



Original Article

The Influence of High Pressure and Temperature on Transport Properties of Liquid Magnesium Oxide

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Abstract: This work provides insights into the effects of both temperature and pressure on structure, dynamics, and diffusion mechanism in liquid magnesium oxide (MgO) systems. The Molecular Dynamics simulation (MDs) method and a kinetic approach are employed in this research. The structure of liquid MgO undergoes changes under compression, primarily consisting of the polyhedral units of MgO_3 , MgO_4 , and MgO_5 at ambient pressure and MgO_5 and MgO_6 at high pressures up to 25 GPa. Meanwhile, the structure of liquid MgO is still composed of the polyhedral units of MgO_3 , MgO_4 , and MgO_5 at different temperatures. The diffusion mechanism in liquid MgO involves the transition of the polyhedral units from MgO_x to $MgO_{x\pm 1}$. We found that two factors contribute significantly to the diffusion process of the liquid MgO system including the mean square of transition d_{tr} and the rate of transition r_{tr} coefficient.

Keywords: The liquid MgO , MD, structure, diffusion.

1. Introduction

Magnesium oxide system MgO is one of the most common components in the Earth's crust. With a high melting point, MgO has many applications in industry as well as in high-tech materials. MgO is the main ingredient in heat-resistant materials, refractory materials [1-5], geophysics [6-11], and medical materials [12, 13]. Low thermal expansion, MgO is used in materials to speed up the enamel's melting process, creating a fluid enamel with high slack and high surface tension. Knowledge of the structure and kinematics of the MgO system under high pressure and temperature conditions is essential to

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optimize new material generation processes and to test geological activities. Therefore, the study of the structure and kinetic properties of MgO has been the subject of many research projects. The research results showed that the structure of the MgO system changes markedly when the compression pressure changes, the first peak position of the radial distribution functions $g_{Mg-Mg}(r)$, $g_{Mg-O}(r)$, $g_{O-O}(r)$ all tend to move to a smaller distance when compressed, but the first peak of $g_{Mg-O}(r)$ has a negligible change [14-16], which proves that the short-range order of MgO is not affected much by pressure. At low pressure, the $Mg-O$ coordination numbers are 3, 4, and 5, when the pressure increases, the coordination number of the system changes to 4, 5, 6. The MD simulation results show that MgO system is composed of the polyhedral units MgO_x ($x = 3, 4, 5, 6...$), when increasing the compressive pressure, the length of the $Mg-O$ bond in MgO_x structural units decreases. The MgO_x polyhedral units tend to bond with each other to form clusters through the spherical oxygen atom. The results of kinetic properties also show that the structure of MgO system has spatial heterogeneity [14], the short-range order is more stable than the intermediate-range order. Regions of atoms move quickly or slowly over time and are unevenly distributed in space. For a liquid MgO system, studies show that the diffusion mechanism through nearest neighbor atom exchange between the structural units [11, 17-19], the simulations of the pressure dependence of the diffusion coefficient in liquid MgO shows that the diffusion coefficient of Mg atom is similar to that of O atom [14]. At a pressure of 0.08 GPa, the diffusion coefficient is about 1.2×10^{-4} cm²/s. When the pressure increases, the diffusion coefficient decreases. At 25.20 GPa, the diffusion coefficient has a value of about 0.5×10^{-4} cm²/s [14].

In this study, we employed MDs method and a kinetic approach to clarify the structure, dynamics and diffusion mechanism in a liquid MgO system under varying temperature and pressure conditions.

2. Calculation Method

Using MDs method with the Lewis-Catlow potential, we constructed the liquid MgO models in the range of temperatures from 3,600 K to 5,000 K at ambient pressure and in the range of pressure from 0 to 25 GPa at temperature of 3,800 K. Detail of the Lewis-Catlow potential can be found in [20]. Firstly, the initial sample is created by randomly placing all atoms in a simulation box with periodic boundary condition. It is heated at temperature of 7,000 K and then cooled down to the desired temperature and pressure. A consequent long relaxation has been done in the NPT ensemble to obtain a sample at ambient pressure and desired temperature which denoted to model M1. The models at different pressures were constructed by compressing model M1 to different pressures, namely 0, 10, 20 and 25 GPa. The models at different temperatures were constructed by heating model M1 to temperatures of 3,600 K; 3,800 K; 4,200 K and 5,000 K. Next, these models are relaxed by 10^7 MD steps to reach equilibrium. The Verlet algorithm is applied with the MD step of $\Delta t = 0.25$ fs. To study the diffusion, the obtained models are additionally relaxed by 2×10^7 MD steps in the NVE ensemble. The diffusion coefficient of atoms in MD model is usually determined via the Einstein equation:

$$D = \lim_{t \rightarrow \infty} \frac{\langle r(t)^2 \rangle}{6t} = \lim_{t \rightarrow \infty} \frac{\langle r(t)^2 \rangle}{6n\Delta t} = K \cdot \lim_{t \rightarrow \infty} \frac{\langle r(t)^2 \rangle}{n} \quad (1)$$

with $\langle r(t)^2 \rangle$ is the mean square displacement (MSD) over time $t = n\Delta t$; n is number of MD steps; $K = \frac{1}{6 \cdot \Delta t}$. Thus, the value of the diffusion coefficient D is defined as the slope of the line representing the dependence of the mean squared displacement on the number of MD steps. Using a kinetic approach in order to clarify the diffusion mechanism in liquid MgO , we track the movements and changes in coordination number of each atom during the simulation. The obtained results show that the diffusion occurs when there is an exchange of O coordination between the structural units MgO_x . Therefore, the diffusion in liquid MgO proceeds via the transition mechanism $MgO_x \rightarrow MgO_{x+1}$. n_{tr} is defined as the total

number of transitions $MgO_x \rightarrow MgO_{x\pm 1}$ per one atom in n MD steps. We have the following equations: $d_{tr} = \lim_{n_{tr} \rightarrow \infty} \frac{\langle r(t)^2 \rangle}{n_{tr}}$ and $r_{tr} = \lim_{n \rightarrow \infty} \frac{n_{tr}}{n}$ where d_{tr} is the mean square displacement of a $MgO_x \rightarrow MgO_{x\pm 1}$ transition and r_{tr} is the rate of a $MgO_x \rightarrow MgO_{x\pm 1}$ transition. Therefore, the diffusion coefficient is determined as following equation:

$$D = K \cdot \lim_{t \rightarrow \infty} \frac{\langle r(t)^2 \rangle}{n_{tr}} \cdot \lim_{t \rightarrow \infty} \frac{n_{tr}}{n} = K \cdot \lim_{n_{tr} \rightarrow \infty} \frac{\langle r(t)^2 \rangle}{n_{tr}} \cdot \lim_{t \rightarrow \infty} \frac{n_{tr}}{n} = K \cdot d_{tr} r_{tr} \tag{2}$$

Thus, the atomic-level diffusion mechanism in liquids MgO system is elucidated by calculating the diffusion coefficient through two Eqs. (1) and (2).

3. Results and Discussion

To assess the reliability of the liquid MgO models, we first computed the partial radial distribution functions (RDFs) $g_{ij}(r)$ between i^{th} and j^{th} atom. These RDFs were then compared to the ones presented in [18], as depicted in Fig. 1. The first peaks observed in $g_{MgMg}(r)$ at 3.20 Å, $g_{MgO}(r)$ at 1.74 Å, and $g_{OO}(r)$ at 2.82 Å indicate a good agreement of the shape, amplitude and position of the peaks with the data reported in [18, 21-23]. Consequently, one can conclude that the constructed models are reliable and serve as a solid foundation for studying the dynamics in the liquid MgO system.

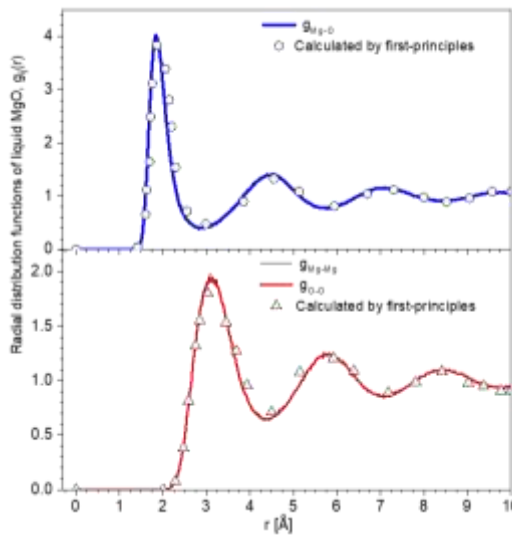


Figure 1. The RDF $g_{ij}(r)$ of liquid MgO model and the data in [18].

