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The Effect of Pressure on Temperature System of ZnO a Molecular Dynamics Prediction

Yahia Chergui *

M'hamed Bougara University, Electrical And Electronic Engineering Institute, Boumerdes 35000, Algeria

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ABSTRACT:

Zinc oxide is a promising semiconductor, due to the chemical bonds; they are between covalent and ionic. This bonding plays a dramatic role in thermodynamic properties under extended pressure and temperature. In this work we analyze the behavior of the effect of pressure on the system temperature of ZnO wurtzite structure; we have been investigated equilibrium parallel molecular dynamics technique and dlpoly_4, using RAVEN supercomputer of Cardiff University(UK), to simulate the evolution in time of system temperature and its equilibrium time in isothermal and isobaric ensemble. Our system contains 2916 atoms of ZnO wurtzite type, under the ranges of pressure 0-200(GPa) and temperature 300-3000(K), where the interatomic interactions are modeled by Buckingham and Coulomb potential for short and long-range interactions respectively; we used equilibrium time of system temperature to know the effect of pressure. Due to the lack of information about the effect of pressure on system temperature, under previous conditions, our results are still a prediction which needs confirmation in future. The thermodynamic behaviors of ZnO have huge importance in nanoscale and macroscale, especially in medicine, pharmacy and geophysics fields.

Keywords: ZnO, MD, phase transition, pressure, temperature.

INTRODUCTION

Zinc oxide is a promising semiconductor in technology, giophysics, and recently in last decade is used in nanotechnology; nano helices [1, 2], nano pins [3-10], nano rods [11-15], tetraped, nano whiskeres [16], nanocompbs [17, 18]. The most stable phase of ZnO is the Wurtzite structure (B4); defines by unit cell parameters a=b= 3.2496(Å), C= 5.204(Å), μ=3/8, and c/a=1.633 where each atom of Zinc is surrounded by four atoms of Oxygen and vice versa [19, 20]. The parameter values of unit cell vary from 3.2475 to 3.250(Å) and from 5.2042 to 5.2075(Å) for the parameters a and c respectively [21]. This deviation due to the volume of unit cell which depend on the free electrons concentrations, on concentrations of foreign atoms and defects, external strains, and temperature [22].

Beside many experimental and theoretical studies on ZnO; this material needs more investigations to know its thermodynamic behavior in nanoscale, especially under extended conditions of pressure and temperature [11, 35], where the heat transfer in nanoscale and the effect of pressure on system temperature still a challenge subject. In this work, the interatomic potential is modeled by Buckingham-Coulomb potential [23, 24], the range of pressure 0-200GPa and temperature 300-3000K product a phase transition from wurtzite to rocksalt at around 10GPa,from rocksalt to wurtzite at around 2GPa, and from rocksalt to zinc blend at 260GPa[4, 6-9]. In this paper, we focus on evolution of system temperature in time and its equilibrium time of isothermal and isobaric ensemble; in order to analyze the effect of pressure on system temperature and the main parameter which control this effect.

II. Calculation Method

In order to save time of calculations, parallel molecular dynamics becomes a powerful tool for simulation; in this work the calculations have been run in RAVEN supercomputer of Cardiff university, using dl_poly_4 software. In this calculations, our sample contains 2916 atoms of ZnO (1458 atoms of Zn2+ and 1458 atoms of O2-), the short-range and long-range interactions are modeled by Buckingham and Coulomb potential respectively [23, 25], where the interactions will be neglected outside the cutoff rc=12(Å). The ensemble of Nose-Hoover (nST) is used to control the relaxation of pressure (10ps) and temperature (10ps)[23]. The timesteps Δt is 0.001ps and for equilibrium and measurement the time is 30000ps, respecting the periodic conditions. The range of pressure and temperature are 0-200GPa and 300-3000K respectively [14]. The crystallographic component vectors of wurtzite according X, Y, and Z are respectivelya(1/2,√3/2,0), a (1/2,-√3/2,0), and a (0, 0,c/a). The bases of atoms in Cartesian coordinates are (0,0,0), (0,0,uc), a(1/2,√3/6,c/a), and a(1/2,√3/6,(μ+1/2)c/a) 5, where the dimensions of the simulation box are (9a)x(9b)x(9c). The MD technique consists of numerically solving a group of differential equations of Newton second Law over all atoms of a simulation box; 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 + ծt [26].

