Study of thermodynamic properties changes of Nickel Oxide by DFT method and Romberg integration up to 5000 °C and 100 GPa

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ABSTRACT

This paper aims to illustrate how Romberg's numerical integration is applied in calculating the values of internal energy, free energy, entropy and heat capacity at constant volume. Which is considered one of the important parameters of thermodynamic properties, and it is the only one that depends on integrations in its calculation. The temperature changes from zero to 5000 °C, while the pressure changes between zero and 100 GPa. The application was made to nickel oxide which remains in its cubic phase in this pressure range, and the Debye temperature values for it are determined by the CASTEP program which including the DFT method exactly by GGA approximation via the PBEsol function. We found that the Debye temperature decreases with increasing pressure and its value at absolute zero is slightly consistent with previous studies, confirming the validity of these results. However, we could not compare with the thermodynamic parameters, which we found to also decrease with increasing pressure, except for the values of internal energy, heat capacity at constant volume and entropy values for low temperatures. Conversely, this exception is adopted for increasing temperature, with most parameters showing an increase with increasing temperature.

Keywords: Romberg integration, DFT method, Debye temperature, thermodynamic properties, NiO.

INTRODUCTION

Numerical analysis is the science of approximation, where numerical methods are used to solve complex problems that cannot be solved by analytical methods [01]. It is also known as the study of numerical mathematical methods to find an approximation solution to some mathematical problems that appear when applying mathematics in its various branches in research and applied sciences and analyzing their approximation, accuracy and stability [02]. Numerical analysis can also be considered as a branch of computer science, it is based on the principle of creating, analyzing and implementing a set of algorithms to access numerical solutions to mathematical problems based on constant changes and fluctuations [03]. These issues and problems may arise in various sciences, whether human, economic, engineering, etc. Numerical analysis is also called numerical methods and quantitative analysis [04].

On the other hand, the exponential growth of numerical computers and their availability in large quantities have increased their use in life; the need to analyze mathematical models in science and engineering has become urgent.In order to solve the complexities present in it, a system emerged in the period (1980-1990) that combines numerical analysis, computer graphics, symbolic mathematical

calculations, and other fields of computer science, in order to facilitate the creation of complex mathematical models of the world, their solution, and their interpretation [05].

For example, some integrations are not easy to calculate, therefore numerical methods areused to calculate them, these methods are multiple, includingMidpoint Rule [06], Trapezoidal Rule [07], Simpson Rule [08] and Romberg Rule [09]... etc. These integrals are used in physics to calculate many parameters, especially those related of changing thermal or thermodynamic properties with the change in temperature. Among these parameters is the heat capacity at constant volume, the internal and free energies of Gibbs and entropy [10].

Knowing the change of these parameters is very important in various life applications, especially in the last time with the entry of the world of nanomaterials. These materials have become increasingly interesting, often used metal oxides such as NiO. This oxide is very important, as it is included in many uses in different domains. As electricity production, it is used as an electrode in fuel cells. Moreover, because of its magnetic properties, it is used in the process of manufacturing nickel salts (such as chloride, nitrates and sulfates), which can be used to make refined nickel oxide. It is also used in the production of active nickel catalysts, in electroplating, in stained glass and decolorization. The oxide in the form of sinter is used in the production of steel and nickel alloys, in addition to providing oxygen for the melting process in order to remove carbon as carbon dioxide [11]. Finally, because it contains nickel, this oxide may be very important in the internal composition of the Earth's subsoil, especially within the range of the Earth's core and the extent to which its magnetic properties affect the Earth's magnetism [12].

There are many works that have studied this oxide, the most important of which are; work Noguchi, Y et.al 1998 [13], Shukla, A et.al 2002 [14], de PR Moreira et.al 2002 [15], Zhang, W et al 2006 [16], Kuneš, J et.al 2007 [17],L. Liu et.al 2008 [18], Chauhan, Ret al 2008 [19], Nwanya, A. C et.al 2015 [20], Potapkin, V et.al 2016 [21], and work Gavriliuk, A. G et.al 2023 [22].

Although these studies were of different interest in several aspects, it can be concluded from most of them that this oxide, under normal conditions and like all similar monoxides, crystallizes in the structure of table salt or phase B1, it remains stable in this structure until above 147 GPa as stated in the experimental study of Noguchi, Y et.al 1998 [13].

These studies did not accurately determine the evolution of the values of many parameters, in particular those mentioned above, which are included in the Thermodynamic properties especially in its first phase. Given the importance of these transactions, especially when using this oxide in nano fields.

This report used numerical integration to study the evolution of these parameters with temperature changes from 0 to 5000 °C, and at different pressures their values vary from 0 to 100 GPa. This integration is presented at the beginning of the presentation of the study method, which follows this presentation. The results are then interpreted and presented, and finally a summary presents the most important results obtained.

