

Measurement of ZnO Atomic Distances under Isothermal and Isobaric Ensembles: A Molecular Dynamics Prediction

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ABSTRACT: Zinc Oxide (ZnO) chemical bonds have stayed between covalent and ionic liaisons; this appears in its thermodynamic behavior and the atomic distances under extended pressure and temperature. In this work, the impact of pressure and temperature is focused on the distance between the atoms of unit cell O-O, O-Zn, and Zn-Zn (1458 atoms of O²⁻ and 1458 of Zn²⁺) under the range of pressure (0-200 GPa) and temperature of range 300-3000K. Molecular Dynamics (MDs) technique and DL_POLY_4 software are employed on the RAVEN Supercomputer of Cardiff University (UK). The interatomic interactions are modeled using Buckingham potential for short-range and Coulomb potential for long-range. This paper calculates and confirms the effect of pressure and temperature on Zn-O bond length which is less than that on Zn-Zn and O-O bonds, also the relationship of these lengths, standard error, standard deviation, the mean, the maximum values of the radial distribution function, the percentage of variation, and finally the validity of Buckingham's potential for ionic and

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covalent chemical liaisons are reported. The obtained results are in the vicinity of available theoretical and experimental data; these results would have great importance in nanotechnology and technology fields, especially in Medicine and Pharmaceutics.

KEYWORDS: ZnO; chemical Bond; Pressure; Temperature; MDs.

INTRODUCTION

Zinc oxide is a very important material that can be used in a variety of applications such as gas sensors [1-5], photocatalysts [6, 7], nanowires [8-15], nanorods [16-26], tetrapod, nanowhiskers [27], nano combs [17,28], nano pins [29, 30] and nano-helices [31, 32]. Zinc Oxide is still a promised semiconductor, gratitude to the kind of involved chemical liaisons; varying between covalent and ionic bonds. The wurtzite structure is the most stable at ambient conditions; the unit cell of ZnO wurtzite type contains four atoms [33 - 36], the parameters of the unit cell of wurtzite are defined as $a = b = 3.242$ (Å), $c = 5.188$ (Å), and the internal relaxation $\mu = 3/8$, where $c/a = 1.633$. The structure is formed by two interpenetrating Zinc (Zn) and Oxygen (O) hexagonal sub-lattices; each atom of Zn is surrounded by four atoms of Oxygen and vice-versa [37]. The above-mentioned parameters take values from 3.2475 to 3.2501 (Å) for a , and from 5.2042 to 5.2075 (Å) for c value [4]. Also, the ratio of c/a is determined from 1.593 to 1.6035 (Å), and μ value is given from 0.383 to 0.3856(Å).

The inter-atomic potential is modeled using Buckingham-Coulomb potential [17, 29], Zinc oxide has a challenge for modeling, due to the complex electronic structures and the existence of ionicity and covalence. Hence, a few potentials are available in one formalism [38]. There is a difference in the electro-negativity between Zn and O, which produces a charge transfer from Zn to O atoms, for rocksalt type (B1), the charge density lines are like a sphere; it is a mark of presence ionic between Zn and O atoms [39]. Zinc oxide has the wurtzite type which transfers to rocksalt under 9 GPa. Due to the approaching energy of Zn-3d and O-2p, they can hybridize together, this hybridization pushes up the valence band level, The last part of the valence band is governed by O-2s orbital and the superior part by the O-2p orbital in zinc oxide. The inferior part of the conduction band is controlled by the Zn-2s orbital. Zinc

oxide in zinc blend type and wurtzite structure is a semiconductor with a direct gap of 0.6(eV) and 0.72 (eV) and an indirect gap of 0.98(eV) for rocksalt type, and an indirect gap of 0.6eV(w), and 0.75(eV)(Zb), for rocksalt the indirect gap is 0.98eV [40-43]. The classical force fields permit to study of physical properties and the temperature impact with consideration of anharmonicities using large systems [33, 44, 45], which can be investigated using Molecular Dynamics (MDs). Although many experimental and theoretical investigations on ZnO have been conducted, there is still a need of more studies in order to determine and predict possible scenarios of phase with structural transitions of different ZnO structures using MDs approach [16, 17]. The MDs approach has been used to simulate isobaric and isothermal ensembles of ZnO under different temperatures and pressures [18-22]. Zinc oxide is a very important material that can be used in a variety of applications such as gas sensors [1-5], photocatalysts [6, 7], nanowires [8-15], nanorods [16-26], tetrapod, nanowhiskers [27], nano combs [17, 28], nano pins [29, 30] and nano-helices [31, 32]. In this paper, the impact of temperature and pressure on the distance between the atoms of the unit cell is focused on using an isobaric and isothermal ensemble, the validity of the potential of ionic and covalent bonds is confirmed, the order and disorder of crystalline and amorphous structures are noted under different pressures and temperatures, finally, the Zn-O length is less affected than Zn-Zn, and O-O bonds lengths; to the best of our knowledge, there is no experimental and theoretical data under the mentioned conditions for comparison with our findings.

