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Ab initio determination on diffusion coefficient and viscosity of FeNi fluid under Earth's core condition

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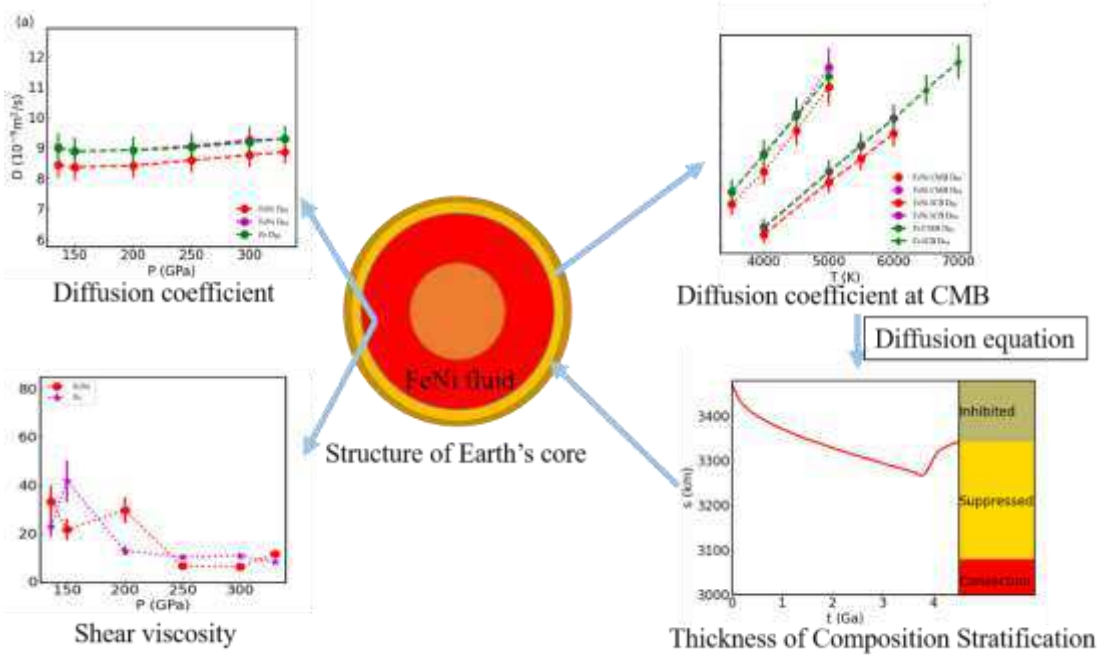
Abstract: The Earth's outer core is mainly composed of Fe and Ni. The compositional stratification and geodynamo of the Earth's core are closely correlated with the transport properties of the fluid in the Earth core. We selected the typical FeNi fluid, and systemically calculated its diffusion coefficient and viscosity under Earth's core condition by quantum molecular dynamics simulation. The diffusion coefficients and viscosity are almost constant along the core adiabatic curve. The self-diffusion coefficients of Ni along the core adiabatic range from 8.37×10^{-9} m^2s^{-1} to 8.87×10^{-9} m^2s^{-1}. The diffusion coefficient increases with temperature increase, while viscosity decrease with temperature increase. The calculations on the transport properties suggest that the Ni impurities have a negligible effect on the diffusion coefficient and viscosity of Earth's core. Combining the self-diffusion coefficient of Ni and the diffusion equation, the thickness of compositional stratification at the top of the core is 138.5 km.

Graphic abstract



1. Introduction

Accurate knowledge of the physical properties under extreme density-temperature conditions is of considerable interest in various fields of physics, including the Earth system [1], planetary physics [2], astrophysics [3], and inertial confinement fusion [4]. The center of the Earth consists of a solid inner core, surrounded by a spherical shell of the liquid outer core. The vigorous convection in the metallic liquid outer core, thus powers the dynamo that sustains the magnetic field. The geodynamo is extremely sensitive to core conditions, which is a very active research topic in Earth science. The viscosity and diffusion coefficients of the Earth core are the main parameters in the convection process.

