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Molecular Dynamics Study the Factors Effecting the Structure of $MgSiO_3$ Bulk

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Abstract

This paper studies the effect of atomic numbers (N), N=2000atoms, 3000atoms, 4000atoms, 5000atoms, 6000atoms at temperature (T), T=300K; N=5000atoms at T=300K, 500K, 1000K, 1500K, 2000K, 2500K, 3000K, 3500K; N=5000atoms at T=300K, 2000K with pressure (P), P=0GPa, 20GPa, 40GPa, 60GPa, 80GPa, 100GPa on the structure of $MgSiO_3$ bulk by Molecular Dynamics method (MD) with Born-Mayer potential (BM), periodic boundary conditions. The results were analyzed through the radial distribution function (RDF), coordination number, angle distribution, size (l), energy (E). The results showed that there are the effects of factors on the structure of $MgSiO_3$ bulk. In addition, with the atomic number (N), temperature (T), different pressures (P) at temperature T=300K, 2000K there are the appearance and disappearance of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg and number of structural units SiO_4, SiO_5, SiO_6, MgO_3, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9 , MgO_{10}, MgO_{11}, MgO_{12}

Keywords: Effect, Atomic Number, Temperature, Pressure, Structure, $MgSiO_3$ Bulk, Molecular Dynamics

1. Introduction

$MgSiO_3$ is a compound of two materials MgO, SiO_2. In it, MgO is a widely used oxide in science and technology as bioactive (Pedone, Menziani, Segre, & Cormack, 2008; Jallot, 2003; Pedone & Menziani, 2009) and SiO_2 is a silicate material with elasticity, density, high viscosity (Kraxner et al., 2008; Schilling et al., 2001; Lin, Chen, Liu, & Li, 2007) and is a main component of the earth's crust & planets (Helfrich & Wood, 2001; Molster et al., 1999; Dorschner et al.,1995). The synthesis of two MgO, SiO_2 material (Kohara et al., 2004) has been extensively studied in recent years (Kalampounias, Nasikas, & Papatheodorou, 2009; Guignard & Cormier, 2008; Sen, Maekawa, & Papatheodorou, 2009; Taniguchi, Okuno, & Matsumoto, 1997). Study the geology of the earth by using the structure of MgO, SiO_2 at high pressure (Sato & Funamori, 2010) and when the pressure is high, the viscosity and diffusion coefficient in $MgSiO_3$ change (Brawer, 1985; Liebau, 1984). There are many methods to study material: Experimental, theoretical and simulation. Experimental methods include: Absorption spectra (Sen, Maekawa, & Papatheodorou, 2009), X-ray diffraction, neutron diffraction performed by Wilding et al. (Wilding, Benmore, Tangeman, & Sampath, 2004) and Raman spectroscopy (Kalampounias, Nasikas, & Papatheodorou, 2009). The theoretical methods include Monte Carlo (MC) method (Guignard & Cormier, 2008) and molecular dynamics (MD) method. Experimental methods show that $MgSiO_3$ is an important component in the process of forming the earth (Williams & Garnero, 1996; Lay, Williams, & Garnero, 1998) and this process occurs at high temperature, high pressure (Fiquet et al., 2010; Nomura et al., 2014; Nomura et al., 2011; Petitgirard et al., 2015). When studying the $MgSiO_3$ material at high temperatures, high pressure is a condition causing equipment and funding difficulties to implement (Labrosse, Hernlund, & Coltice, 2007) such as: it is not impossible to the study structure at 100GPa pressure at the present time, to solve this problem, it is necessary to use theoretical models (Karki, Bhattarai, & Stixrude, 2007; Stixrude & Karki, 2005). Along with that method, melting is performed at pressures below 10GPa (Sanloup et al., 2013). To overcome these difficulties, some studies have used alternative SiO_2 to study the structure at high pressure (Sanloup, 2016). The results show that the coordination number increase from 4 to 6 at pressure (P), P=5÷40GPa (Meade, Hemley, & Mao, 1992; Sato & Funamori, 2008; Sato & Funamori, 2010; Benmore et al., 2010) and coordination number is 6 when P=101.5GPa. Brillouin scattering (Murakami & Bass, 2010) showed the effect of P=140GPa on the deformation of the material. Recently, the results show that coordination number can be greater than 6 and the pressure can be up to 172GPa (Prescher et al., 2017;

Kono et al., 2016). However, the results of SiO_2 (Murakami & Bass, 2011) do not provide direct information on the structure of $MgSiO_3$. In addition, the results show that Mg in $MgSiO_3$ has coordination number of 6 and octahedral structure (Wilding et al., 2004) (With four neighboring atoms O with a Mg-O link of 2.08Å and two neighboring atoms O with a Mg-O link of 2.50Å), or coordination number of 4 with a tetrahedral structure with an Mg-O link of 2.04Å (Taniguchi et al., 1997) and a MgO with a coordination number of 4 or 5. Recent results show that Mg has a coordination number of 6 (Shimoda & Okuno, 2006) and $MgSiO_3$ has phase transition temperature (T_m), T_m=2150K. When the temperature increases (T) near the crystallization temperature (T_g), the viscosity increases (Kohara et al., 2004). The linking length of $MgSiO_3$ with simulation method is 2.28Å, neutron diffraction method and X-ray diffraction method combined with Monte Carlo method (MC) is 2.23Å (Sato & Funamori, 2010). With the simulation method, the coordination number of Mg is 5 or 6 and the coordination number of 6 is dominant (Spera et al., 2011; Kohara et al., 2011). With the combination of X-ray diffraction method, neutron diffraction method with Monte Carlo simulation method, the coordination number of Mg in $MgSiO_3$ is 4 or 5 Taniguchi et al., 1997; Spera et al., 2011; Kohara et al., 2011; Shimoda & Okuno, 2006; Klotz et al., 1995; Cormier & Cuello, 2011; Lee et al., 2005; Kubicki & Lasaga, 1991; Benmore et al., 2011; Al-Hasni & Mountjoy, 2014). However, with other results, the coordination number is greater than 5.1 (Lee et al., 2005) and $MgSiO_3$ structure is synthesized MgO_4, MgO_5 with SiO_4. This shows that experimental methods and simulation methods are the main tool to study $MgSiO_3$ structure at amorphous state, liquid state, and especially to study the structure at room temperature and phase transition temperature at high pressure with a linking length of Mg-O of 1.9÷1.96Å (Matsui & Kawamura, 1980). Meanwhile, Kubicki and Lasagna have studied Mg in a deformed model with 3 or 4 neighboring atoms O, the bonding length of Mg-O is 2Å and O-O is 2.2Å (Kubicki & Lasagna, 1991; Kubicki & Lasaga, 1991). With the recent results, the linking length of Mg-O is 2.07Å and the coordination number is 5 or 7. However, factors effecting the structure as atomic number, temperature and pressure at different temperatures have not been elucidated and what will happen to the structure if the pressure is high at room temperature 300K, high temperature 2000K, this is very interesting and necessary for applications in the glass industry and Earth.