Calculation method

The main objective of MDs calculations is to solve numerically the second law of Newton and to find the macroscopic properties from microscopic properties,

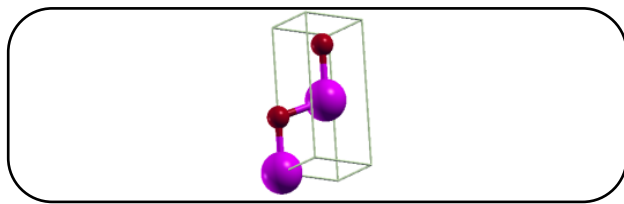


Fig. 1: Unit cell of ZnO wurtzite structure (NASA Goddard Space Institute Collaboration), the zinc and oxygen atoms are magenta and red spheres respectively.

using physical statistics calculations; the calculations have been run on the RAVEN supercomputer in the Chemistry and Physics Departments of Cardiff University (UK) using DL_POLY_4 software. The atomic interactions of the system are given using Coulomb-Buckingham potential, with a cut-off radius of $r_{\text{cut}} = 12$ (Å); outside this distance, the short-range interactions are insignificant [31,32]. To control the temperature and pressure, the Nose-Hoover constant NPT (N number of atoms, P is the applied pressure, and T is the temperature of the system) is employed [17]; with a thermostat relaxation time of 10 (ps) for each pressure and temperature.

Thus given an initial configuration of positions and velocities at the time (t), the positions, velocities, and acceleration can be calculated at a later time $t + \delta t$ [33], where the time step is $\delta t = 1$ (fs) while Verlet algorithm is employed for integration. Each run is made up 300,000 time steps; 300 (ps) is enough to reach the equilibrium state of the system. The simulation box with the periodic boundary conditions contains 2916 atoms of ZnO (1458 Zn^{2+} ions and 1458 O^{2-} ions) equivalent to a box of size $9x \times 9y \times 9z$ with $a = b = 3.242$ (Å), and $c = 5.188$ (Å) see Fig. 1. For the long-range Coulomb interactions, The Ewald Sum method is applied [34]. The error bar of molar volume calculations is also determined between 0.0027 and 0.0064 (Å).

RESULTS AND DISCUSSION

In the ZnO force fields, there are Columbian and van der Walls interatomic interactions; the non-Columbian interactions between Zn-O and Zn-Zn are repulsive where the Buckingham potential is used for this description [1, 2]. The hexagonal unit cell of ZnO wurtzite structure is shown in Fig. 1; the Zn^{2+} cations are surrounded by four O^{2-} anions and vice-versa. The effect of pressure and temperature are analyzed on Zn-O, Zn-Zn, O-O bond length; according to available data under ambient

conditions, the bond length of Zn-O is around 1.97 (Å), 1.76 (Å), and 1.90 (Å) [31,32]; while O-O bond length is around 2.35 (Å); the findings of our work are in the vicinity of theoretical and experimental results as we will describe later in this paper.

Zn-O bond length

Under high pressure and temperature

Fig. 2 shows the behavior of the Zn-O bond length of the wurtzite phase under high pressure and temperature in the ranges of 0-200 (GPa) and 1500-3000(K). Under the range of 0-20 (GPa), this bond decreased for both temperatures of 1500 (K) and 2000 (K), this is because the pressure effect is more than that of temperature. However, at 2500(K), the length of Zn-O is maintained fixed because of the equilibrium between the act of pressure and temperature. While at 3000K; it increases because of the solid-liquid phase where the melting degree of ZnO is 2228 (K) [35].

Under the range of pressure 20-120 (GPa) and at all temperatures, the length of Zn-O converges smoothly to the same variations, except between 80 (GPa) and 120 (GPa) where there is another phase transition [32]. Finally, under the range 120-200 (GPa) and at 1500 (K) and 2000 (K), the bond length has the same behavior(the same phase), However, at 2500 (K) it is still bit linear because of the balance between temperature and pressure till 180 (GPa), where it converged to around 1.90 (Å) at all temperatures under 200 (GPa), this is due to the same type of rocksalt structure, with an exception at 3000 (K) where it increased to 1.98 (Å); Nevertheless, the dropping and jumping of bond length is translated by phase transitions between ZnO structures [32].

Under high pressure and low temperature

Fig. 3 displays Zn-O bond length under 0 - 200(GPa) and both temperatures of 300(K) and 500(K), the bond length drops more under the range of 0-20 (GPa) at 500 (K) than at 300 (K), this because of the effect of pressure that produces the phase transition from ZnO wurtzite type to rocksalt [36 - 41]. While between 20 - 40 (GPa), it becomes linear under 500 (K), while it drops under 300 (K) due to the different phases, however under the range of pressure 0-40 (GPa) and at 300 (K); the length of Zn-O bond decreases smoothly, due to the effect of temperature is not significant.