II- Study method
II-1-1 Romberg Rule in calculating integration

Romberg's integration is based primarily on the semi-deviant base, which provides for the integration of the $f(x)$ function in the period [a, b] after it is divided into n of the partial periods $[x_{i-1}, x_i]$by points $x_i$where $x_i - x_{i-1} = $ and $i = 1, \dots, n$considering$x_0 = a, , x_n = b$ it will be [9]

$$\int_a^b f(x)\, dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{n-1} f(x_i)\right] - \frac{b-a}{12}h^2 f''(\mu) \qquad (1)$$

$$a < \mu < b, \quad = \frac{b-a}{n}, \quad x_i = a + ih, \quad i = 1, 2, \dots, n-1$$

If $_k = \frac{b-a}{n_k} = \frac{b-a}{2^{k-1}}$the formula for Trapezoidal Rule is in the form:

$$\int_a^b f(x)\, dx = \frac{h_k}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{2^{k-1}-1} f(a + h_k i)\right] - \frac{b-a}{12}h_k{}^2 f''(\mu)$$

Assuming that:

$$R_{1,1} = \frac{h_1}{2}\{f(a) + f(b)\} = \frac{b-a}{2}\{f(a) + f(b)\} \qquad (2)$$

$$R_{2,1} = \frac{h_2}{2}\{f(a) + f(b) + 2f(a + h_2)\} = \frac{b-a}{4}\left\{f(a) + f(b) + 2f\left(a + \frac{b-a}{2}\right)\right\}$$

$$R_{2,1} = \frac{1}{2}\left\{R_{1,1} + h_1 f\frac{1}{(a+2}h_1)\right\} \qquad (3)$$

$$\mathbf{R_{3,1}} = \frac{h_3}{2}\{f(a) + f(b) + 2[f(a + h_3) + f(a + 2h_3) + f(a + 3h_3)]\}$$

$$\mathbf{R_{3,1}} = \frac{h_3}{2}\left\{f(a) + f(b) + 2[f(a + \frac{b-a}{4}) + f(a + \frac{b-a}{2}) + f(a + 3\frac{b-a}{4})]\right\}$$

$$\mathbf{R_{3,1}} = \frac{1}{2}\left\{\mathbf{R_{2,1}} + h_2[f\left(a + \frac{1}{2}h_2\right) + f(a + \frac{3}{2}h_2)\right\} \tag{4}$$

Generally:

$$\mathbf{R_{k,1}} = \frac{1}{2}\left\{\mathbf{R_{k-1,1}} + h_{k-1}\sum_{i=1}^{2^{k-1}}f\left(a + (i - \frac{1}{2})h_{k-1}\right)\right\}, k = 2, 3, \dots, n \tag{5}$$

II-2 -2 Determination of thermodynamic Properties

Many Thermodynamic properties parameters are calculated based on Debye's model. In this study, we are interested in addressing both internal and free energies, entropy and heat capacity at constant volume. These properties can be further understood in many references, including [23-25] where:

Internal energy can be calculated from the following relationship [26]:

$$U = 9Nk_BT(\frac{T}{\theta_D})^3\int_0^{x_D}\frac{x^3}{e^x - 1}dx \tag{6}$$

N is the number of molecules, k_B is the Boltzmann'sconstant and T is the temperature.

And

$$\mathbf{x_D} = \frac{\hbar\omega_D}{k_BT} = \frac{\theta_D}{T} \tag{7}$$

$\hbar$ is the Plank's constant and ω_D is the vibration frequency.

This relationship can be written as follows:

$$U = \bar{U}\int_0^{x_D}f_U(x)\,dx \tag{8}$$

where:

$$\bar{U} = 9Nk_BT(\frac{T}{\theta_D})^3, \qquad f_U(x) = \frac{x^3}{e^x - 1}$$

While the free energy or Gibbs function is written as follows [27]:

$$F(V; P, T) = E(V) + PV + A_{Vib}(\theta(V); T) \tag{9}$$

where E (V) is the total energy as a function of the initial cell volume, PV is equivalent to the hydrostatic pressure constant, θ(V) is the Debye temperature, and A_{Vib} is vibration term, which can be written using the Debye phonon density of states model:

$$\mathbf{A_{Vib}} = nkT\left[\frac{9\theta}{8T} + 3\ln\left(1 - e^{\frac{-\theta}{T}}\right) - D\left(\frac{\theta}{T}\right)\right] \tag{10}$$

where n presents the number of atoms in the initial cell, $D\left(\frac{\theta}{T}\right)$ represents the Debye integral.

$$\mathbf{F} = 9RZT\int x^2\ln\left(1 - e^{-\frac{\theta_D}{T}x}\right)dx \tag{11}$$

This relationship can also be written as follows:

$$F = \bar{F}\int_0^{x_D}f_F(x)\,dx \tag{12}$$

where:

$$\bar{F} = 9RZT, \qquad f_F(x) = x^2\ln\left(1 - e^{-\frac{\theta_D}{T}x}\right)$$

Entropy is calculated from the second law of thermodynamic with the following relationship [27]:

$$\mathbf{S} = 9RZ\frac{\theta_D}{T}\int x^3\left[\frac{1}{e^{\frac{\theta_D}{T}x} - 1} - \ln\left(1 - e^{-\frac{\theta_D}{T}x}\right)\right]dx \tag{13}$$