2. Calculation Method

Initially, $MgSiO_3$ bulks with atomic number (N), N=2000 atoms, 3000 atoms, 4000 atoms, 5000 atoms, 6000 atoms were randomly placed into the cube by Molecular Dynamics (MD) method with the Born-Mayer (BM) potential and recirculating boundary conditions (Dung, 2018).

$$U_{ij}(r)=\frac{Z_iZ_je^2}{r}+A_{ij}\exp(-B_{ij}r_{ij})-\frac{C_{ij}}{r_{ij}^6} \quad (1)$$

In which: $U_{ij}(r)$ (eV) is the pairing potential energy; r_{ij}(Å) is the distance between atoms; The coefficients A_{ij}, B_{ij}, C_{ij} are determined from elastic and network constants; Z_i, Z_j are the charges of ions i and j, respectively, shown in Table 1.

Table 1. The parameters of $MgSiO_3$ bulk

	Si-Si	Si-O	O-O	Si-Mg	O-Mg	Mg-Mg
A_{ij} (eV)	0	1137.9639	2024.686563	0	1042.37635	0
B_{ij} (Å^{-1})	0	3.4373187	3.739716	0	3.25918353	0
C_{ij} (Å^{-1})	0	0	3.3052647	0	0	0
Z_i(e)	0	2.4	-1.2	0	1.2	0

Initially, all samples at temperature (T), T=7000K were lowered temperature to T=300K with a heating rate of 10^6K/s and time of each simulation step MD was 0.478fs; $MgSiO_3$ bulks with 5000 atoms were increased in temperature from T=300K to T=500K, 1000K, 1500K, 2000K, 2500K, 3000K, 3500K at pressure (P), P=0GPa; $MgSiO_3$ bulk model with 5000 atoms at temperature T=300K, 2000K increases at pressure from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa. With $MgSiO_3$ bulk obtained, run 10^5 step recovery statistics, run $2x10^5$ step NVT (with constant atomic number, volume, the temperature), run $2x10^5$ step NVP (with constant atomic number, volume, pressure) and run $4x10^5$ step NVE (with constant atomic number, volume, energy) to the system reaches equilibrium. With samples at equilibrium, study the structure through radial distribution function (RDF), coordination number, energy (E), size (l), angle distribution and phase transition temperature (T_m) through energy (E), temperature (T) and temperature of the system complying with the formula Nosé-Hoover (Nos´e, 1984; Hoover, 1985).

3. Results and Discussion

3.1 Effect of Atomic Number

$MgSiO_3$ bulk with atomic number (N), N=2000 atoms at a temperature (T), T=300K have structural shape, size (l), energy (E) and radial distribution function (RDF), the results are shown in Figure 1, Figure 2 and Figure 3.

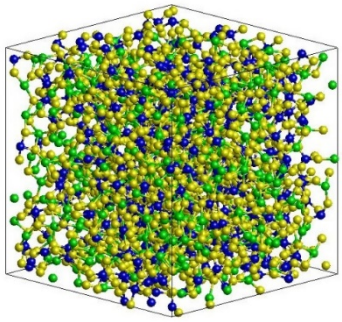

Figure 1. Structure shape of $MgSiO_3$ bulk with 2000 atoms at 300K temperature.

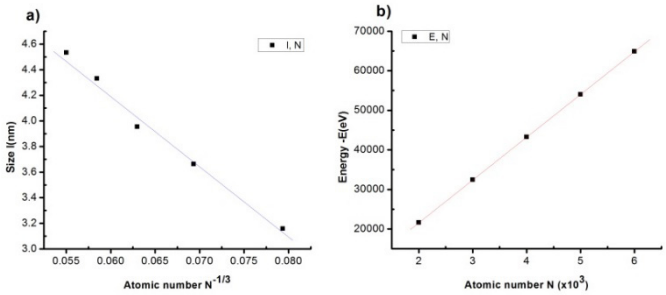

Figure 2. The energy, size of $MgSiO_3$ bulk at temperature 300K with different atomic numbers

The results show that $MgSiO_3$ bulk with atomic number (N), N=2000 atoms at temperature (T), T=300K has cube-shaped and made of three atomic types (Figure 1) (blue of Mg dark, green of Si, and yellow O), size (l), l=3.157nm, energy (E), E=-21623.33eV. When increasing atomic number (N), from N=2000 atoms to N=3000 atoms, 4000 atoms, 5000 atoms, 6000 atoms lead to an increase in size (Figure 2), satisfying the formula: $l = 7.6 - 56N^{-1/3}$, energy of sample decreases and proportional to N^{-}. The results show that l proportional to $N^{-1/3}$ and E proportional to N^{-}. This result is perfectly consistent with previously published results such as crystallization temperature (T_g) in proportion to $N^{-1/3}$ (Qi et al., 2001) and size (l or D) is proportional to $N^{-1/3}$ with Ni nanoparticles or CuNi nanoparticles (Dung, 2018; Nguyen, 2017; Nguyen et al., 2017). To find out this, research the radial distribution function (RDF), the results are shown in Figure 3, Table 2a and Table 2b.