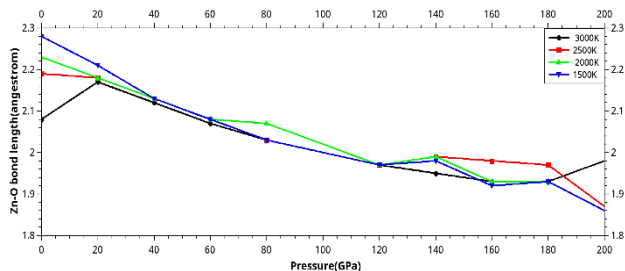


Fig. 2: Zn-O bond length under 0-200 (GPa) and 1500-3000(K) range

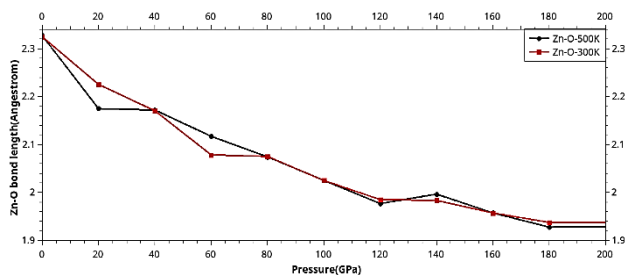


Fig. 3: Zn-O bond length under the range of pressure 0-200 (GPa) and at 300 (K) and 500 (K).

Under the range of 40 - 80 (GPa) and at 500 (K), the length of Zn-O drops fluidly, while at 300 (K), it reduces to 60 (GPa) and becomes stable pending 80 (GPa). In this range of 40-80 (GPa), the effect of temperature is more significant than the pressure. Under 80-120 (GPa), there is the selfsame shift of Zn-O bond length. From 120 (GPa) to 200 (GPa), Zn-O has the same behavior and changes by the same value approximately from zinc oxide structures to rocksalt [32, 36 - 41]. Table 1 exhibits a comparison of our results with other work.

Due to the small segment of temperature between 300K and 500K, and due to ionic and covalent of ZnO liaisons, the behavior of Zn-O is approximately similar, with the exception under the range 0-60GPa where there is a bit of influence of the segment of temperature of 200K; that difference is explained by the phase transition; the parameters of the unit cell of ZnO are changed.

Under low pressure and low and high temperature

Fig. 4 shows the Zn-O bond length under 0-15(GPa) and at 300-3000 (K) range of temperature. At both temperatures of 300 (K) and 500 (K) and under the range of pressure 0-5 (GPa); the bond length of Zn-O is 2.34 (Å) which is dropped under the range of 5 - 10 (GPa); this is due to the phase transition from wurtzite to rocksalt [36 - 41]. This bond length is converged to around 2.25 (Å) under

Table 1: Behavior of Zn-O bond length at low temperatures (300 (K) and 500 (K)) and under 0 (GPa). Reference a is [42-45].

	Zn-O length(Å)	
	This work 0 (GPa)	Other work
300	2.32	1.972-1.90 ^a
500	2.33	-

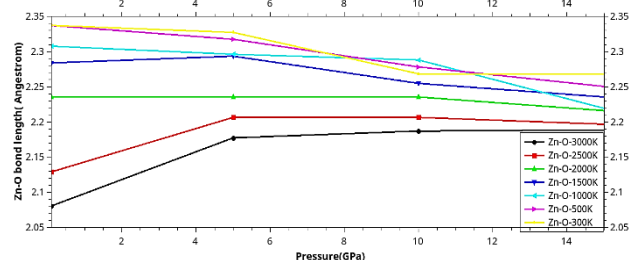


Fig. 4: Behavior of Zn-O bond length under low pressure (0-15(GPa)) and low and high temperature (300-3000(K)).

15 (GPa) at all temperatures. Under 1000 (K), the Zn-O length is linear around 2.31 (Å) under 0 - 10 (GPa), however, it decreased to around 2.25 (Å) under 15 (GPa). At 1500 (K) and under 0-5 (GPa); the structure is stable, where the phase is changed between 5 (GPa) and 10 (GPa)[48], and becomes stable under the range of 10-15 (GPa). The length of this bond is a bit linear under 2000 (K), so the phase is stable. Under both temperatures of 2500 (K) and 3000 (K) and in the range of 0-5 (GPa), Zn-O length is raised and has different values under 0 (GPa) due to the solid-liquid phase under 3000 (K) [35]. Under the range of pressure 5 - 15 (GPa) the bond length becomes steady; it is the phase of rocksalt structure [40 - 43].