In the same way, this relationship can always be written as follows:

$$S = \bar{S}\int_0^{x_D}f_S(x)\,dx \tag{14}$$

where:

$$\bar{S} = RZ\frac{\theta_D}{T}, \qquad f_S(x) = x^3\left[\frac{1}{e^{\frac{\theta_D}{T}x} - 1} - \ln\left(1 - e^{-\frac{\theta_D}{T}x}\right)\right]$$

According to the Debye's law, the mathematical formula for thermal capacity can be written on the following way [27]:

$$C_V = 9R \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx \tag{15}$$

In the same way, this relationship can always be written as follows:

$$C_V = \overline{C_V} \int_0^{x_D} f_{C_V}(x)\, dx \tag{16}$$

where:

$$\overline{C_V} = 9R \left(\frac{T}{\theta_D}\right)^3, \qquad f_S(x) = \frac{x^4 e^x}{(e^x - 1)^2}$$

II-3 Determination of Debye temperature

From previous relationships in particular the x value is related to an important amount, this amount is the variable temperature basically by pressure change. Debye temperature is estimated through the information of density value and the longitudinal and transversal wave velocities, that given the following relationship [25]:

$$\theta_D = \frac{h}{k_B} \left[\frac{9nN_A\rho}{4\pi(M_{O^{-2}} + M_{Ni^{+2}})\left(\frac{1}{V_P{}^2} + \frac{2}{V_S{}^2}\right)}\right]^{\frac{1}{3}} \tag{17}$$

n is the number of atoms in the initial cell of the crystal where it is estimated here as 2.

Debye temperature is an elastic parameters, therefore CASTEP code (Cambridge Total Energy Package) [28], in its modern version has become calculating this parameter directly. This program is based on the DFT method (Density Functional Theory), which is one of the most important methods used in theoretical physics and chemistry and by which we can determine the properties of a multiparticle system, the total energy of the system, the electron density of the orbitals, the physical and optical parameters of the matter ...... etc, and it is one of the most used methods in quantum calculations to solve the Schrödinger equation due to the possibility of applying it to various (multivariate) systems [29].

This method involves many approximations, as we used GGA (Generalized Gradient Approximation) [30-31], which has developed and become stronger due to its multiple possibilities of use, in 2008 the PBEsol approximation used here and explained in detail in [32]appeared. We have adopted the borders of the region of Brillion 10 x 10 x 10 and cut-off energy estimated at 630 eV, these values enable to provide a very close calculation with very reliable results. In this program, you must go through an important step in order to calculate elastic properties, which is the first step in the calculation called geometric improvement, which identifies a lot of initial parameters especially those of structural properties.

III- Results and interpretation
III-1 Study of Debye temperature

With the exception of Debye temperature values at 50 and 80 GPa pressures, it is clear from figure (1) and table (1) this temperature is approximately decreasing in the form of a semi-parabola whose focus is at zero pressure, i.e mean second-degree polynomials. This exception is due to the deviation in its values from this change, which is limited to a width of 160.01 K. Figure (1) presents the change in Debye temperature to the NiO structure up to 100 GPa pressure, and Table (1) includes Debye temperature values for this oxide at 0, 50 and 100 GPa pressures.

The Debye temperature obtained in our study at zero pressureis close to that of the experimental work [13], as our value is 5.42 K.
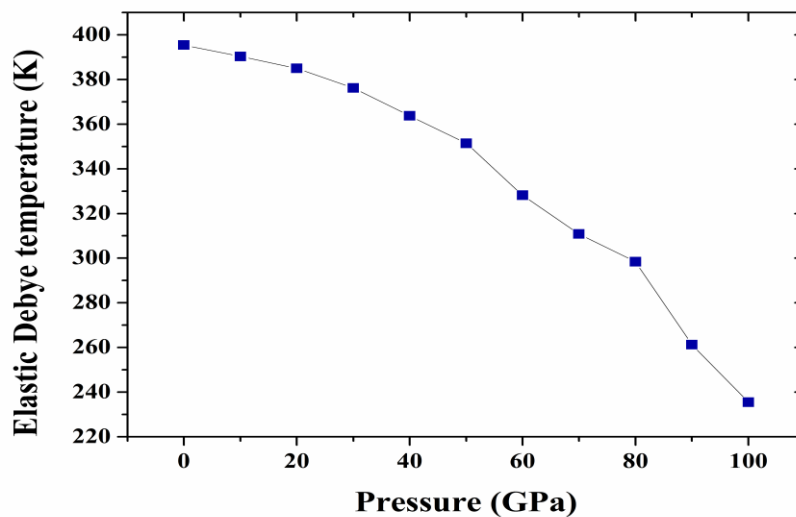
Figure 1: Change in the Debye temperature for NiO structure up to 100 GPa pressure.

Table 1: Presents Debye temperature values for NiO at pressures 0, 50 and 100 GPa.

Pressure (GPa)	0	50	100
Debye temperature (K)	395.62	351.38	235.41

III-2 Study the thermodynamic properties
III-2-1 The internal energy

Through Table (2) and Figure (2) it can be seen that the internal energy of nickel oxide is constantly increase linearly with the increase in temperature within a range its width of about 250 kjoule/moule, with a slope that is close whatever the pressure by 49.72 joule/moule.K. The values of this energy are very close with the change in pressure, but in fact they are increasing by the increase in pressure and it is apparent from figure (3).