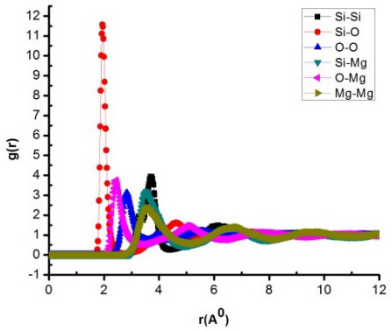

Figure 3. The radial distribution function of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg at temperature 300K

Table 2a. The linking length of Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg with different atomic numbers

Atoms number (atoms)	r_{ij} (Å)					
	Si-Si	Si-O	O-O	Si-Mg	O-Mg	Mg-Mg
2000	3.7	1.94	2.82	3.54	2.44	3.58
3000	3.72	1.94	2.82	3.54	2.42	3.6
4000	3.68	1.96	2.82	3.52	2.42	3.58
5000	3.68	1.94	2.84	3.56	2.42	3.6
6000	3.72	1.94	2.82	3.5	2.42	3.56

Table 2b. Height of radial distribution function of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg with different atomic numbers

Atoms number (atoms)	$g_{ij}(r)$					
	Si-Si	Si-O	O-O	Si-Mg	O-Mg	Mg-Mg
2000	3.93	11.57	3.12	3.2	3.75	2.37
3000	3.93	12.29	3.09	3.07	3.94	2.25
4000	3.78	11.69	3.16	3.23	3.71	2.46
5000	3.87	11.88	3.03	3.07	3.85	2.3
6000	3.87	11.23	3.09	3.1	3.73	2.39

The results show that $MgSiO_3$ bulk with N=2000 atoms at T=300K has the first peak position of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg has to occupy a dominant position corresponding to linking length of ~~is~~ 3.7Å, 1.94Å, 2.82Å, 3.54Å, 2.44Å, 3.58Å (Figure 3, Table 2a) and the height of the radial distribution function g(r) has a corresponding value of 3.93, 11.57, 3.12, 3.2, 3.75, 2.37. When increasing N, from N=2000 atoms to N=3000 atoms, 4000 atoms, 5000 atoms, 6000 atoms, the first peak position of RDF and g(r) of the links are not significantly changed (Table 2a and Table 2b). This shows that the linking length of Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg does not depend on the atomic number, there is no far distant order, but close order exists. To confirm the accuracy of the results, study the coordination numbers of the links in Table 3a, Table 3b.

Table 3a. The coordination number of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg at temperature 300K, pressure 0GPa with different atomic numbers

Atoms number (atom)	Si-Si	Si-O	O-O	Si-Mg	O-Mg	Mg-Mg
2000	5	5	12	6	2	6
3000	5	5	13	6	2	7
4000	5	6	13	7	2	7
5000	5	5	13	6	2	6
6000	5	6	13	6	2	7

Table 3b. The density of coordination number of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg at temperature 300K, pressure 0GPa with different atomic numbers

Atoms number (atom)	Si-Si	Si-O	O-O	Si-Mg	O-Mg	Mg-Mg
2000	100	206	290	85	390	74
3000	176	338	421	141	618	119
4000	206	407	587	178	855	160
5000	263	545	702	229	1028	203
6000	324	639	854	240	1205	234

The results show that, with N=2000 atoms then the coordination number of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg has the corresponding value of 5, 5, 12, 6, 2, 6. When increasing N, from N=2000 atoms to N=3000 atoms, 4000 atoms, 5000 atoms, 6000 atoms, the coordination number of links Si-Si and O-Mg has constant value; the coordination numbers of links Si-O, O-O, Si-Mg, Mg-Mg are variable but not significant (Table 3a) and the density of coordination numbers of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg increases (Table 3b).

The cause of the change in coordination number, the density of coordination numbers is due to heterogeneity in the sample: the increase in the number of atoms leads to the size (l), the energy (E) of the samples increases, the bonding length of Si-Si, Si-O, O-O, Si-Mg, O-Mg increases leads to structural change. Next, using the visual method to study the number of structural units and the density of structural units of TOx links (T is Si or Mg), x=4, 5, 6, 7, 8, 9, 10, 11, 12, results in Figure 4, Table 4a and Table 4b.

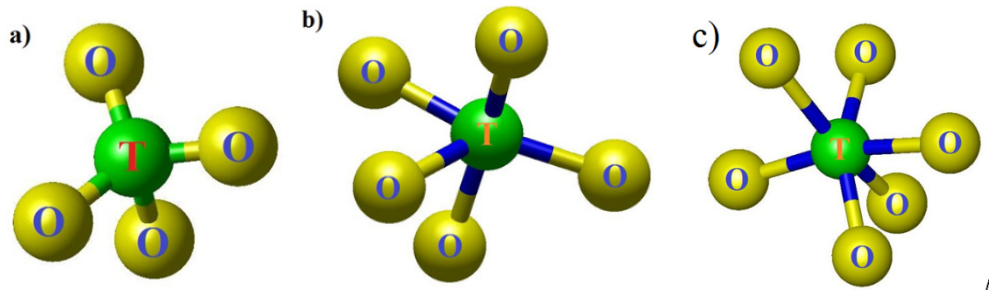

Figure 4. The number of structural units of TO_x (T is Si or Mg) with x=4 (Figure a), x=5 (Figure b), x=6 (Figure c), ... (Dung, 2018)

Table 4a. The number of structural units of SiO_x, MgO_x of $MgSiO_3$ bulk at temperature 300K, pressure 0GPa with different atomic numbers

Atoms number (atom)	2000	3000	4000	5000	6000
SiO_4 (degrees)	100	105	105	105	105
SiO_5 (degrees)	90	90	90	90	90
SiO_6 (degrees)	85	90	85	90	85
MgO_3 (degrees)	0	0	0	0	0
MgO_4 (degrees)	90	95	95	95	95
MgO_5 (degrees)	90	90	90	90	80
MgO_6 (degrees)	85	60	60	60	60
MgO_7 (degrees)	60	60	60	60	60
MgO_8 (degrees)	60	60	60	60	60
MgO_9 (degrees)	60	60	60	55	60
MgO_{10} (degrees)	60	60	55	55	60

Table 4b. The density of structural units of SiO_x, MgO_x of $MgSiO_3$ bulk at temperature 300K, pressure 0GPa with different atomic numbers