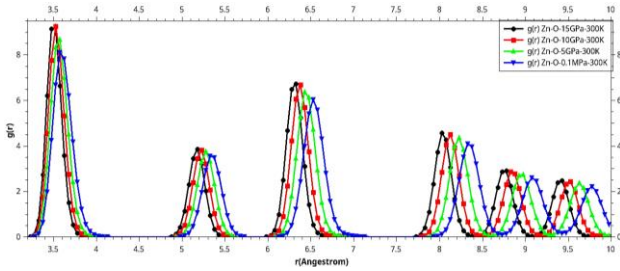
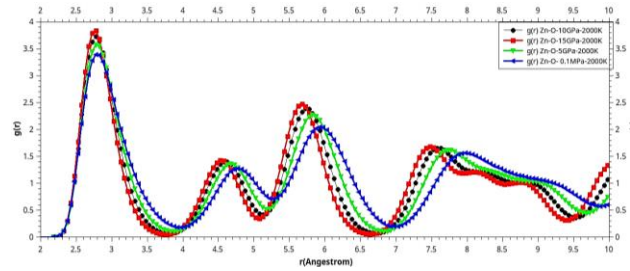
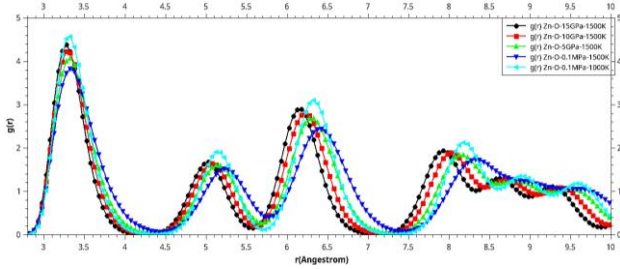
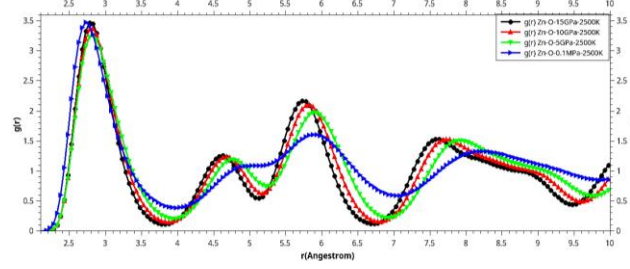
To calculate the bond length, a radial distribution function is used, where the x -coordinate in the middle of the first peak gives the distance between the reference atom and the first neighbor; see Fig. 5 - 8.

In order to summarize the calculations in Fig. 5-8; Table 2 lists the values of the mean value of radial distribution function $g(r)$, the standard error (SE), standard deviation (SE), the minimum value, and the maximum value of $g(r)$ under the low pressure (0-15 (GPa)) and under both temperatures of 300K, and 2500(K).

The radial distribution functions of the bonds O-O, Zn-Zn, and Zn-O under both temperatures of 300 (K) and 3000 (K) and under the pressure of 0.1(MPa) are depicted in Fig. 9, the high temperature provokes the disorder of the system (curved peaks), increases the distance between the reference atom and its neighbors, and decreases $g(r)$.

Table 2: Zn-O bond mean value of $g(r)$, standard error, standard deviation, minimum and maximum of $g(r)$ at 300 (K) and 2500 (K).

P (GPa)	Temperature 300 (K)					Temperature 2500(K)				
	Mean $g(r)$	SE	SD	$g(r_{\min})$	$g(r_{\max})$	Mean $g(r)$	SE	SD	$g(r_{\min})$	$g(r_{\max})$
0.1	1.0007	0.1029	1.4959	0	8.1083	1.0756	0.0384	0.5630	0	3.4735
5	0.9788	0.1063	1.5452	0	8.6699	1.0125	0.0411	0.6190	0	3.2662
10	0.9708	0.1081	1.5716	0	9.2598	0.9897	0.0436	0.6405	0	3.3735
15	0.9534	0.1091	1.5853	0	9.2125	0.9736	0.0446	0.6551	0	3.4700

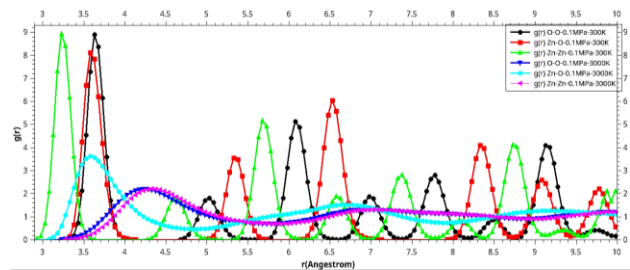
**Fig. 5: Correlation function of Zn-O bond under 0-15(GPa) and 300(K)****Fig. 7: Correlation function of Zn-O under 0-15(GPa) and at 2000 (K).****Fig. 6: Correlation function of Zn-O bond under 0.1(MPa) and at 1000 (K) and 1500 (K).****Fig. 8: Correlation function of Zn-O bond under 0-15 (GPa) and at 2500 (K).**

In the previous curves, the radial distribution function $g(r)$ gives the probability of finding an atom at a distance r from the origin, so it describes the internal structure of materials, and $\rho g(r)$ is the linear density where $\rho = N/V$ (N is the number of atoms and V is the volume of the system); the sharpened peaks signify the order structure of atoms, whereas the disorder is interpreted by curved peaks. It is noted that the distance between two atoms is augmented with increasing temperature and reduces with rising pressure.