III. Results and Discussion

We focus in this work to show the evolution of system temperature in time, to extract the equilibrium time depends to pressure and temperature; in order to see the effect of pressure, the dependence of system temperature in time of ZnO wurtzite structure under the range of temperature 300-3000K and low pressure 0.1MPa-15GPa is shown in figure1.

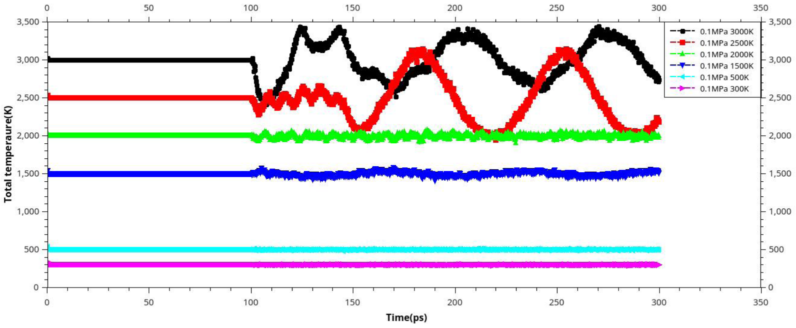

Figure1: Evolution in time of system temperature of ZnO wurtzite structure under low pressure (0.1MPa-15GPa) and under low and high temperature (300-3000K).

As it is noticed from figure 1, the period of time of 300ps is enough for equilibrium state, which confirm the validity of interatomic potential of Buckingham-Coulomb; this objective permit us to extend the conditions of pressure to high values under the range of 0-200GPa.

Under low temperature 300K and 500K and the pressure of 0.1MPa; the system temperature is approximately linear, where the fluctuations are insignificant, while increasing the temperature to 1500K 2000K, the system temperature is started to fluctuate, which means that the effect of temperature is more than the effect of pressure. However it is clear that under high temperature of 2500K and 3000K; there is a dramatically fluctuations, due to the phase transition from solid to liquid [21], where the effect of pressure (0.1MPa) is neglected.

Under isobaric ensemble of 5GPa and under the range of temperature 300-3000K; the evolution of system temperature in time tends to equilibrium as shown in figure 2, under high temperature, it becomes bit linear less than under lowest one, also the effect of temperature on the system atoms need around 100ps for influencing; it is the required time for the heat transfer.

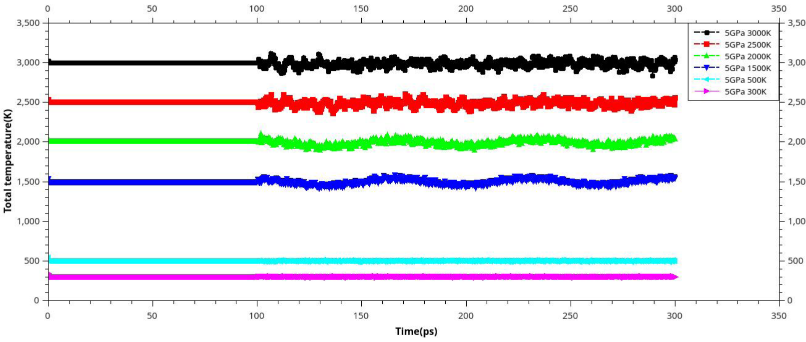

Figure2: Evolution of system temperature in time under low and high temperature 300-3000K and at 5GPa.

The effect of pressure on system temperature is becoming clear, under increasing the pressure from 5GPa to 10 and 15GPa (see figure 3 and 4); we use here an isobaric ensemble as previous cases and we change the temperature from low to high value.

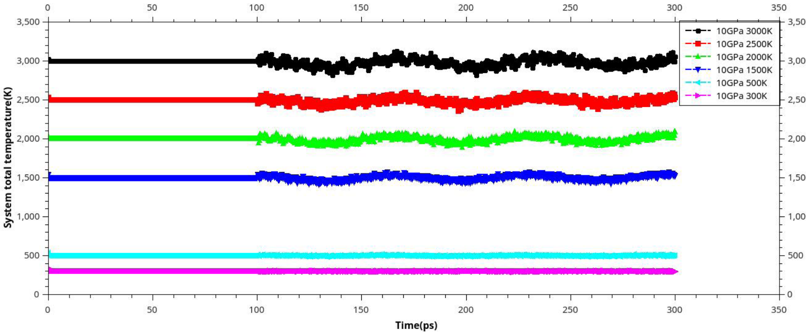

Figure3: The evolution of system temperature in time under the 10GPa and low and high temperature 300-3000K.

