-dimensional self-consistent computer simulation of a geomagnetic field reversal. Nature 377:203–209

Iida T, Guthrie RIL (1988) The physical properties of liquid metals. Clarendon, Oxford

Jephcoat AP, Mao HK, Bell PM (1986) Static compression of iron to 78 GPa with rare gas solids as pressure-transmitting media. J Geophys Res 91(B5):4677–4684

Kuang W, Bloxham J (1997) An Earth-like numerical dynamo model. Nature 389:371–374

Levesque D, Verlet L, Kurkijarvi J (1973) Computer "experiments" on classical fluids. IV. Transport properties and time-correlation functions of the Lennard-Jones liquid near its triple point. Phys Rev A 7(5):1690–1700

Lumb LI, Aldridge KD (1991) On viscosity estimates for the Earth's outer core and core-mantle coupling. J Geomagn Geoelectr 43:93–110

Mao HK, Wu Y, Chen LC, Shu JF, Jephcoat AP (1990) Static compression of iron to 300 GPa and $Fe_{0.8}Ni_{0.2}$ alloy to 260 GPa: implication for composition of the core. J Geophys Res 95:21 737–21 742

Nasch PM, Manghnani MH (1994) Sound velocity measurements in liquid iron by ultrasonic interferometry. J Geophys Res, 99(B3):4285–4291

Nasch PM, Manghnani MH, Secco RA (1997) Anomalous behavior of sound velocity and attenuation in liquid Fe-Ni-S. Science 277:219–221

Poirier JP (1988) Transport properties of liquid metals and viscosity of the Earth's core. Geophys J 92:99–105

Secco RA (1995) Viscosity of the outer core. In: Ahrens TJ (ed) Mineral physics and crystallography, a handbook of physical constants. American Geophysical Union, Washington DC, pp 218–226

Singh AK, Mao HK, Shu JF, Hemley RJ (1998) Estimation of single-crystal elastic moduli from polycrystalline X-ray diffraction at high pressure: application to FeO and iron. Phys Rev Lett 80:2157–2160

Smylie DE (1999) Viscosity near Earth's solid inner core. Science 284:461–463

Stacey FD (1992) Physics of the Earth (3rd edn). Brookfield Press, Brisbane, Australia

Stixrude L, Cohen RE, Hemley RJ (1998) Theory of minerals at high pressure. In: Hemley RJ (ed) Ultrahigh-pressure mineralogy: physics and chemistry of the Earth's deep interior (Reviews in Mineralogy vol. 37) Mineralogical Society of America, Washington DC, pp 639–671

Sutton AP, Chen J (1990) Long-range Finnis-Sinclair potentials. Philos Mag Lett 61:139–146

Svendsen B, Anderson WW, Ahrens TJ (1989) Ideal Fe-FeS, Fe-FeO phase relations and Earth's core. Phys Earth Planet Inter 55:154–186

Zarestky J, Stassis C (1987) Lattice dynamics of γ-Fe. Phys Rev B 35(9):4500–4502