Zn-Zn bond lengths

Under high pressure and high temperature

Under the range of pressure 0-200(GPa) and 1500-3000(K) of temperature, the behavior of Zn-Zn bond length is shown in Fig. 10. It is noted that at all temperatures and under the range of pressure 0-80 (GPa), Zn-Zn bond length

**Fig. 9: Correlation function of Zn-O, O-O, and Zn-Zn bonds under 0.1 (MPa) and at 300 (K) and 3000 (K).**

is lowered smoothly with a bit of the same variations, due to the different phase transitions of Zinc Oxide [32, 44], Whereas, under the range of pressure 80-140 (GPa), Zn-Zn is assembled fluently to the same value under all temperatures. Under the range of pressure 140-200 (GPa), Zn-Zn length is reunited to the same length at both temperatures of 1500(K) and 2000(K).

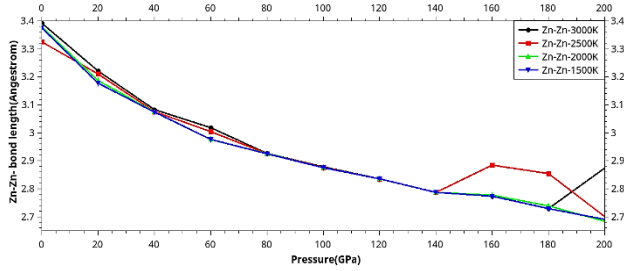


Fig. 10: Bond length of Zn-Zn under high pressure 0-200 (GPa) and high temperature 1500-3000 (K).

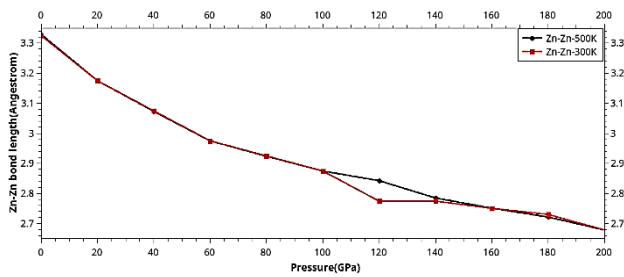


Fig. 11: Zn-Zn bond length under 0-200 (GPa) and at 300 (K) and 500 (K).

However, at 3000 (K), the length of the bond is increased to around 2.9 (Å) because of the deformation of the unit cell. While, at 2500 (K) the bond length rises under 140 (GPa) to around 2.865 (Å), and becomes linear between 160 (GPa) and 180 (GPa) because of the phase transition [48]. Finally, it drops to 2.70 (Å) under 200 (GPa) at all temperatures, it is noted that at around 2.7 (Å), the structure is the rocksalt one [32].

Under high pressure and low temperature

Fig. 11 depicts the behavior of Zn-Zn bond length under high pressure (0-200(GPa)) and low temperature (300 (K) and 500 (K)); the bond length dropped smoothly under all pressures from around 3.32 (Å) to 2.68 (Å), with the exception under the range of pressure 100-140 (GPa) [32].

Under low pressure and low and high temperature

Under low pressure (0-15(GPa)) and the temperature of the range (300-3000(K)), Zn-Zn bond length is shown in Fig. 12; under 0-10 (GPa) and at both temperatures of 300 (K) and 500 (K), the length of the bond decreased a similar manner, while under the range of pressure 10-15 (GPa) at 500(K); it becomes linear at 500(K) due to equilibrium between pressure and temperature, but it dropped to around 3.18(Å) at 300(K). At 1000K and under 0 - 5(GPa), the bond length decreased than becomes

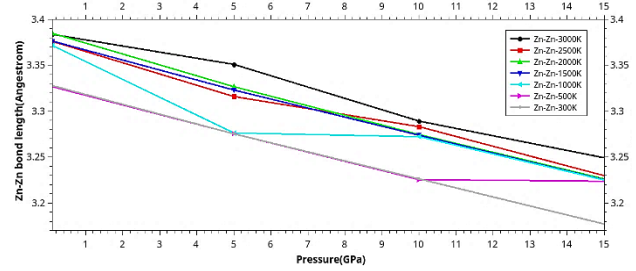


Fig. 12: Zn-Zn bond length under 0-15 (GPa) and at 300-3000 (K).

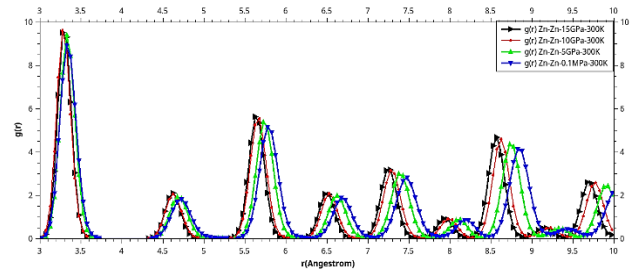


Fig. 13: Correlation function of Zn-Zn bond under 0-15(GPa) and at 300 (K).