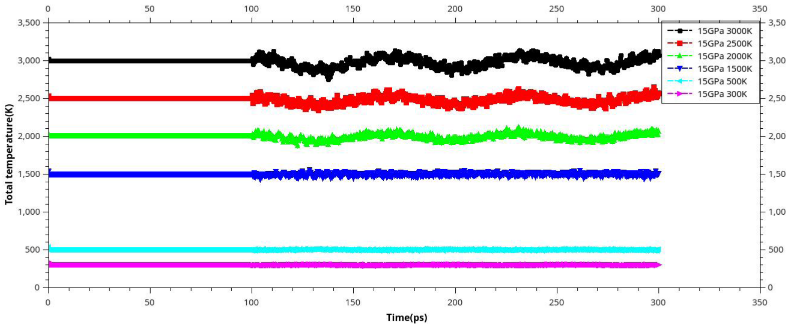

Figure4: The evolution of system temperature in time, under 15GPa and low and high temperature (300-3000K).

We extend the low pressure (0.1MPa-15GPa) to high value 0-200GPa using always isobaric ensemble, with changing the temperature from low to high degree, as shown in figures 5-7

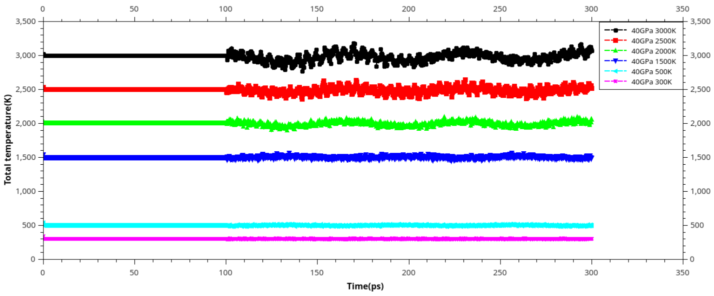

Figure5: The evolution of system temperature in time under 40GPa and low and high temperature (300-3000K).

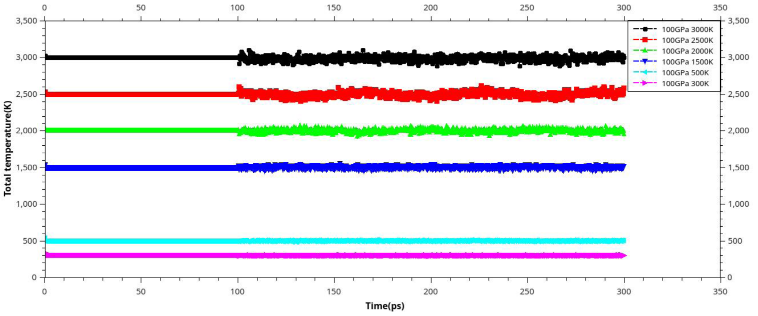

Figure6: The evolution of system temperature in time under 100GPa and low and high temperature (300-3000K).

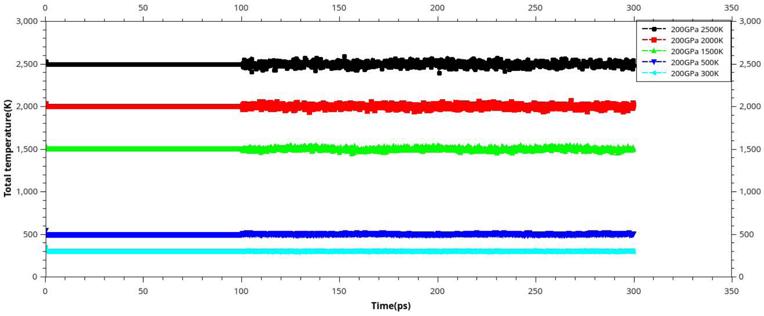

Figure7: The evolution of system temperature in time under 200GPa and low and high temperature (300-3000K).

In previous isobaric ensemble in figures1-7 and under the low and high temperature; due to the influence of high pressure, the atoms of ZnO wurtzite structure become closer to each other, which prevent the impact of temperatures, therefore it can be neglected under high pressure, while under low pressure and high temperature the consequence of temperature is significant especially down more than melting degree of ZnO (2228K)[27].