Atoms number (atom)	2000	3000	4000	5000	6000
SiO_4	14	35	10	46	25
SiO_5	325	511	613	840	829
SiO_6	470	574	1050	1016	1593
MgO_3	0	0	0	0	0
MgO_4	7	23	9	33	47
MgO_5	58	123	116	202	274
MgO_6	141	251	313	401	522
MgO_7	198	242	430	429	483
MgO_8	102	95	249	196	147
MgO_9	21	21	56	41	23
MgO_{10}	3	1	6	5	3

The results show that, for N=2000 atoms, the number of structural units of SiO_x is SiO_4, SiO_5, SiO_6, and MgO_x are MgO_3, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9, MgO_{10}, MgO_{11}, MgO_{12} (Figure 4). Angle distribution of SiO_4, SiO_5, SiO_6 là 100^0, 90^0, 85^0 and MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9, MgO_{10} is 90^0, 90^0, 85^0, 60^0, 60^0, 60^0,

60^0. The density of structural units of SiO_4, SiO_5, SiO_6, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9, MgO_{10} is 14, 325, 470, 7, 58, 141, 198, 102, 21, 3. When increasing atomic number N, from N=2000 atoms to N=3000 atoms, 4000 atoms, 5000 atoms, 6000 atoms, the angle distribution of SiO_5, MgO_7, MgO_8 is constant and the angle of SiO_4, SiO_6, MgO_4, MgO_5, MgO_6, MgO_9, MgO_{10} has no significant change (Table 4a, Table 4b). The obtained results were consistent with the results (Lee et al., 2005) and showed the influence of N on structural characteristics such as r, g(r), number of structural units, number of density of structural units, coordination number, density of coordination number and l is proportional to $N^{-1/3}$ and E is proportional to N^{-1}.

3.2 Influence of Temperature

$MgSiO_3$ bulk 5000 atoms, using visualization method at temperature T=300K, the result of structural shape and transition temperature is shown in Figure 5, radial distribution function in Figure 6.

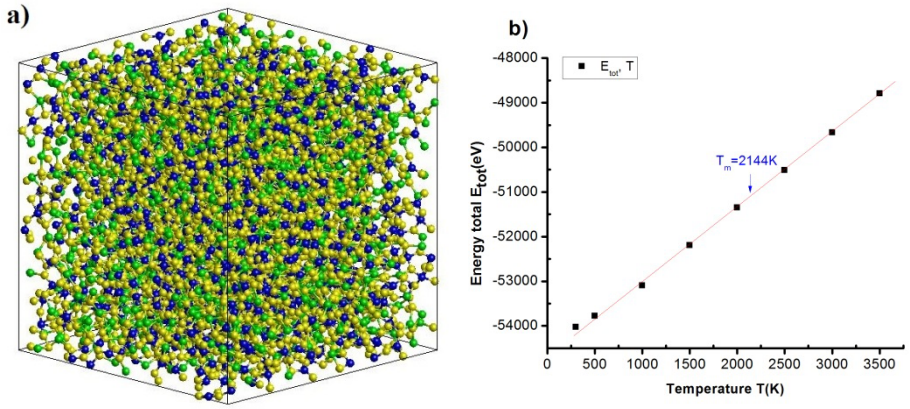

Figure 5. The structural shape of $MgSiO_3$ bulk 5000 atoms at temperature 300K (Figure a), phase transition temperature of $MgSiO_3$ bulk model with 5000 atoms at different temperatures (Figure b)

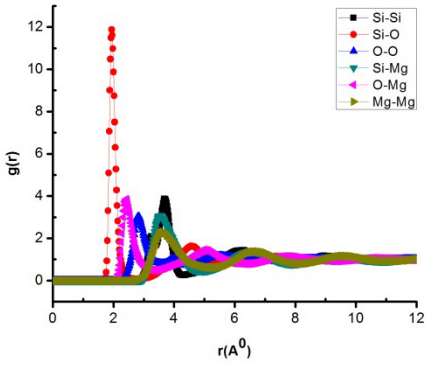

Figure 6. The radial distribution function of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg at temperature 300K

Table 5a. The bond length of Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg at different temperature

Temperature (K)	r_{ij} (Å)					
	Si-Si	Si-O	O-O	Si-Mg	O-Mg	Mg-Mg
300	3.68	1.94	2.84	3.56	2.42	3.6
500	3.7	1.94	2.84	3.54	2.42	3.64
1000	3.72	1.92	2.84	3.62	2.42	3.8
1500	3.66	1.88	2.88	3.72	2.4	3.94
2000	3.62	1.88	2.88	3.76	2.34	3.8
2500	3.64	1.86	2.94	3.8	2.36	3.84
3000	3.58	1.86	2.9	3.78	2.3	3.92
3500	3.6	1.82	3	3.82	2.26	4.1

Table 5b. The height of the radial distribution function of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg at different temperatures

Temperature (K)	$g_{ij}(r)$ Si-Si	Si-O	O-O	Si-Mg	O-Mg	Mg-Mg
300	3.87	11.88	3.03	3.07	3.85	2.3
500	3.71	10.65	2.89	2.97	3.4	2.29
1000	3.37	8.91	2.56	2.76	2.71	1.98
1500	3.03	8.73	2.19	2.48	2.48	1.68
2000	2.83	8.5	2.06	2.29	2.32	1.52
2500	2.73	8.52	1.98	2.12	2.27	1.44
3000	2.63	8.67	1.97	2.06	2.25	1.38
3500	2.7	8.79	1.97	1.98	2.25	1.34

The results show that $MgSiO_3$ bulk model with 5000 atoms at temperature T=300K have cube-shaped (Figure 5a), size l=4.236nm, energy E=-70306.32eV. When T increases, from T=300K to T=500K, 1000K, 1500K, 2000K, 2500K, 3000K, 3500K, l increases from l=4.236nm to l=4.348nm, 4.398nm, 4.583nm, 4.731nm, 4.884nm, 5.071nm, 5.257nm and E increases leads to a phase transition temperature (T_m), T_m=2144K (Figure 5b). This result is consistent with the empirical results (Kohara et al., 2004). The results show that, at temperature T=300K, the first peak of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg of the radial distribution function is dominant and the bonding length is 3.68Å, 1.94Å, 2.84Å, 3.56Å, 2.42Å, 3.6Å (Figure 6, Table 5a). When increasing the temperature (T), from T=300K to T=500K, 1000K, 1500K, 2000K, 2500K, 3000K, 3500K, the first peak position of the links was not changed significantly (Table 5a), and g(r) decreased sharply (Table 5b). Combined with the above results, the increase in temperature leads to E, l increase and atomic density decrease. This shows that the internal molecular distance between the links does not depend on temperature leading to the non-existence of distant order but there is always the existence of close order. In order to confirm the accuracy of the results, research the coordination number, the density of coordination number of the links and the results are shown in Figure 7.