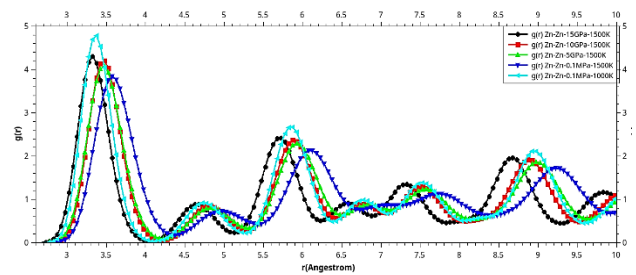


Fig. 14: Correlation function of Zn-Zn under 0-15 (GPa) and at 1500 (K)

linear between 5(GPa) and 10(GPa), later it dropped and decreased at 300K because of the effect of pressure. Under 0-5 (GPa) range and at 1000 (K) the bond length drops from 3.37 (Å) to 3.29 (Å), it remains constant between 5 (GPa) and 10 (GPa), and later it converged to around 3.23(Å); these variations of Zn-Zn bond length is due to the phase transition [32]. At the range of temperature 1500-2500(K), the Zn-Zn length is decreased a bit homogeneously under the pressure range of 0-15(GPa). Nevertheless, under 3000(K) the length of this bond has a similar variation to under 2500(K) but with higher values; the variations of the Zn-Zn length correspond to the phase transitions of ZnO structures [32].

In order to explain the previous values of Zn-Zn bond lengths, Figs. 13-16 illustrate the value of radial distribution function $g(r)$ versus the distance between atoms under low pressure and high temperature.

Table 3: Zn-Zn bond data mean value of $g(r)$, standard error, standard deviation, minimum and maximum value of $g(r)$ at 300 (K) and 2500 (K).

P (GPa)	Temperature 300 (K)					Temperature 2500 (K)				
	Mean $g(r)$	SE	SD	$g(r_{\min})$	$g(r_{\max})$	Mean $g(r)$	SE	SD	$g(r_{\min})$	$g(r_{\max})$
0.1	1.0452	0.1067	1.4561	0	8.9300	1.0119	0.0329	0.4688	0	2.4712
5	1.0623	0.1106	1.5130	0	9.3987	0.9890	0.0400	0.5675	0	3.0528
10	1.0395	0.1121	1.5336	0	9.6164	0.9741	0.0414	0.5893	0	3.1857
15	1.0073	0.1124	1.5424	0	9.5189	0.9592	0.0420	0.5990	0	3.2623

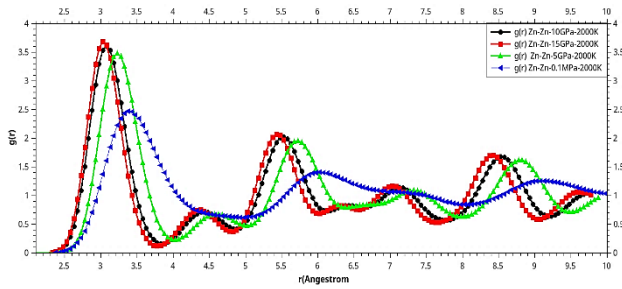


Fig. 15: Correlation function of Zn-Zn under 0-15 (GPa) and at 2000 (K).

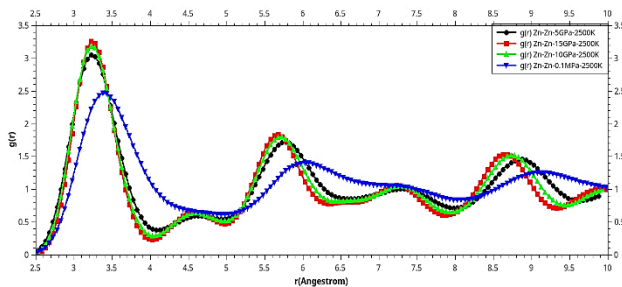


Fig. 16: Correlation function of Zn-Zn under 0-15(GPa) and at 2500 (K).

The data of previous Fig. 13-16 are listed in Table 3. As a general conclusion the maximum value of the radial distribution function, the standard error, and the standard deviation are augmented by increasing the pressure, whereas the mean value of $g(r)$ is reduced.

O-O bond lengths

Under high pressure and high temperature

At all temperatures and under the range of pressure 0-80 (GPa) as depicted in Fig. 17; the curves decreased smoothly and converged to neighbor values. Under the range of 80-140 the bond length of O-O is lowered, except at 2000 (K); the curve drops and rises to join the other curves at around 2.70 (Å), this is due to the attainment of melting degree 2228 (K) of ZnO [44]. It is noted that the converged curves produce a similar phase, while the jumping or rising of the curves tends to another phase of ZnO structures [32].

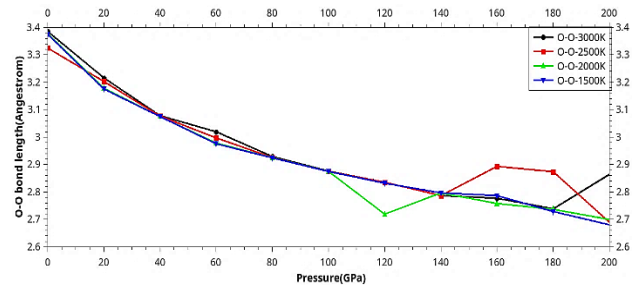


Fig. 17: Bond length of O-O under the range of 0-200 (GPa) and at the range of temperature 1500 -3000 (K).