The main parameters in character the geodynamo and stable stratification are molecular diffusion coefficients and viscosity. The analysis of compositional stratification is mostly based on the diffusion

equation [5], which correlated the thickness of the layer with the diffusion coefficients. In the early reported paper, the diffusion coefficient is mostly adopted as 3×10^{-9} m^2s^{-1}, and this corresponds to a 60 to 70 km thickness of compositional stratification [5]. It is difficult to get the accurate diffusion coefficient and viscosity values under Earth's core condition experimentally [6]. Now, quantum molecular dynamics (QMD) can give a direct and accurate estimation of the transport coefficients [7]. The QMD results show that the self-diffusion coefficient of Fe is 5.2×10^{-9} m^2/s, and viscosity is 8.5 mPa s [8]. Recently, light element effects on transport properties are also considered, such as Fe-Si-O fluid [9], Fe-O fluid [10, 11], Fe-S fluid [12].

The QMD results of viscosity are far lower than the values inferred from seismic and other measurements [13, 14]. Early in 1998, it is inferred that the viscosity of the inner core is 1.22×10^{11} Pa s [15]. Geodynamic estimation by Buffett inferred viscosity is less than 10^{16} Pa s [16]. The theoretical value for viscosity varies largely by different methods, from ~0.1 mPa s [14] to 10^{11} Pa s [15]. QMD calculation shows that the viscosity is 13 mPa s and diffusion coefficients 5×10^{-9} m^2s^{-1} at the inner-core boundary(ICB), and 12 mPa and 4×10^{-9} m^2s^{-1} at the core-mantle boundary (CMB) [17]. The viscosity is about several mPa s for MD results of FeNi fluid [18]. Though there were limitations in MD, the early report MD results claim that Ni has a negligible effect on viscosity [19].

However, the self-diffusion coefficient and viscosity of Fe-Ni fluid at Earth's core condition has never been calculated by QMD. As the second constitute elements in the Earth's core, how Ni affects the transport coefficients and the compositional stratification are still waiting solved questions. In this paper, we calculated the diffusion coefficients and viscosity of Fe-Ni fluid under Earth's core condition by the precisely QMD methods, and give a simple analysis of temperature effect on transport properties of Fe-Ni fluid. Furthermore, we used the accurate self-diffusion coefficient to give a further discussion about its effect on the compositional stratification and evolution of Earth's core.

2. Methods and calculations

2.1. Transport property

The theory equations are collected from Ref. [7, 20-22]. Diffusion coefficients can be calculated by either mean-squared displacements or velocity autocorrelation functions by equilibrium molecular simulation. The self-diffusion coefficient D_i calculated by the Einstein equation is

$$D_i = \frac{1}{3}\int_0^\infty \left\langle \mathbf{V}_i(t)\,\mathbf{V}_i(0)\right\rangle dt, \tag{1}$$

where $V_i(t)$ is the velocity of atom i at time t.

The shear viscosity calculated by Einstein relation is

$$\eta = \lim_{t\to\infty} \frac{V}{2tk_BT}\left\langle \left(\int_0^t P_{xy}(t')\,dt'\right)^2 \right\rangle, \tag{2}$$

where p_{xy} is the off-diagonal elements of the pressure tensor.

We adopt empirical fits to the integrals of the autocorrelation function. Both D_i and η have been fit to the function in the form of $A[1-exp(-t/\tau)]$, where A and τ are free parameters. The fractional statistical error in calculating a correlation function C for molecular dynamics trajectories [23] can be given by

$$\frac{\Delta C}{C} = \sqrt{\frac{2\tau}{T_{traj}}}, \tag{3}$$

where T_{traj} is the length of the trajectory and τ is the correlation time of the function. In the present paper, we generally fitted over a time interval of [0,4τ-5τ].

2.2. Thickness of compositional stratification

The compositional stratification on the top of the outer core is caused by the diffusion of the light elements [5, 24]. The basic assumptions in this paper are that the Earth's core is spherical homogeneous, and the self-diffusion coefficient of light elements is in order of that of Fe and Ni. The basic structure in Earth's core includes the inner core, convection zone, and stratified layer (Figure 1).