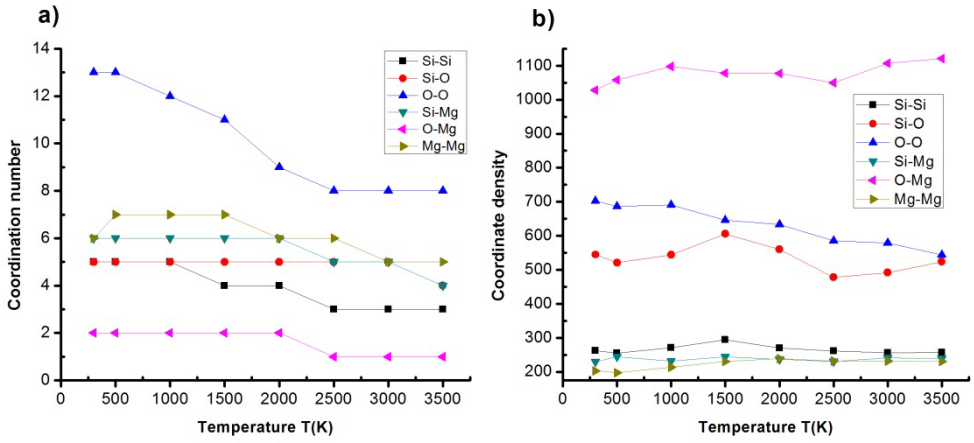

Figure 7. The coordination number (Figure a), coordination number density (Figure b) at different temperatures

The results show that $MgSiO_3$ bulk model with 5000 atoms at temperature T=300K has a coordination number of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg is 5, 5, 13, 6, 2, 6. When increasing T from T=300K to T=500K, 1000K, 1500K, 2000K, 2500K, 3000K, 3500K, the coordination number of the links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg has a large change value (Figure 7a). The coordination number-density of the links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg has negligible value changes (Figure 7b). The main cause of the changes link and density of coordination number is due to the heterogeneity in the sample: When the temperature increases, l, E increases of and the length of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg changes lead to structural change. Next, studying structural unit number SiO_x, MgO_x in $MgSiO_3$ bulk model with 5000 atoms, the results are shown in Table 6.

Table 6a. Number of structural units SiO_x, MgO_x of $MgSiO_3$ bulk model with 5000 atoms at different temperatures

Temperature (K)	300	500	1000	1500	2000	2500	3000	3500
SiO_4 (degrees)	105	105	105	105	100	100	100	100
SiO_5 (degrees)	90	90	90	90	90	90	90	90
SiO_6 (degrees)	90	90	85	85	85	80	85	80
MgO_3 (degrees)	0	95	0	105	95	105	100	100
MgO_4 (degrees)	95	95	100	95	95	95	95	100
MgO_5 (degrees)	90	90	90	95	90	90	60	60
MgO_6 (degrees)	60	60	60	60	60	60	60	60
MgO_7 (degrees)	60	60	60	60	55	60	60	55
MgO_8 (degrees)	60	60	55	55	55	60	55	55
MgO_9 (degrees)	60	50	55	55	55	55	55	55
MgO_{10} (degrees)	55	50	55	55	55	0	0	0

Table 6b. Number of structural units SiO_x, MgO_x of $MgSiO_3$ bulk model with 5000 atoms at different temperatures

Temperature (K)	300	500	1000	1500	2000	2500	3000	3500
SiO_4	46	40	42	155	237	285	309	306
SiO_5	840	765	709	676	563	434	347	288
SiO_6	1016	1022	834	340	178	127	87	70
MgO_3	0	1	0	5	10	29	33	33
MgO_4	33	23	16	49	70	109	105	93
MgO_5	202	157	110	165	172	162	145	133
MgO_6	401	351	282	276	235	140	120	116
MgO_7	429	447	418	250	171	64	56	58
MgO_8	195	237	328	129	73	16	15	20
MgO_9	40	80	132	39	18	3	3	4
MgO_{10}	5	10	28	7	3	0	0	0

The results show that, $MgSiO_3$ bulk model with 5000 atoms at temperature T=300K has structural units is SiO_4, SiO_5, SiO_6, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9, MgO_{10} with an angle distribution of 105^0, 90^0, 90^0, 95^0, 90^0, 60^0, 60^0, 60^0, 60^0, 55^0 and a density of structural units is 46, 840, 1016, 33, 202, 401, 429, 195, 40, 5. When temperature T is increased, from T=300K to T=500K, 1000K, 1500K, 2000K, 2500K, 3000K, 3500K, SiO_5, MgO_6 have a constant value of 90^0, 60^0, other angle distributions and number density of structural unit has change value as MgO_3 appears at T=500K, disappears at T=1000K and stabilizes at 1500K; MgO_{10} disappears at T=2500K and SiO_4, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9 have a variable angle distribution and the densities of angle distribution changed (Table 6a, Table 6b). With the disappearance of MgO_{10} at T=2500K, it raises the question of whether this is a phase transition temperature or not. The results show that in the temperature range from T=2000K to T=2500K the number of structural units of SiO_4, SiO_5, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9, MgO_{10} has a big change, leading to the disappearance of structure units MgO_{10}. To answer the above questions, continue to study the structure at temperatures 300K, 2000K with different pressure values.

3.3 Effect of Pressure

3.3.1 Effect of Pressure at Temperature 300K

$MgSiO_3$ bulk model with 5000 atoms at temperature T=300K with pressure P=0GPa, 20GPa, 40GPa, 60GPa, 80GPa, 100GPa, results are shown in Figure 8.