Fig. 2 illustrates the fraction of polyhedral units MgO_x , where x ranges from 3 to 6, in the models of liquid MgO at various pressures and temperatures. These polyhedral units form the structure of the liquid MgO . In Fig. 2a, it is evident that the structure of liquid MgO varies significantly with pressure. At lower pressures, the predominant polyhedral units are MgO_3 , MgO_4 and MgO_5 , while at higher pressures, the structure is mainly composed of MgO_5 and MgO_6 . The fraction of these structural units undergoes significant changes as the pressure increases. The considered pressures have a notable influence on the structure of liquid MgO . As the pressure increases, there is a transition from a network structure primarily composed of MgO_3 and MgO_4 to a network structure dominated by MgO_5 and MgO_6 . In Fig.

2b, the structure of liquid MgO at different temperatures (ranging from 3,600 K to 5,000 K) primarily consists of structural units MgO_3 , MgO_4 , and MgO_5 . The fractions of these structural units exhibit slight variations with temperature. Specifically, the percentages of MgO_4 and MgO_5 units slightly decrease, while the proportion of MgO_3 units slightly increases. Notably, the majority of the polyhedral units are still MgO_4 , forming a tetrahedral network structure. This result is in good agreement with the data reported in [16, 18, 21-23], the average coordination number is 4 for liquid MgO . A significant aspect of the diffusion process is the relationship between the MSD $\langle r(t)^2 \rangle$ and the MD steps n . This relationship allows us to determine the diffusion coefficient D , by applying Einstein's Eq. (1), which has been detailed in section 2.

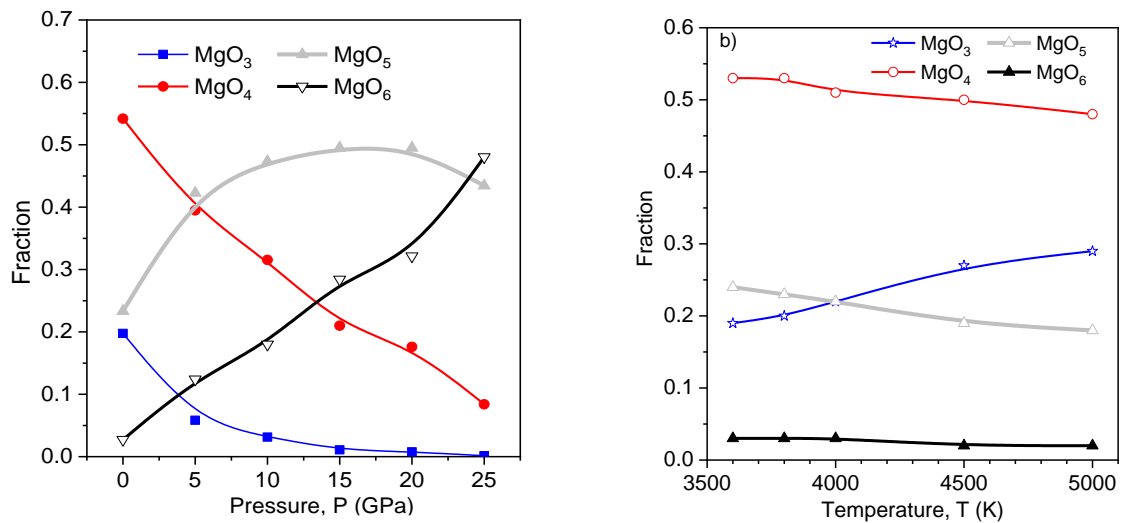


Figure 2. The fraction of polyhedral units in liquid MgO models at different pressure (a) and temperatures (b).