We have been seen that the period of time 300ps is enough to achieve the equilibrium of system, beneath the range of temperature 300-3000K and 0-200GPa range of pressure; we extract the equilibrium time to see the relationship with the applied pressure.

Figure 8 shows dependence between equilibrium time and low pressure (0.1MPa-15GPa), and low, and high temperature in the range of 300-3000K; it is noticed that the equilibrium time increases with increasing temperature, beneath low pressure (0.1MPa and 5GPa), while it decreases with increasing the pressure (10GPa and 15GPa), in these isobaric ensembles, the curves are bit linear, due to the proportionality between equilibrium time, pressure and temperature.

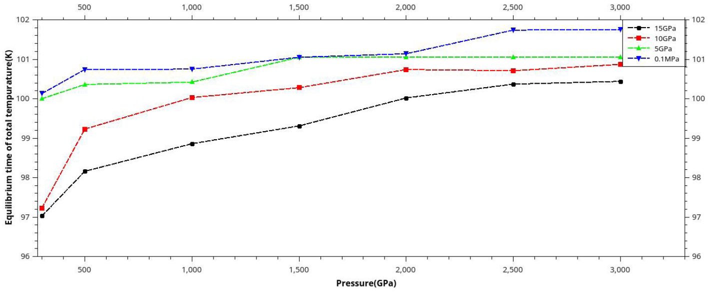

Figure 8: Equilibrium time of system temperature in isobaric ensembles(low pressure) versus temperature under the range of 300-3000K.

In isothermal ensembles under the range of temperature 300-3000K and low pressure as shown in figure 9; under 300K and less than 5GPa the equilibrium time is constant till 5GPa, which means the same phase structure of ZnO wurtzite type, while between 5GPa and 10GPa there is dropping of equilibrium time; it is the area of phase transition from wurtzite to rocksalt. After 10GPa there is a stability of equilibrium time, due to the same phase of rocksalt [4, 6].Down 1000K and 1500K, the equilibrium time has the same variations till 5GPa, where it is changed at 10GPa, because the phase transition. However under high temperature 1500-3000K and less than 5GPa; there is nearly the same values of equilibrium time , in other side the system tends approximately the same limit under 2500K and 3000K[21]. It is noted that under all temperatures at 15GPa, the equilibrium time of system temperature converges to one limit (one phase of rocksalt) [4, 6].

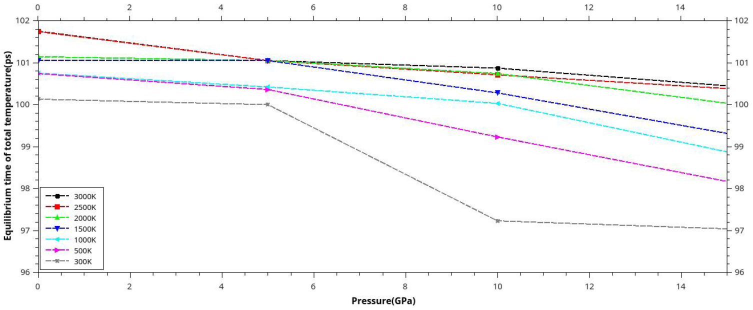

Figure 9: Equilibrium time of system temperature in isothermal ensembles (low pressure) versus pressure under the range of 300-3000K

IV. Conclusion

Equilibrium parallel molecular dynamics, dl_poly_4 software, and Buckingham- Coulomb are investigated to analyze the impact of pressure on system temperature of 2916 atoms of ZnO type; we have seen that the evolution of system temperature in time achieved the equilibrium in enough time of 300ps. It is noticed that beneath low pressure 0.1MPa, and at low temperature (300K and 500K); the influence of pressure is more than the trace of temperature, due to no fluctuations. However, increasing temperature (1500-3000K), increases the fluctuations under 0.1MPa, but under the range of pressure 5-15GPa, the fluctuations are dropped and tends to be bit linear and limit to one value. Generally, we can conclude that; high temperature is insignificant under high pressure, and becomes only a weak function. The equilibrium time decreases with increasing the pressure and vice versa with temperature. Using equilibrium time of system temperature can be used to justify the phase transition, which needs confirmation in future.

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