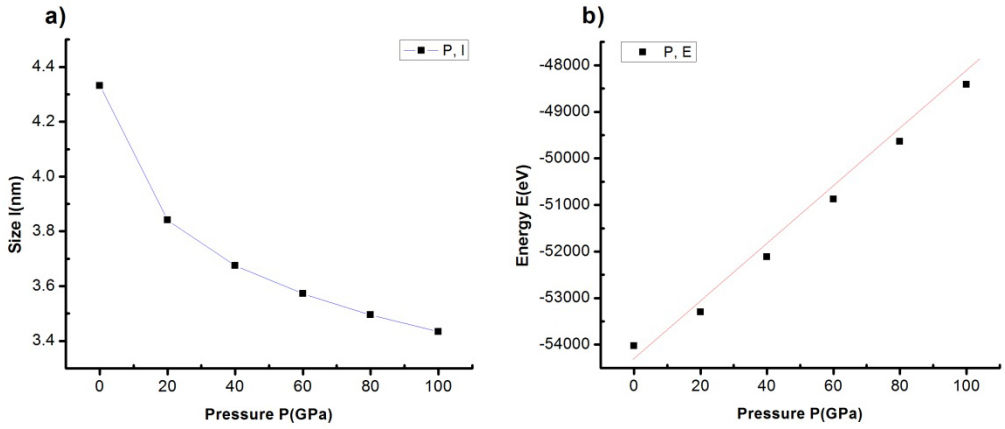

Figure 8. The relationship between pressure, size (Figure a), pressure, energy (Figure b) of $MgSiO_3$ bulk at temperature 300K

The results show that, $MgSiO_3$ bulk model with 5000 atoms at pressure P=0GPa has size l=4.332nm, energy E=-54028.51eV. When increasing P from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa leading to l decreases from l=4.332nm to 3.434nm (Figure 8a) and E increases from E=-54028.51eV to -48415.37eV (Figure 8b). To confirm this, study structure of the links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg, the results are shown in Figure 9.

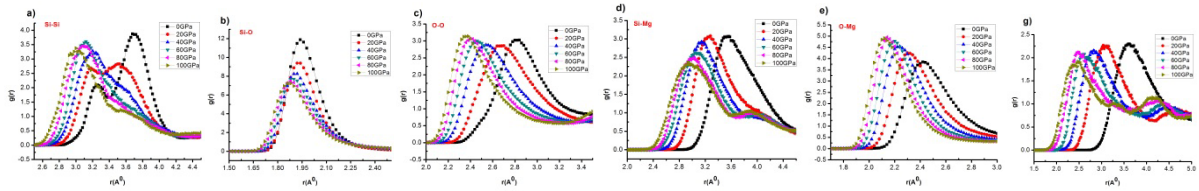

Figure 9. The radial distribution function of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg at temperature 300K with different pressures

The results show that $MgSiO_3$ bulk model with 5000 atoms at pressure P=0GPa, temperature T=300K has the first pick position of RDF is r=3.68Å, the height of RDF is g(r)=3.87. When increasing P, from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa, the first peak position of RDF gradually shifted to left and height g(r) increased with links O-Mg, Si-Si and reduced with links Si-O, O-O, Si-Mg, Mg-Mg (Figure 9). To confirm this, study the coordination number and the density of coordination number, results are shown in Figure 10.

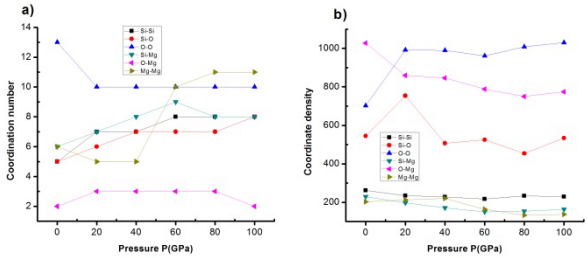

Figure 10. The coordination number (Figure a), the density of coordination number (Figure b) at different pressures

The results show that $MgSiO_3$ bulk model with 5000 atoms at temperature T=300K with pressure P=0GPa has a coordination number of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg is 5, 5, 13, 6, 2, 6. When increasing P from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa, the coordination number of the links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg has great change value (Figure 10a). The density of coordination number of links Si-Si,

Si-Mg, Mg-Mg has changed insignificantly, while the density of coordination number of links O-O, Si-O, O-Mg have great change value (Figure 10b). The reason for the change of links, coordination number and density of coordination number are the heterogeneity in sample, because: increasing P leads to size l decreases, increasing energy E and the linking length of Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg changes leading to structural changes. Next, studying the number of structural units, the density of structural units of SiO_x, MgO_x, the results are shown in Table 7a and Table 7b.

Table 7a. The number of structural unit SiO_x, MgO_x of $MgSiO_3$ bulk model with 5000 atoms at temperature 300K with different pressures

Pressures (GPa)	0	20	40	60	80	100
SiO_4 (degrees)	105	0	0	0	0	0
SiO_5 (degrees)	90	85	85	0	0	0
SiO_6 (degrees)	90	85	85	80	80	80
MgO_3 (degrees)	0	0	0	0	0	0
MgO_4 (degrees)	95	0	0	0	0	0
MgO_5 (degrees)	90	85	0	0	0	0
MgO_6 (degrees)	60	80	75	75	85	75
MgO_7 (degrees)	60	65	70	70	70	70
MgO_8 (degrees)	60	65	65	65	65	65
MgO_9 (degrees)	55	65	65	65	65	65
MgO_{10} (degrees)	55	60	60	60	60	60
MgO_{11} (degrees)	0	60	55	60	60	60
MgO_{12} (degrees)	0	55	55	55	0	50

Table 7b. The density of structural unit SiO_x, MgO_x of $MgSiO_3$ bulk model with 5000 atoms at temperature 300K with different pressures

Pressures (GPa)	0	20	40	60	80	100
SiO_4	46	0	0	0	0	0
SiO_5	840	40	4	0	0	0
SiO_6	1016	1691	692	362	166	73
MgO_3	0	0	0	0	0	0
MgO_4	33	0	0	0	0	0
MgO_5	202	2	0	0	0	0
MgO_6	401	46	22	6	9	7
MgO_7	429	349	285	166	215	142
MgO_8	195	905	998	876	989	899
MgO_9	41	891	1023	1317	1242	1301
MgO_{10}	5	298	419	580	532	680
MgO_{11}	0	32	81	91	86	102
MgO_{12}	0	2	2	8	0	5