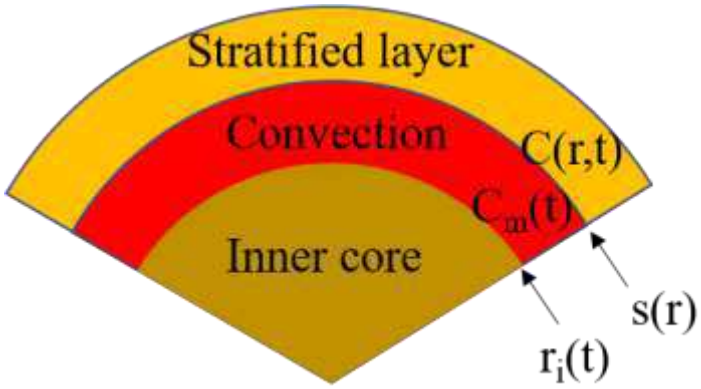


Figure 1 Structure of the Earth's core. r is the radial distance from the Earth center, r_c is the radius of the core-mantle boundary, and s(t) is the location between stratified layer and the convection region of the outer core at time since the presence of inner core. C is the concentration of the light element.

In the stratified layer ($s(t)<r<r_c$), the concentration of light element satisfied the diffusion equation

$$\rho\frac{\partial C(r,t)}{\partial t}=-\nabla\mathbf{I}(r,t) \tag{4}$$

where ρ is the density at stratified layer, $\rho=1.23\times10^4$ kg/m^3, C(r, t) is the concentration at radius r and time t, $\boldsymbol{I}(r,t)$ is the diffusion flux and ∇ is coordinate partial.

$$\mathbf{I}(r,t)=-\rho D(t)\left(\nabla C(r,t)+\frac{\alpha_c}{\rho H}\nabla P\right) \tag{5}$$

where $D(t)$ is the self-diffusion coefficient of the light element and is calculated as a function of temperature. α_c is the chemical expansion coefficient, H is the heat of mixing, P is the pressure at radial r, and t is the time. Neglecting the time and location effect on α_c and H. For simplicity, α_c~1.0. H is $H=\left(\frac{\partial\mu}{\partial c}\right)_{P,T}$ (partial chemical potential with concentration c at constant pressure P and temperature T) and can be calculated directly from ab initio simulations. On the other hand, H is simplified as $\frac{RT}{M_LC\left(1-C\bar{M}/M_L\right)}\approx\frac{RT}{M_LC}$, where R=8.314 JK^{-1}mol^{-1}, $\bar{M}$ and M_L are the molar mass of mixtures and light element, respectively.

In the convection region ($r_i(t)<r<s(t)$), $r_i(t)$ is radius of the inner-core at time t. As the regrious convection, oxygen concentration is homogeneous $C_m(t)$. oxygen conservation

$$\frac{4\pi\rho}{3}\left(s^3(t)-r_i^3(t)\right)\frac{dC_m(t)}{dt}=-4\pi s^2(t)\mathbf{I}_r\left(s^-,t\right)+\Phi(t) \tag{6}$$

where $I(s^-,t)$ is the radial component of the flux in the convection zone, and Φ(t) is light element accumulation due to the growth of the inner-core.

$$\Phi(t)=4\pi r_i^2(t)\rho C_m(t)\frac{dr_i(t)}{dt} \tag{7}$$

$r_i(t)$ is the radius of the inner core at time t. dr_i/dt is directly from the parametrized model [25-27]

$$r_i(t)=r_i(t_1)\sqrt{(t-t_0)(t_1-t_0)} \tag{8}$$

where $r_i(t_1)$ (1221km) is the radius at present time, t_1=4.5 Ga, t_0 is the time the inner core begins to grow. As the high thermal conductivity of pure Fe [28], the age of the inner core is within 1.0 Ga, we adopt t_0=3.85 Ga.