Fig. 3 expresses the dependence of MSD on MD steps in liquid MgO at various pressure and temperature. Notably, the plot reveals distinct straight lines. Despite some fluctuations, the results indicate that MSD $\langle r(t)^2 \rangle$ remains a linear function of simulation time. As a consequence, the diffusion coefficient D can be determined by examining the slopes of these lines. Additionally, the MSD exhibits a significant decrease as the pressure increases (see Fig. 3a). As a result, the D of Mg atoms decreases with higher pressure. Conversely, the slopes of the lines increase as the temperature rises. Consequently, the diffusion coefficient of Mg atoms increases with higher temperatures. These values are presented in Table 1.

Table 1. The diffusion coefficient D of Mg atom in liquid MgO , which is determined by equation (1) at different pressure and temperature

P (GPa)	0	10	20	25
D ($10^{-4}cm^2/s$)	1.27	0.96	0.73	0.57
T (K)	3600	4200	4500	5000
D ($10^{-4}cm^2/s$)	1.12	1.53	1.96	2.47

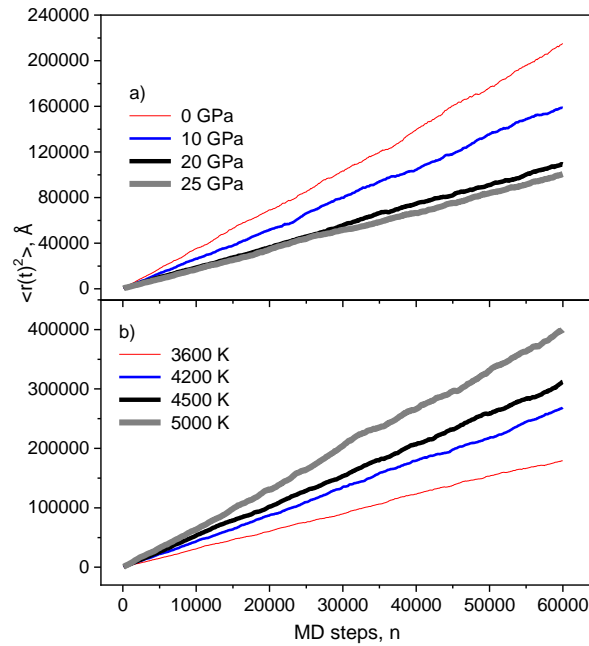


Figure 3. The dependence of $\langle r(t)^2 \rangle$ as a function of MD steps n at different pressure (a) and different temperatures (b).

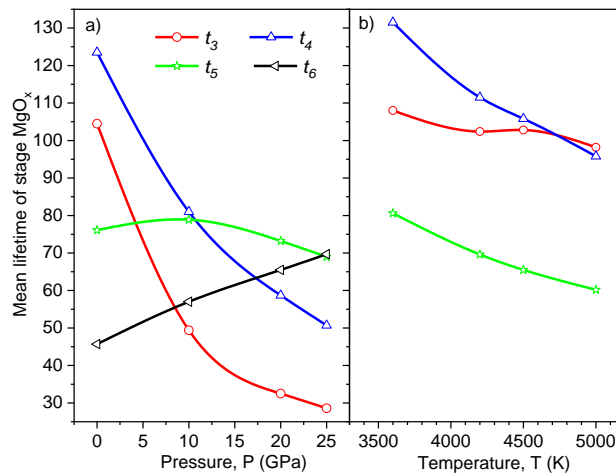


Figure 4. The mean lifetime of stage MgO_x ($x = 3 - 6$) at different pressure (a) and temperatures (b).

At atmosphere pressure, the D of Mg is $1.27 \times 10^{-4} \text{ cm}^2/\text{s}$. When the pressure increases up to 25 GPa, the D of Mg decreases by 2.23 times, to $0.57 \times 10^{-4} \text{ cm}^2/\text{s}$. Meanwhile, as the temperature increases, the D of the atoms in liquid MgO increases. It means that diffusion is obviously easier at higher temperatures. Especially, in the investigated temperature range, the D of Mg increased from $1.12 \times 10^{-4} \text{ cm}^2/\text{s}$ at 3600 K to $2.47 \times 10^{-4} \text{ cm}^2/\text{s}$ at 5000 K. This value is in good agreement with the result in [14, 18], which showed that at ambient pressure, the diffusion coefficient of Mg is about $1.2 \times 10^{-4} \text{ cm}^2/\text{s}$ at 3,800 K and $1.5 \times 10^{-4} \text{ cm}^2/\text{s}$ at 4,000K. As analyzed above, the network structure of liquid MgO is made up of basic structural units MgO_x with $x = 3, 4, 5$ at low pressure; $x = 4, 5, 6$ at high pressure and