The difference often increases by increasing pressure, which is proven after the temperature 250 °C almost. the lowest value of this difference is estimated at 60.66 joule/moule and this is at absolute zero and between two pressures 0 and 10 GPa, while its highest value is estimated at 478.73 joule/moule and this is at 5000 °C and between the two pressures 90 and 100 GPa.

Where Figure (2) presents the change in the internal energy of the NiO structure calculated relative to the values of the pressures studied with the change in temperature. While, Figure (3) presents the change in the internal energy difference of the NiO structure with the change in temperature from 0 to 5000 °C by taking its value at zero pressure as a reference, where -A calculated at pressures 0, 10, 20, 30, 40 and 50 GPa and -B calculated at pressures 50, 60, 70, 80, 90 and 100 GPa. Table (2) presents the most important values of the internal energy, free energy, entropy and heat capacity at constant volume at 0, 50 and 100 GPa pressures.
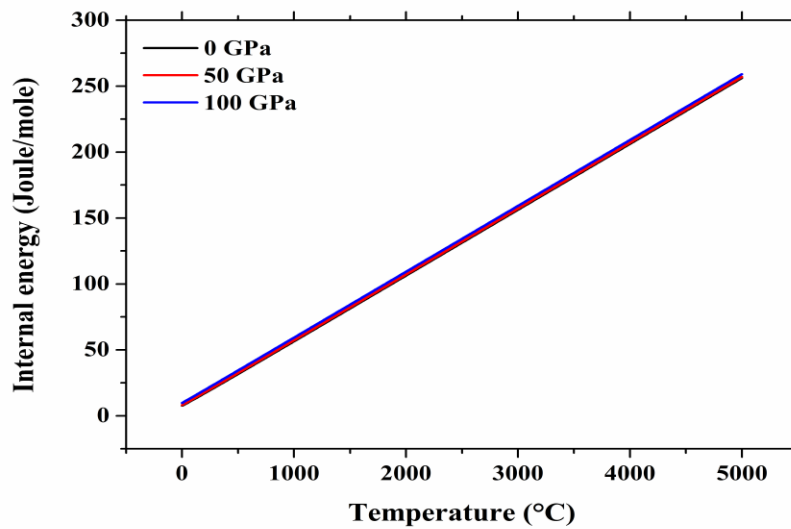
Figure 2: Change in the internal energy for NiO structure calculated at pressures 0, 50 and 100 GPa with the change in temperature from 0 to 5000 °C.
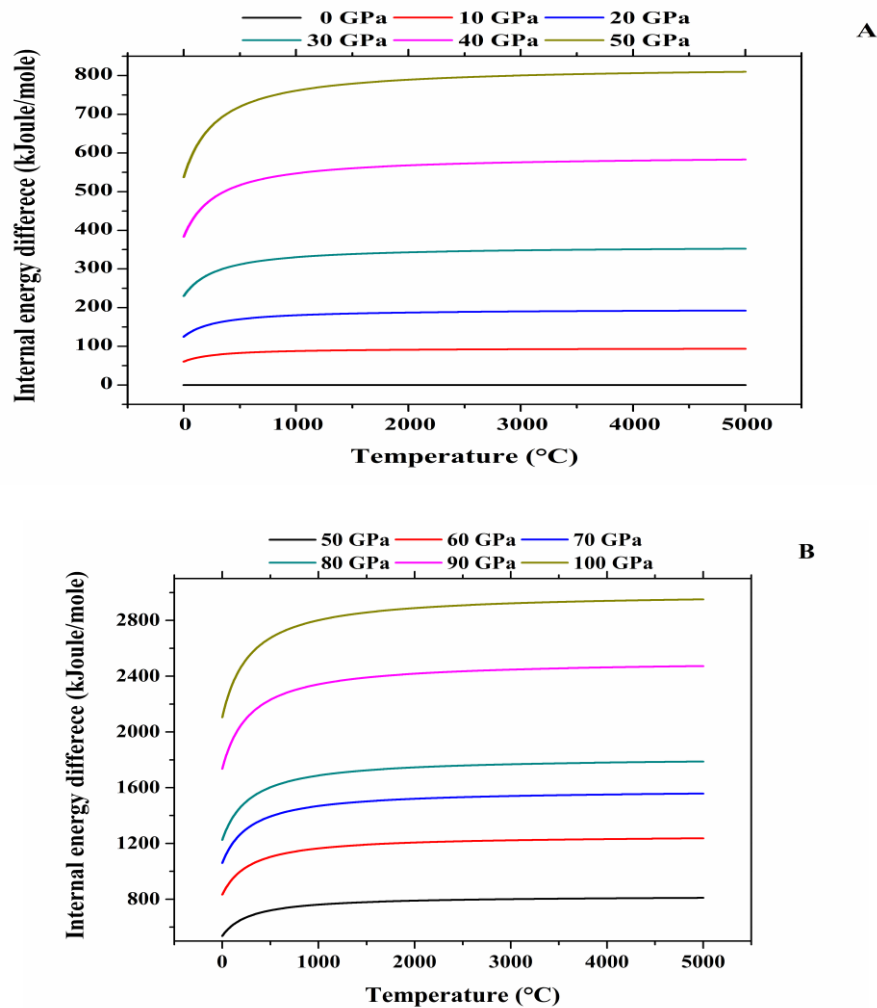

Figure 3: Change in the difference in internal energy for NiO structure with the change in temperature from 0 to 5000 °C by taking its value at zero pressure as a reference.