The boundary condition is that light element concentration at the CMB is equal to that at the lower mantle $C_{eq}(T,P)$. For continuous condition

$$\mathbf{I}_r\left(s^+,t\right)=\mathbf{I}_r\left(s^-,t\right)$$

$$\frac{dC_m(t)}{dt}=\frac{\partial C(r,t)}{\partial t}+\frac{ds(t)}{dt}\left(\frac{\partial C(r,t)}{\partial r}\right)_{r=s^+} \tag{9}$$

where s^+ represents the side of the stratified layers near the interface. Integration Eqs. (4) and (6) with the boundary conditions Eq.(9), the s(t) and *C(r, t)* are collected. From Eqs. (4) and (6), with the initial and boundary conditions (Eq. (9)), the *C(r, t)*, $C_m(t)$, and *s(t)* are numerically calculated.

In the analysis of stratification, the dynamic model [29] shows: (a) If $T'_{eq}>0$, convection is uninhibited at the top of the outer core. (b) If $T'_{eq}<0$ with $Q_{CMB}<Q_k$, convection is inhibited, but not suppressed at the top of the outer core. (c) If $T'_{eq}<0$ with $\Delta C(r)>0$ (radial gradient of light element), convection is suppressed at the top of the outer core.

2.3. Calculation details

Ab initio molecular dynamics were performed using the Vienna ab initio simulation package (VASP) [30, 31]. The ion-electron interaction was represented by the projector augmented wave (PAW) [32, 33]. The generalized gradient approximation with Perdew, Burke, and Ernzerhof corrections was employed [34]. The electronic states were populated following the Fermi-Dirac distribution [35]. In this paper, we selected 128 atoms as the cell. Ni atoms were randomly distributed in the cell, with 12 Ni atoms and others are Fe atoms, and the corresponding atom ratio are 9.375 at.%. Plane wave cutoff is 400 eV enough to make sure that the pressure is converged within 1% accuracy. Time dependent mean square displacement to check system in the liquid state. The selected time step is 1ps in all the calculations. To get the convergence transport coefficients, the total time is more than 20 ps. The core-mantle boundary (CMB) pressure 136 GPa, inner-core boundary (ICB) pressure 330 GPa, and pressures along the core adiabatic 150 GPa, 200 GPa, 250 GPa, 300 GPa. The analytical expressions of state profiles along the adiabatic curve were given by following Labrosses [25, 36].

3. Results and discussion

3.1. Self-diffusion coefficient

Our QMD calculations on self-diffusion coefficient of pure Fe liquid agree with the early reported QMD results [7]. The self-diffusion coefficients of Fe and Ni are comparable, in the orders of 10^{-9} m^2s^{-1}. Our calculated self-diffusion coefficients of Fe are consistent with the ab initio calculated results of pure Fe [8], Fe-Si-O fluid [9], and Fe-O fluid[11]. Self-diffusion coefficients of Fe along the core adiabatic are in the range of [8.88, 9.30]$\times10^{-9}$ m^2s^{-1}. Self-diffusion coefficients of Ni along the core adiabatic are in the range of [8.37, 8.87]$\times10^{-9}$ m^2s^{-1}. The self-diffusion coefficient of Fe-Ni fluid along the core adiabatic is almost kept constant (Figure 2(a)). The self-diffusion of Ni is a little smaller than that of Fe at the same pressure and temperature condition. This can be easily explained that the atom mass of Ni is a little higher than that of Fe. Considering the pressure and temperature effect (Figure 2(b)), the self-diffusion coefficient is higher when at same pressure with higher temperature or the same temperature with lower pressure. The diffusion coefficient shows a monotonic rise with increasing temperature. Self-diffusion coefficient of Fe at CMB ranges from (7.79±0.40)$\times10^{-9}$ m^2s^{-1} at 3500K to (11.87±0.64)$\times10^{-9}$ m^2s^{-1} at 5000K. The self-diffusion coefficient of Ni at CMB ranges from (7.38±0.38)$\times10^{-9}$ m^2s^{-1} at 3500K to (11.22±0.60)$\times10^{-9}$ m^2s^{-1} at 5000K.