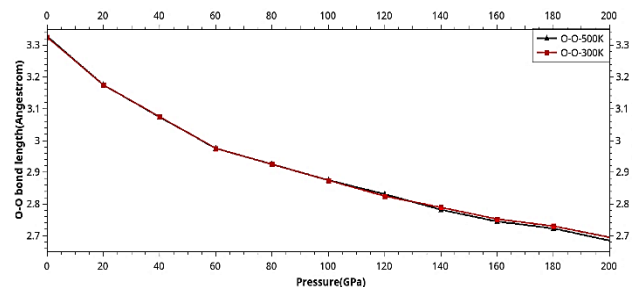


Fig. 18: the bond length of O-O at low temperatures (300(K) and 500(K)) and under high pressure 0-200 (GPa).

Under high pressure and low temperature

Due to the small segment of temperature between 300 (K) and 500 (K) and under high pressure of the range 0-200 (GPa); the bond length of O-O decreases quietly with the same disparity under all pressures from wurtzite parameters to rocksalt one (Fig. 18) [36 - 38].

This work is in the vicinity of available data under ambient conditions as mentioned in Table 4, there are no results for comparison under used conditions of pressure and temperature.

Under low pressure and low and high temperature

The effect of pressure under the range of 0.1MPa - 15GPa and at low temperature (500 (K) and 300(K)) on the bond lengths of O-O is summarized in Fig. 19; under 500(K), this length is dropped under the range of (0.1MPa - 15GPa) and becomes stable under (10-15GPa) due to the transition

Table 4: Comparison with available data of O-O bond length of wurtzite phase at low temperature (300 (K) and 500 (K) and under 0.1 (MPa), where reference a is [37 - 39], and reference b is [42-45].

Temperature (K)	this work	other work
300	3.32	(3.188)(2.35-2.95) ^a - - (2.35)(2.85-2.98) ^b
500	3.33	-

Table 5: Bond of O-O mean value of $g(r)$, standard error, standard deviation, the minimum and maximum value of $g(r)$.

P(GPa)	Temperature 300 (K)					Temperature 2500 (K)				
	Mean $g(r)$	SE	SD	$g(r_{\min})$	$g(r_{\max})$	Mean $g(r)$	SE	SD	$g(r_{\min})$	$g(r_{\max})$
0.1	1.0125	0.1037	1.4381	0	8.8905	1.0120	0.0328	0.4676	0	2.4623
5	1.0437	0.1082	1.4997	0	9.3773	0.9990	0.0397	0.5604	0	3.0483
10	1.0128	0.1096	1.5191	0	9.5840	0.9838	0.0412	0.5833	0	3.1803
15	0.9863	0.1103	1.5295	0	9.4814	0.9592	0.0420	0.5992	0	3.2579

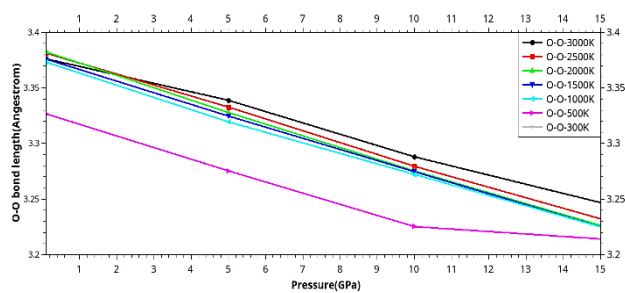


Fig. 19: the bond length of O-O under low pressure (0-15(GPa)) and at low and high temperature (300-3000(K)).

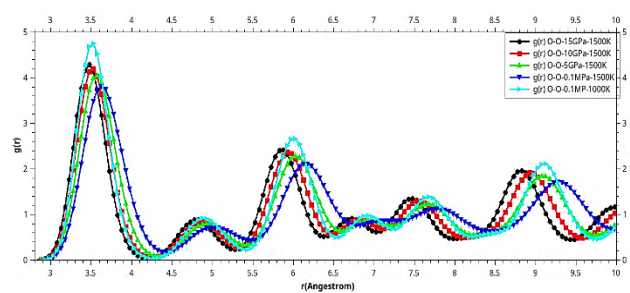


Fig. 21: Correlation function of O-O under 0-15 (GPa) and at 1500 (K) and 1000 (K).

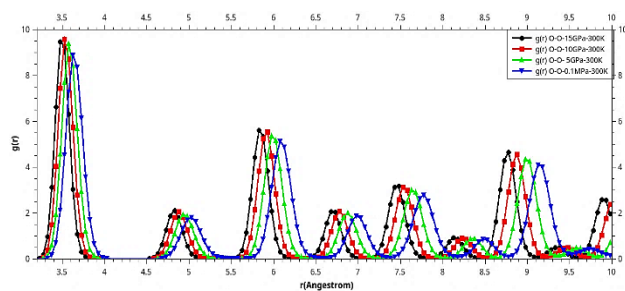


Fig. 20: Correlation function of O-O under 0-15 (GPa) and at 300 (K).