A Calculated at pressures 0, 10, 20, 30, 40 and 50 GPa.
B Calculated at pressures 50, 60, 70, 80, 90 and 100 GPa.

III-2-2 The free energy
Where Figure (4) presents the change in the free energy of the NiO structure calculated relative to the values of the pressures studied with the change in temperature. While, Figure (5) presents the change in the free energy difference of the NiO structure with the change in temperature from 0 to 5000 °C by taking its value at zero pressure as a reference, where; A calculated at pressures 0, 10, 20, 30, 40 and 50 GPa and B calculated at pressures 50, 60, 70, 80, 90 and 100 GPa.
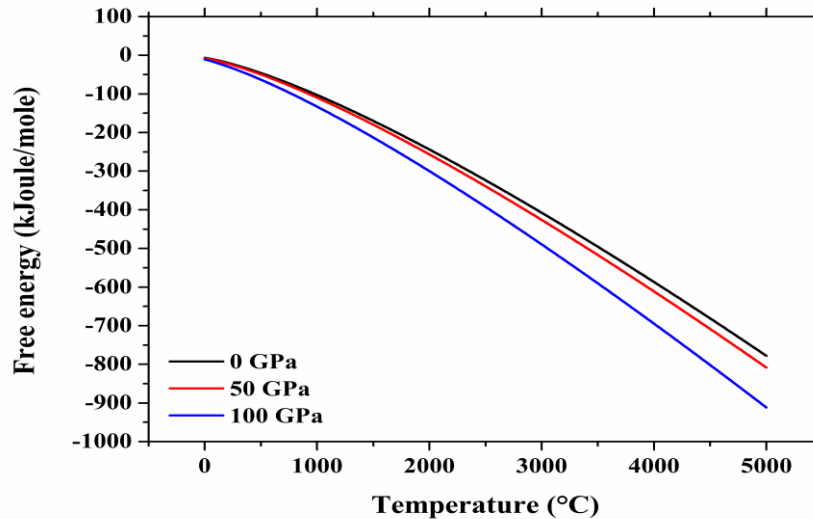

Figure 4: Change in the free energy for NiO structure calculated at pressures 0, 50 and 100 GPa with the change in temperature from 0 to 5000 °C.

Table 2: Presents the most important values of internal energy, free energy and entropy and heat capacity at constant volume calculated at pressures 0, 50 and 100 GPa with the change in temperature from 0 to 5000 °C.

	Temperature (K)	Pressure (GPa)		
		0	50	100
Internal energy (kJoule/mole)	0	7.64	8.17	7.64
	5000	256.22	257.03	256.22
Free energy (kJoule/mole)	0	-6.21	-7.14	-6.21
	5000	-777.94	-808.24	-777.94
Entropy (Joule/K.mole)	0	49.75	52.46	49.75
	5000	56.66	56.22	56.66
heat capacity at constant volume (Joule/K.mole)	0	45.11	46.08	48.17
	5000	49.97	49.97	49.97