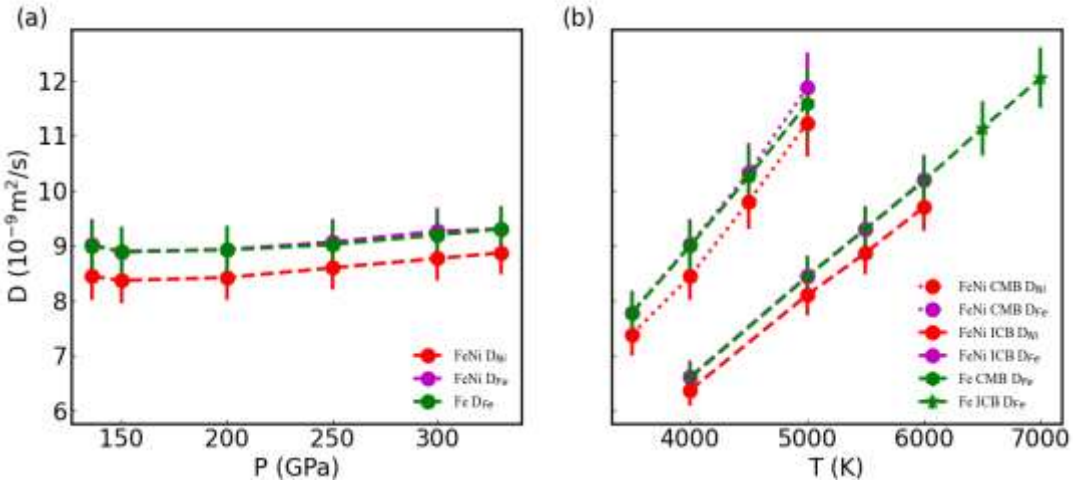


Figure 2 The self-diffusion coefficients (D_{Fe} and D_{Ni}) of Fe and FeNi fluid under Earth's core conditions. (a) is along the core adiabatic, and (b) is temperature variation at CMB and ICB.

3.2. Shear viscosity

The viscosity of Fe-10%Ni fluid is lower than pure Fe, under ICB, CMB, or the chosen OC condition, or along the adiabatic curves (Figure 3). The QMD result is different from the early reported MD results, which point out Ni has a negligible effect on bulk viscosity of liquid iron, about ~mPa s [19]. However, a clear conclusion is that Ni decrease viscosity under all Earth outer core condition in these QMD simulations. Furthermore, the QMD results of viscosity are far lower than the values inferred from seismic and other measurements [13, 14], and other model inferred results. With increasing pressure, the shear viscosity increases.

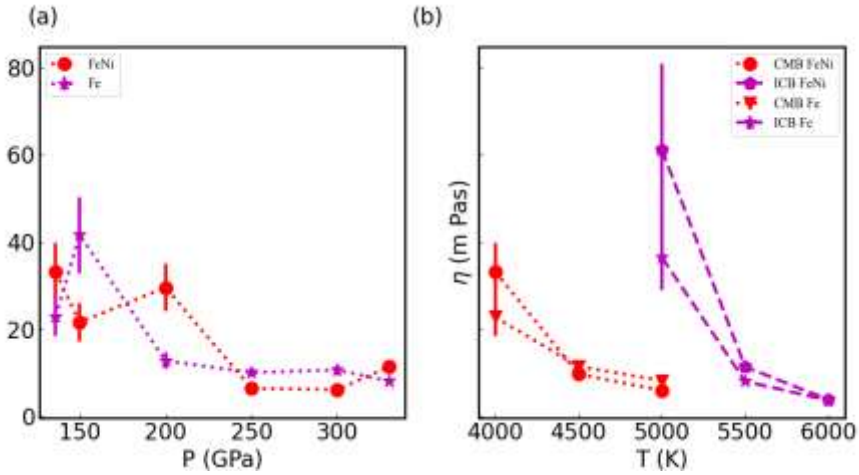


Figure 3 Viscosity of the pure Fe and FeNi fluid under Earth's core condition. (a) is viscosity along the adiabatic curve and (b) is viscosity under inner-core (136 GPa) and core-mantle (330 GPa) boundary pressure with different temperatures. The Fe and FeNi labels correspond to pure Fe and FeNi fluid results, respectively.