$x = 3, 4, 5$ at different temperatures. Our investigation reveals that each atom goes through a series of stages during which its coordination number remains unchanged, indicating the existence of distinct structural units with specific lifetimes. This implies that each polyhedral unit has a certain lifetime, determining the duration before it converts into another polyhedral unit. The lifetime of polyhedral unit MgO_x ($x = 3 - 6$) is very different, as depicted in Fig. 4.

In considered pressure range, Fig. 4a shows that at low pressure, the lifetime of the structural unit MgO_4 is the largest. As the pressure increases, the lifetime of MgO_3 and MgO_4 decreases sharply, meanwhile, the lifetime of MgO_6 structural units increases. Namely, the lifetime of MgO_3 and MgO_4 decreases from 123.5 and 104 to 50.7 and 28.6 MD steps, respectively. The lifetime of MgO_6 polyhedral units increases from 45.7 to 69.7 simulation time steps. The lifetime of MgO_5 structural units increases from 76.1 at 0 GPa to 78.9 at 10 GPa, then reduced to 69 simulation time steps at 25 GPa pressure. Thus, the polyhedral unit of MgO_4 is the most stable at low pressure and the least stable at high pressure. In contrast, the structural unit of MgO_6 is the most stable at high pressure. There is a transition of MgO_4 tetrahedral units to MgO_6 octahedral units under compression. In considered temperature, Figure 4b indicates that at each certain temperature, in the liquid MgO , there are coexistence of three isolated phases MgO_3 , MgO_4 and MgO_5 , their lifetime is different. The lifetime of MgO_5 polyhedral units is the smallest, so the atom in MgO_5 has a large mobility. The MgO_5 phase forms mobile region in the model. The dynamical heterogeneity in liquid MgO is therefore due to the heterogeneity of the distribution of MgO_x polyhedral units. Due to the very different lifetimes of MgO_x structural units, thus the number of transitions occurring in different structural units is different. Therefore, dynamics in liquid MgO is studied through the transition mechanism of $MgO_x \rightarrow MgO_{x\pm 1}$ structural units. The results indicate that the diffusion occurs when there is coordination O exchange between MgO_x polyhedral units. It means that there is a break and re-formation of the bond between Mg and O atoms to convert from one MgO_x polyhedral unit to another MgO_x polyhedral unit called the $MgO_x \rightarrow MgO_{x\pm 1}$ transition. Since then, the diffusion coefficient is determined through the MSD of a $MgO_x \rightarrow MgO_{x\pm 1}$ transition d_{tr} and the rate of a $MgO_x \rightarrow MgO_{x\pm 1}$ transition v_{tr} by Eq. (2.2).

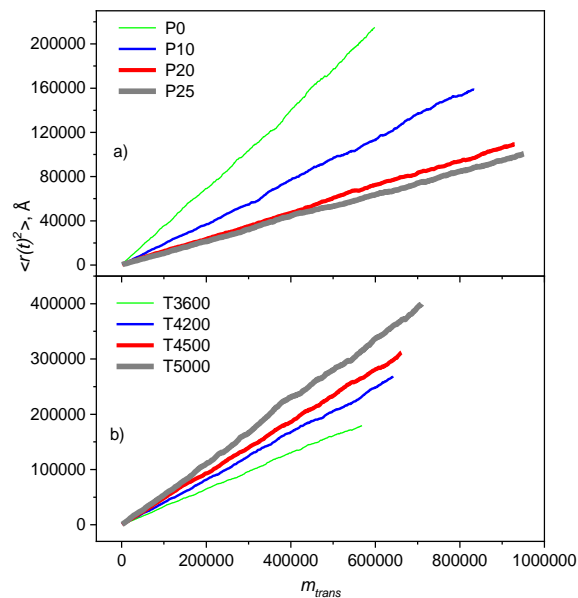


Figure 5. The dependence of $\langle r(t)^2 \rangle$ as a function of n_r at different pressure (a) and different temperatures (b).