From Figure (4) and Table (2) note that the free energy of nickel oxide decreases in a nonlinear manner with the increase in temperature, in the range of at least an estimated 770.36 kjoule/moule for zero pressure, but for the pressure of 100 GPa the domain of its change is estimated at 899.28 kjoule/moule. Also, its value at absolute zero is not zero, if its values also decrease with the increase in pressure, where its value are estimate at 6.21 kjoule/moule and 10.74 kjoule/moule at the previous two pressures respectively.
It also notes that the difference is increasing with the increase in temperature, and this is also clearly determined by figure (5). This figure also shows that this difference is increasing with the increase in pressure, with the lowest difference estimated at 99.58 joule/moule at absolute zero and between two pressures 0 and 10 GPa, while its highest value is estimated at 26.99 kjoule/moule and this is at 5000 °C and between the two pressures 90 and 100 GPa.
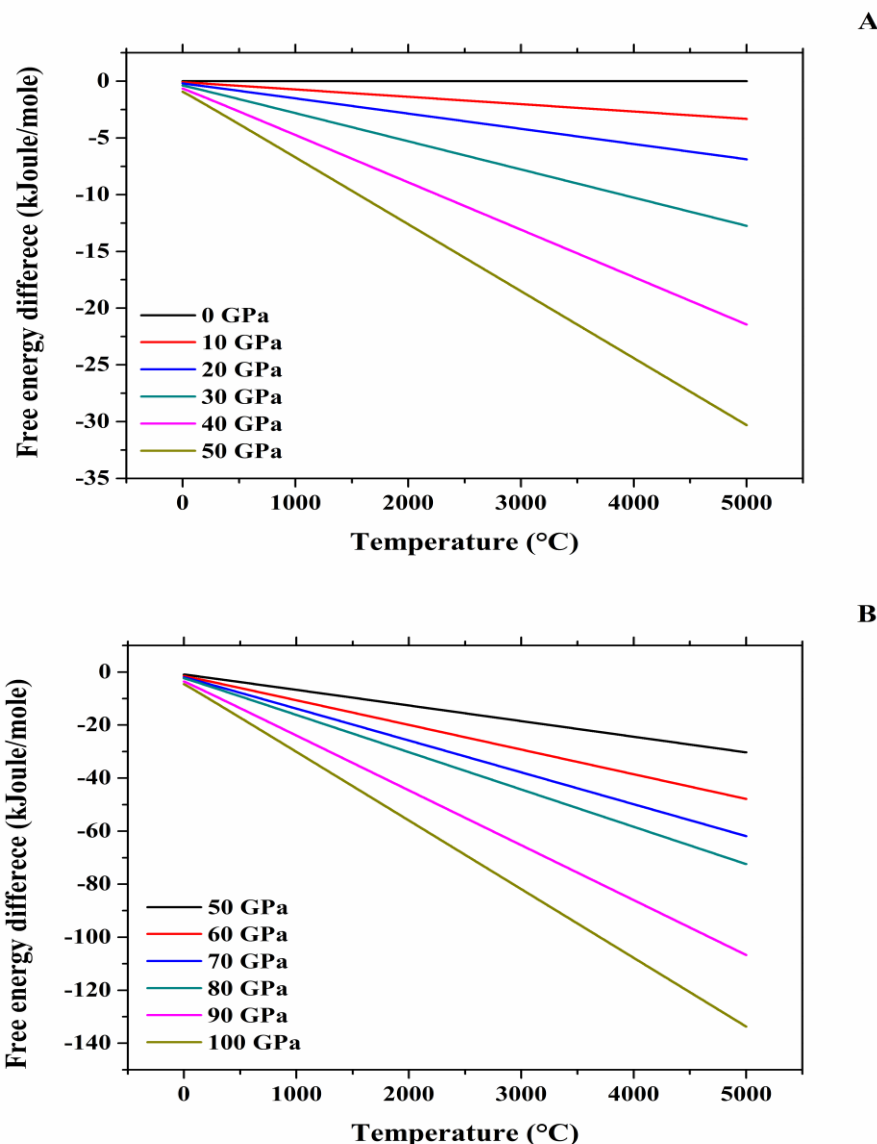
Figure 5: Change in the difference in the free energy for NiO structure with the change in temperature from 0 to 5000 °C by taking its value at zero pressure as a reference.
-A Calculated at pressures 0, 10, 20, 30, 40 and 50 GPa.
-B Calculated at pressures 50, 60, 70, 80, 90 and 100 GPa.

III-2-3 The entropy

Figure (6): presents the change in entropy of NiO structure calculated at pressures 0, 50 and 100 GPa with the change in temperature from 0 up to 5000 °C.

Figure (7): presents the change in the entropy difference of the NiO structure with the change in temperature from 0 to 5000 °C by taking its value at zero pressure as a reference, where A- calculated at pressures 0, 10, 20, 30, 40 and 50 GPa and B- calculated at pressures 50, 60, 70, 80, 90 and 100 GPa.

From Table (2) and the above two figures note that the entropy of nickel oxide increases with the increase in temperature up to certain temperatures, which are decreasing with the increase in pressure, the entropy value reaches a maximum value whatever the pressure, estimated at approximately 63 joule/K.mole. After these temperatures the value of entropy decreases, but somewhat slowly. Their values are at absolute zero at non-pressure, while higher for the largest pressure values. The range of change of this entropy is limited between 14 and 8 joule/K.mole, for the two pressures mentioned above respectively. It can also be seen that the values of this parameter do not maintain a specific arrangement, as they are rearranged after certain temperatures compared to their values for each pressure. This makes the difference decreasing before and after these temperatures, taking a value for zero pressure as a

reference, it is at two specific temperatures. Before pressure 50 GPa this temperature is estimated at 520 °C, while above this pressure it is estimated at 480 °C.
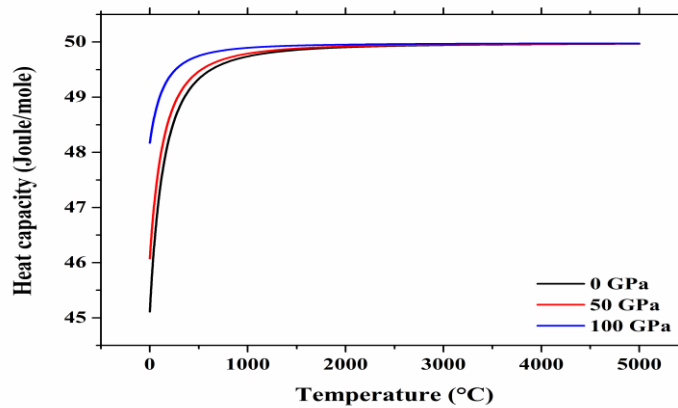

Figure 6: Change in the entropy for NiO structure calculated at pressures 0, 50 and 100 GPa with the change in temperature from 0 to 5000 °C.