3.3. Temperature effect and physical laws

The Stokes-Einstein relation gives a connection between the diffusion and shear viscosity through the expression

$$F_{SE}\left[D,\eta\right]=\frac{D\eta}{k_BTa}=C_{SE}, \tag{10}$$

where a is an effective atomic diameter. C_{SE} ranges from 1/6π(0.053) to 1/4π(0.080) from Ref. [37]. The Stokes-Einstein relation can be used to predict the viscosity and diffusion coefficients of liquid Earth's outer core from its structural properties. Examination of the Stokes-Einstein relation with respect to $1/ak_BT$. Application Stokes-Einstein relation for Fe-Ni systems [18]. Under the same pressure and constituent, both the viscosity and diffusion coefficients increase with temperature. However, neither the

viscosity nor diffusion coefficients do not strictly exhibit Arrhenius behaviors. We analyzed the Stokes-Einstein expression as a function of temperature. Within the expected fitting error of ~20% for determining viscosity from the simulations, the QMD results are bounded by the classical values of C_{SE} from below and the Chisolm-Wallace (0.18±0.02) liquid metal value from above.

3.4. Thickness of compositional stratification

The stratified layer is calculated by assumption that uniform compositional enrichment or net subadiabatic CMB flux are driving stratification, shown in Figure 4. The self-diffusion coefficient is correlated with the stratification. Usually, a big diffusion coefficient corresponds to high sensitivity of the concentration with time evolution. Only Fe and Ni components, the composition stratification is impossible. With the addition of O, it is more reasonable [38]. If the diffusion coefficient of light elements is of the same magnitude as Fe and Ni, the thickness of compositional stratification derived from diffusion equation [5] is 138.5 km. On top of the outer core is classified into three zones [29]. Compared with the total stratification from thermal conductivity of thermal conductivity in FeNi fluid [39], r>3341.5 km scale is inhibited, 3079 km<r<3341.5 km is prohibited, and r<3079 km is uninhibited convection.

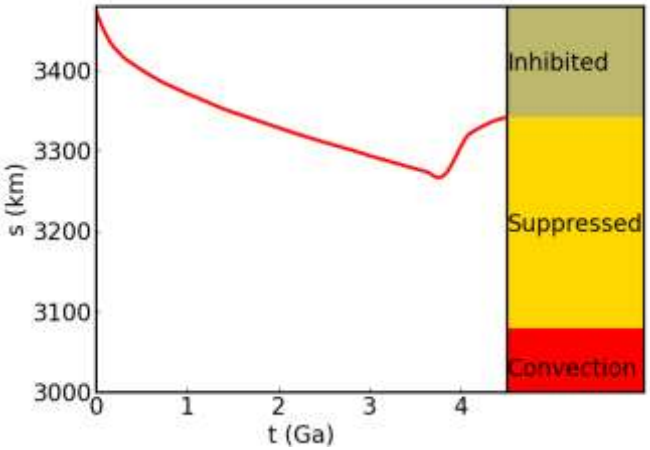


Figure 4 Evolution of stratification during the whole Earth's time. On the right of the figure, the inhibited, suppressed and convection zones at present are labeled.

4. Conclusion

Ab initio molecular dynamics estimates self-diffusion coefficient and viscosity of outer core are important for several purposes. Self-diffusion coefficients of Ni along the core adiabatic range from 8.37×10^{-9} m^2s^{-1} to 8.87×10^{-9} m^2s^{-1}. At the core-mantle boundary, the diffusion coefficient increases with temperature increase, while viscosity decrease with temperature increase. In addition, the self-diffusion coefficient of Ni was adopted in the diffusion equation, which shows that the thickness of the compositional stratification on top of the outer core is 138.5 km. The ab initio calculated ion transport properties offer an insight into the evolution of the Earth's deep interior.

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Data availability

The data that support the findings of this study are available from the corresponding author(s) upon reasonable request.

Author contributions

Wei-Jie Li designed and planned the project of this research, conducted the ab initio calculation, wrote the paper and plot all the figures. Cong Wang, Zi Li, Ping Zhang, Yong Lu, Zhe Ma, Qian Jia, Xue-Bin Cheng, and Han-Dong Hu discussed the interpretation of the calculation results. All authors contributed

to the preparation the manuscript and have approved the submitted version of the manuscript.

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