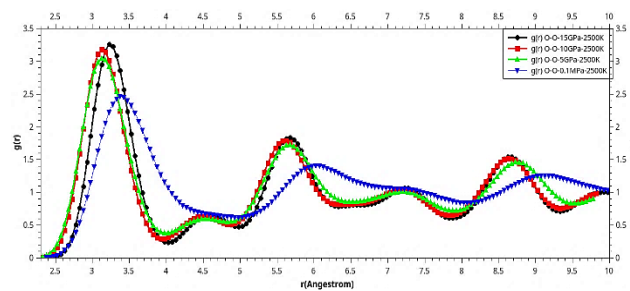


Fig. 22: correlation function of O-O bond under 0-15 (GPa) and at 2500 (K)

from wurtzite structure to rocksalt [10 - 13, 32]. However, under the range of 0(MPa)-15(GPa) and 1000 - 2000(K), the O-O bond length is reduced similarly from around 3.38(Å) to 3.23(Å) which means converging to the same structure of ZnO. Whereas, at 3000(K), the length of this bond is more than that; at all temperatures due to the phase of solid-liquid [32, 44]. We can clarify the data of previous curves in the following Figs. 20-22 of radial distribution functions.

The detailed data of the bond O-O are noted in Table 5.

It should be noted that the behavior of the bond length of O-O under low pressure and at low temperature

of 300(K) as mentioned in Table 5 is similar to that of Zn-Zn bond, where the maximum of the radial distribution function, the standard error, and the standard deviation are augmented with rising pressure, but the mean value of $g(r)$ is decreased, because of the decrease of the probability of finding an atom near the reference.

In order to confirm the validity of the interatomic potential, the calculations, and the results of this work.

Figs. 23-25 shows the error bar of ZnO bond length measurements, which is in the vicinity of available theoretical and experimental literature.

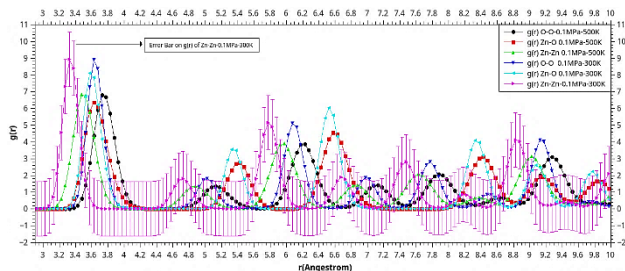


Fig. 23: Error bar of Zn-Zn bond correlation function under 0.1 (MPa) and at 300 (K) and 500 (K)

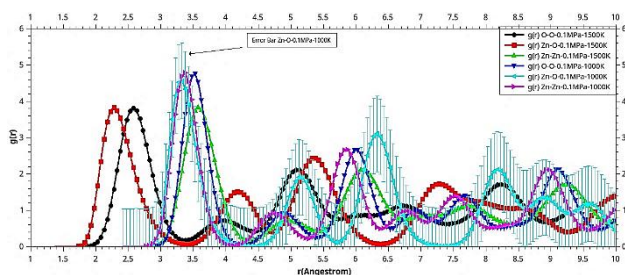


Fig. 24: Error bar of Zn-Zn bond (RDF) under 0.1 (MPa) and at 1000 (K) and 1500 (K)

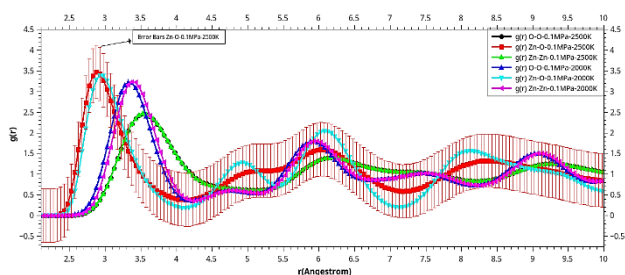


Fig. 25: Error bar of O-O bond (RDF) under 0.1 (MPa) and at 2000 (K) and 2500 (K)

CONCLUSION

Under an extended range of temperature and pressure, the behavior of ZnO wurtzite structure and its chemical bond lengths are analyzed using MD technique and DL_POLY software; Under low pressure and high temperature, the length of Zn-Zn, Zn-O, and O-O are enlarged due to the effect of temperature is significant compared with pressure, while under both high pressure and temperature, the effect of temperature is neglected; not that the variation of Zn-O bond is less than Zn-Zn and O-O lengths because of the strongest potential. The parameters of the unit cell are changed under the effect of temperature and pressure, which permits the phase transition between ZnO structures. Although the modeling of interatomic potential is a challenge for ionic-covalent bonds; the potential of Buckingham is in agreement with available data under ambient conditions. This work helps

the materials design for new structures, also it is very important in Medicine, Pharmacy, Geophysics, and especially in nanoscale for ZnO nanoparticles.

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