III-2-4 The heat capacity at constant volume

Figure (8) presents the change in the heat capacity at constant volume of the NiO structure calculated at pressures 0, 50 and 100 GPa with the change in temperature from 0 to 5000 °C. While, figure (9) presents the change in the difference in the heat capacity at constant volume of the NiO structure with the change in temperature from 0 to 5000 °C by taking its value at zero pressure as a reference, where -A calculated at pressures 0, 10, 20, 30, 40 and 50 GPa and -B calculated at pressures 50, 60, 70, 80, 90 and 100 GPa.
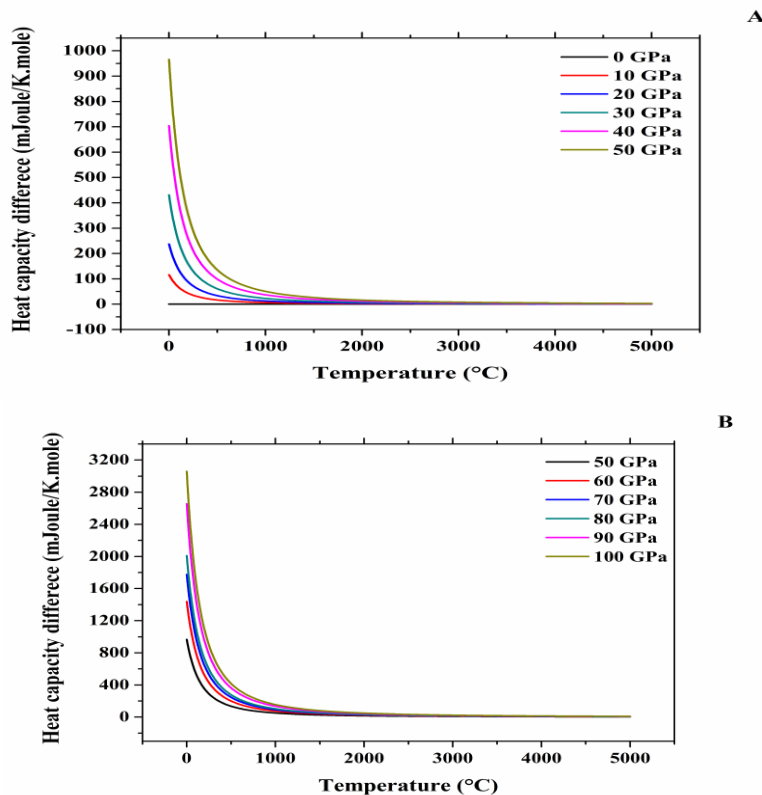

Figure 7: Change in the difference in the entropy for NiO structure with the change in temperature from 0 to 5000 °C by taking its value at zero pressure as a reference.
-A Calculated at pressures 0, 10, 20, 30, 40 and 50 GPa.
-B Calculated at pressures 50, 60, 70, 80, 90 and 100 GPa.

Which through them and table (2) show that heat capacity values are increasing with the increase in pressure, being at absolute zero the lowest value of it for zero pressure. In addition, at this pressure the range of change of this capacity is greater, which is estimated at 1.80 joule/K.mole. While the lowest range to change it is for 100 GPa pressure, which is estimated at 4.85 joule/K.mole. This capacity is greatly increased with the increase in temperature, but this increase is even faster only until certain values of temperatures and then slows down dramatically to the point of almost constant after it. These temperatures are increasing with the decrease in pressure; at the temperature close to 3000 °C the heat capacity value is almost constant regardless of the increase in pressure or temperature. Before this temperature, the difference is decreasing with the increase in temperature, between the two pressures 0 and 10 GPa is estimated at 0.12 joule/moule as its lowest value, while its highest value is estimated at 0.41 joule/moule and this is between the two pressures 90 and 100 GPa.
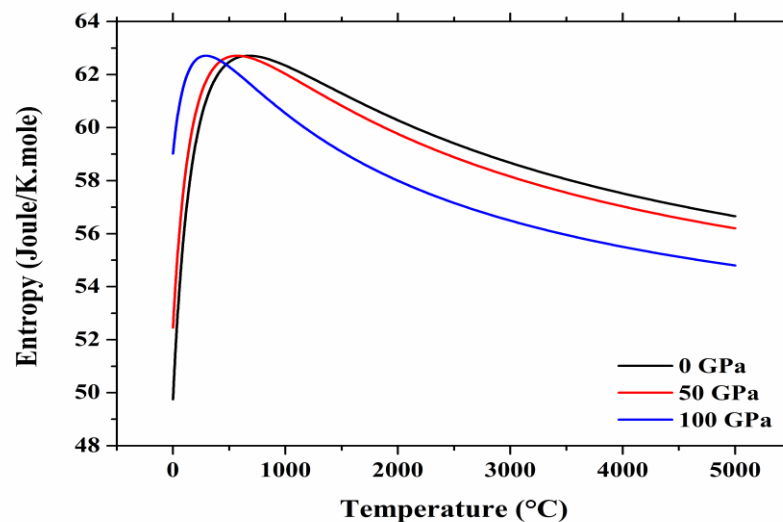

Figure 8: Change in the heat capacity at constant volume for NiO structure calculated at pressures 0, 50 and 100 GPa with the change in temperature from 0 to 5000 °C.