The result show that $MgSiO_3$ bulk model with 5000 atoms at temperature T=300K, pressure P=0GPa has structural units are SiO_4, SiO_5, SiO_6, MgO_3, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9, MgO_{10}, MgO_{11}, MgO_{12} corresponding to the angle distribution of 105^0, 90^0, 90^0, 0^0, 95^0, 90^0, 60^0, 60^0, 60^0, 60^0, 55^0, 55^0, 0^0, 0^0. When increasing P, from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa leading to angle distribution and the number density of structural unit SiO_4, SiO_5, SiO_6, MgO_3, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9, MgO_{10}, MgO_{11}, MgO_{12} has a very large change as SiO_4, MgO_4 disappear at P=20GPa; MgO_{11}, MgO_{12} appear at P=20GPa and angle distribution of SiO_5, MgO_5 decrease at P=20GPa; SiO_5 disappears at P=60GPa; angle distribution SiO_6 decreases at P=20GPa and angle distributions MgO_8, MgO_9, MgO_{10} increase at P=20GPa (Table 7a) and changes in the density of structural units are very big (Table 7b).

3.3.2 Effect of Pressure at Temperature 2000K

$MgSiO_3$ bulk model with 5000 atoms at temperature T=2000K with pressure P=0GPa, 20GPa, 40GPa, 60GPa, 80GPa, 100GPa, results are shown in Figure 11.

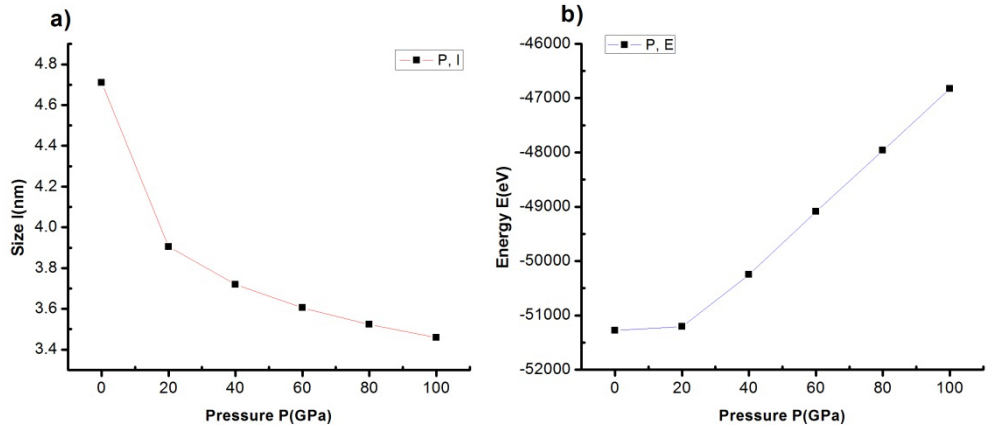

Figure 11. The relationship between pressure and size (Figure a), pressure and energy (Figure b) of $MgSiO_3$ bulk model with at temperature 2000K with different pressures

The result show that, $MgSiO_3$ bulk model with 5000 atoms at temperature T=2000K with pressure P=0GPa has size l=4.711nm, energy E= -51279.79eV. When increasing P from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa leads to l decreases from l=4.711nm to l=3,458nm (Figure 11a), E increases from E=-51279.79eV to E=-46823.94eV (Figure 11b). To confirm this, study the structure of the links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg, results are shown in Table 8a, Table 8b.

Table 8a. The linking length of Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg at temperature 2000K with different pressures

Pressure	r_{ij} (Å)					
P (GPa)	Si-Si	Si-O	O-O	Si-Mg	O-Mg	Mg-Mg
0	3.66	1.86	2.88	3.74	2.34	3.82
20	3.44	1.9	2.66	3.34	2.28	3.08
40	3.26	1.9	2.56	3.2	2.22	2.88
60	3.18	1.9	2.48	3.14	2.18	2.7
80	3.12	1.88	2.44	3.04	2.16	2.66
100	3.06	1.88	2.38	3.06	2.12	2.48
Results			2.2 (Kubicki & Lasaga, 1991)		1.9-1.96 (Matsui & Kawamura, 1980) 2.07 (Shimoda & Okuno, 2006), 2.04 (Taniguchi et al., 1997) 2.05, 2.08 (Wilding et al., 2004) 2.0 (Kubicki & Lasaga, 1991; Kubicki & Lasagna, 1991)	

Table 8b. The height radial distribution function of link Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg at temperature 2000K with different pressures

Pressure (GPa)	$g_{ij}(r)$					
	Si-Si	Si-O	O-O	Si-Mg	O-Mg	Mg-Mg
0	2.89	8.31	2.05	2.18	2.32	1.56
20	2.66	5.48	2.17	2.47	2.7	1.85
40	2.91	5.25	2.28	2.42	3.03	1.91
60	3.06	5.08	2.38	2.3	3.24	1.91
80	3.16	5.1	2.47	2.25	3.43	1.98
100	3.24	5.09	2.54	2.15	3.55	1.92

The result show that, $MgSiO_3$ bulk model with 5000 atoms at temperature T=2000K with pressure P=0GPa, the first peak position of links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg are r=3.66Å, 1.86Å, 2.88Å, 3.74Å, 2.34Å, 3.82Å (Table 8a) and the height of first peak position of RDF g(r)=2.89, 8.31, 2.05, 2.18, 2.32, 1.56 (Table 8a). When increasing P, from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa leads to the first peak position of RDF moves gradually to the left and g(r) increases with links Si-Si, O-O, Si-Mg, O-Mg, Mg-Mg and reduces with link Si-O. The results are consistent with results (Wilding et al., 2004; Taniguchi et al., 1997; Lee et al., 2005; Matsui & Kawamura, 1980; Kubicki & Lasagna, 1991; Shimoda & Okuno, 2006). To confirm this, study the coordination number and the density of coordination number, as shown in Figure 12.