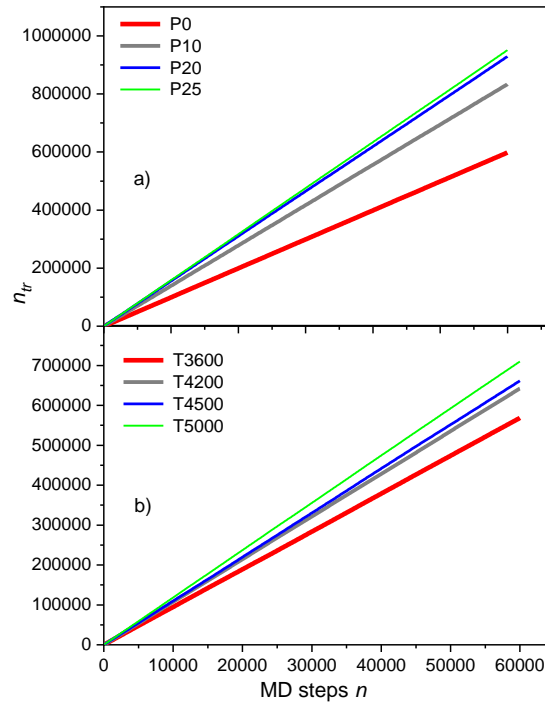


Figure 6. The dependence of n_{tr} as a function of MD steps n at different pressure (a) and temperatures (b).

Figs. 5 and 6 show the dependence of MSD $\langle r(t)^2 \rangle$ on n_{tr} and n_{tr} on n , respectively. It is clear that the straight lines are observed and the d_{tr} and r_{tr} were determined from the slopes of these lines. These values are shown in Table 2.

Table 2. Dynamical characteristics of liquid MgO models. d_{tr} is the MSD of a $MgO_x \rightarrow MgO_{x\pm 1}$ transition and r_{tr} is the rate of a $MgO_x \rightarrow MgO_{x\pm 1}$ transition. The diffusion coefficient D^* is determined by new equation (2)

P (GPa)	0	10	20	25
$r_{tr} (10^{-3})$	10,20	14,24	15,92	16,20
$d_{tr} (A^2)$	0,34	0,18	0,12	0,09
$D^* (10^{-4} \text{ cm}^2/\text{s})$	1.29	0.96	0.72	0.56
T (K)	3600	4200	4500	5000
$r_{tr} (10^{-3})$	9,85	10.3	11.28	12.15
$d_{tr} (A^2)$	0,32	0.39	0.46	0.56
$D^* (10^{-4} \text{ cm}^2/\text{s})$	1.15	1.48	1.89	2.48

The results show that the number of transitions is a linear function of the MD steps n and the MSD is a linear function of the number of transitions n_{tr} . As the pressure increases, the MSD of a $MgO_x \rightarrow MgO_{x\pm 1}$ transition d_{tr} decreases, but the number of transitions increases, i.e the rate of a $MgO_x \rightarrow MgO_{x\pm 1}$ transition r_{tr} increases (see Table 2). The increase in the number of transitions when the pressure increases is due to the repetition of the neighboring O atom jumping in and out leading to many transitions, but these transitions are inefficient. This result leads to an increase in r_{tr} but the diffusion process is still slow. On the other hand, d_{tr} decreases more strongly than the increase of

r_{tr} . Whereas, r_{tr} increases 1.59 times (from 10.2×10^{-3} to 16.2×10^{-3}) but d_{tr} decreases in 3.78 times (from 0.34 to 0.09). Consequently, the diffusion coefficient D decreases under compression. In contrast, when the temperature increases, both values r_{tr} and d_{tr} increase, leading to an increase in the diffusion coefficient D . Especially, at high temperatures, the diffusion coefficient of Mg increased by 2.54 times. The increase/decrease of d_{tr} indicates whether the chemical bond between Mg and O is weak/strong. When d_{tr} is larger, the chemical bond between Mg-O is weaker, conversely, the smaller d_{tr} , the stronger the chemical bond between Mg-O. Calculation of the diffusion coefficient D by the new method- Eq. (2.2) is also compared with the Einstein Eq. (2.1) shown in Fig. 7.