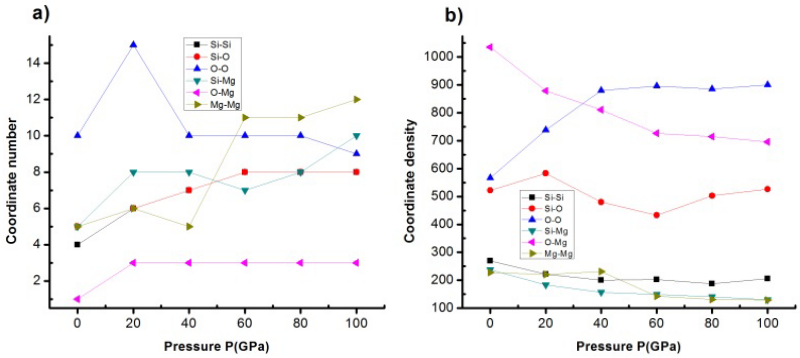

Figure 12. The coordination numbers (Figure a), the coordinate numbers density (Figure b) at temperature 200K with different pressures

The result show that, $MgSiO_3$ bulk model with 5000 atoms at temperature T=2000K with pressure P=0GPa has the coordination numbers of the links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg are 4, 5, 10, 5, 1, 5. When increasing P, from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa leading to the coordination numbers of the links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg have great change value (Figure 12a). The density of coordination numbers of the links Si-Si, Si-Mg, Mg-Mg changes significantly and the density of coordination numbers of links O-O, Si-O, O-Mg, O-Mg are greatly changed (Figure 12b). The cause of the changes of the links, coordination number and density of coordination numbers is the heterogeneity in the sample, because: When increasing P leads to l, E increase, length of the links Si-Si, Si-O, O-O, Si-Mg, O-Mg, Mg-Mg changes leading to structural change. Next, study the number of structural units of the links SiO_x, MgO_x, the results are shown in Table 9a and Table 9b.

Table 9a. The angle distribution of the number of structural units SiO_x, MgO_x at temperature 2000K with different pressures

Pressure (GPa)	0	20	40	60	80	100
SiO_4 (degrees)	100	0	0	0	0	0
SiO_5 (degrees)	90	85	85	0	0	0
SiO_6 (degrees)	85	85	80	80	85	85
MgO_3 (degrees)	100	0	0	0	0	0
MgO_4 (degrees)	95	0	0	0	0	0
MgO_5 (degrees)	65	0	0	0	0	0
MgO_6 (degrees)	60	80	75	75	75	70
MgO_7 (degrees)	60	70	70	70	70	70
MgO_8 (degrees)	60	65	65	65	65	65
MgO_9 (degrees)	55	60	65	65	65	65
MgO_{10} (degrees)	0	60	60	60	60	60
MgO_{11} (degrees)	0	55	55	55	55	55
MgO_{12} (degrees)	0	55	55	55	55	55

The results show that $MgSiO_3$ bulk model with 5000 atom at temperature T=2000K with pressure P=0GPa has structural units are SiO_4, SiO_5, SiO_6, MgO_3, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9, MgO_{10}, MgO_{11}, MgO_{12}

corresponding to the angle distribution of 105^0, 90^0, 85^0, 100^0, 95^0, 65^0, 60^0, 60^0, 60^0, 55^0, 0^0, 0^0, 0^0. When increasing P, from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa leading to SiO_4, SiO_5, SiO_6, MgO_3, MgO_4, MgO_5, MgO_6, MgO_7, MgO_8, MgO_9, MgO_{10}, MgO_{11}, MgO_{12} have great change value when SiO_4, MgO_4, MgO_3, MgO_5 disappear at P=20GPa, MgO_{10}, MgO_{11}, MgO_{12} appear at P=20GPa and angle distribution SiO_5 decreases at P=20GPa and angle distribution MgO_8, MgO_9 increase at P=20GPa (Table 9a) leads to very big change of the density of structural unit (Table 9b). The results show that the influence of factors on the structure of $MgSiO_3$ bulk is very big.

Table 9b. The density of angle distribution of the number of structural units SiO_x, MgO_x at temperature 2000K with different pressures

Pressure (GPa)	0	20	40	60	80	100
SiO_4	271	0	0	0	0	0
SiO_5	537	69	5	0	0	0
SiO_6	150	983	429	136	57	22
MgO_3	25	0	0	0	0	0
MgO_4	109	0	0	0	0	0
MgO_5	177	0	0	0	0	0
MgO_6	172	22	9	7	8	5
MgO_7	84	179	128	137	154	131
MgO_8	23	598	617	677	742	759
MgO_9	4	848	1011	1064	1073	1161
MgO_{10}	0	544	648	622	597	590
MgO_{11}	0	173	181	158	123	123
MgO_{12}	0	26	27	19	13	8

4. Conclusion

The results show that, $MgSiO_3$ bulk has cube-shaped, nano-size and is determined by Molecular Dynamics (MD) method with Born-Mayer (BM) potential and periodic boundary conditions. Successfully determine the influence of atomic number, temperature (T), pressure (P) at T=300K, 2000K to the structure of $MgSiO_3$ bulk. Especially, at T=2000K, when increasing P, from P=0GPa to P=20GPa, 40GPa, 60GPa, 80GPa, 100GPa leading to the first peak position of RDF moving gradually to left and height g(r) increases with the links Si-Si, O-O, Si-Mg, O-Mg, Mg-Mg and decreases with the link Si-O. The results are consistent with the results (Wilding et al., 2004; Taniguchi et al., 1997; Lee et al., 2005; Matsui & Kawamura, 1980; Kubicki & Lasagna, 1991; Shimoda & Okuno, 2006). The reason is due to the size effect, when atomic number increases (temperature), the size increases, the energy decreases (increases) and when the pressure increases leading to size decreases, energy increases: When increasing P at T=300K the number of structural unit SiO_4, MgO_4 appears at P=20GPa and MgO_{11}, MgO_{12} disappear at P=20GPa; MgO_5 disappears at P=40GPa, SiO_4 disappears at P=60GPa. When increasing P at T=2000K, MgO_{10}, MgO_{11}, MgO_{12} appear at P=20GPa; SiO_4, MgO_3, MgO_4, MgO_5 disappear at P=20GPa; SiO_4 disappears at P=60GPa. This shows that, when increasing P, the structure at T=300K is always more stable at high temperature T=2000K leading to the number of structural units, the density of structural units at T=2000K has a very big change.

Conflict of interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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