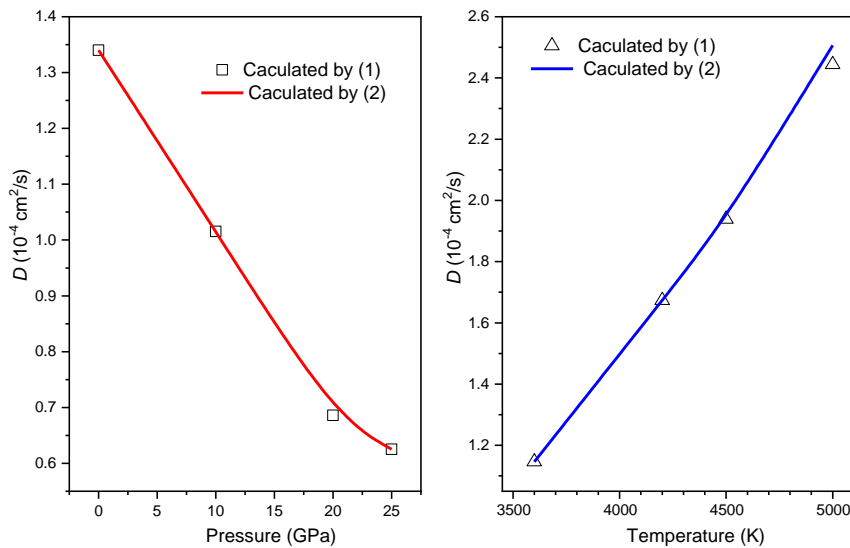


Figure 7. The diffusion coefficient for Mg of MgO liquid at different pressure (a) and different temperatures (b).

The results show a good agreement between two calculation results. This again proves that the diffusion mechanism in liquid MgO is indeed through the change in neighboring O atoms between MgO_x structural units or in other words through the transition mechanism of structural unit $MgO_x \rightarrow MgO_{x \pm 1}$. Overall, under compression, the diffusion coefficient D in liquid MgO decreases. This is primarily due to two factors: a decrease in the mean square of a transition d_{tr} and an increase in the rate of a transition coefficient r_{tr} . However, it's important to note that the decrease in d_{tr} is more prominent compared to the increase in r_{tr} , resulting in an overall decrease in D . On the other hand, when the temperature is increased, the diffusion coefficient D in liquid MgO increases. This can be attributed to the simultaneous increase in both the coefficients r_{tr} and d_{tr} . As a result, the overall diffusion is enhanced, leading to a higher value of D . It is worth noting that the diffusion mechanism in liquid MgO involves the transition of structural units from MgO_x to $MgO_{x \pm 1}$. This transition mechanism contributes to the diffusion process within the system.

4. Conclusions

This research highlights the relationship between temperature, pressure, and the structural components of liquid MgO . By elucidating the differences in structure and dynamics, MD simulations provide valuable insights into the behavior of liquid MgO under varying temperature and pressure

conditions. The results offer a deeper understanding of the changes that occur in the system. Under compression, the structure of liquid MgO primarily consists of three main polyhedral units, namely MgO_3 , MgO_4 , and MgO_5 , at ambient pressure. However, at pressures up to 25 GPa, the structure is mainly composed of MgO_5 and MgO_6 . This observation suggests that the structural arrangement of liquid MgO undergoes significant modifications as pressure increases. Similarly, when examining the effects of temperature on the structure, it was found that the composition of the polyhedral units remains consistent. In both scenarios, the presence of MgO_3 , MgO_4 , and MgO_5 structural units is evident, indicating their importance in the overall structure of liquid MgO . The presence of dynamical heterogeneity in the liquid MgO model is more pronounced when comparing different temperatures rather than different pressures. This distinction is attributed to the significant variations in the lifetimes of the MgO_x structural units within the system. It is this disparity in lifetimes that ultimately gives rise to the observed dynamical heterogeneity in the liquid MgO model. This transition mechanism contributes to the diffusion process within the system. Therefore, it can be concluded that the diffusion in liquid MgO is facilitated by the transition of structural units $MgO_x \rightarrow MgO_{x+1}$, playing a significant role in the overall dynamics of the system.

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