CONCLUSION

In this work, we were interested in illustrating the importance of using Romberg integration in calculating some important parameters of thermodynamic properties, which most previous studies on nickel oxide did not care about. Especially when the pressure changes from 0 to 100 GPa, the temperature changes between 0 and 5000 ° C. This is done by identifying Debye temperature values at the pressures of the study, which were determined using the CASTEP program by determining the function of PBEsol from the GGA approximation, DFT method that appeared in 2008. Therefore, we were able to see that:

- There is a decrease in Debye temperature of nickel oxide when pressure increases, by nonlinear manner.
- Most thermodynamic parameters are increasing with the increase in pressure, other than free energy and entropy for high temperatures. The same exception depends for an increase in temperature, as the rest of the parameters are often increasing as well.
- At absolute zero the values of our study results correspond to Debye temperature. While we could not compare the rest of the other parameter values due to their unavailability.

In the future, it is possible to suggest a number of research directions that always fall within this scope, which are:

- The study can be directed to apply its results within a certain range, such as studying the possibility of the presence of this oxide in the Earth's layers.
- Investing in the results of this study to calculate other parameters, such as heat capacity at constant pressure, thermal expansion, thermal conductivity, etc.
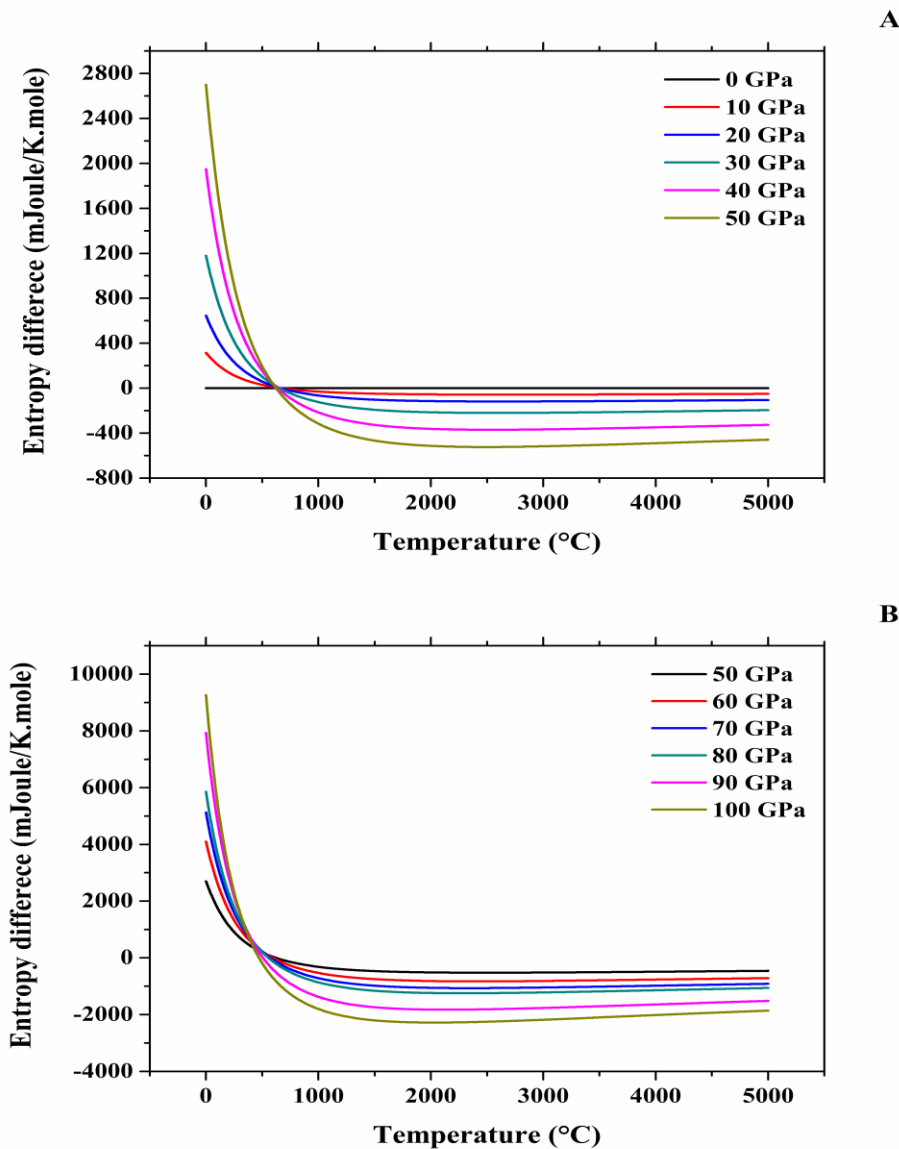
Figure 9: Change in the difference in the heat capacity at constant volume for NiO structure with the change in temperature from 0 to 5000 °C by taking its value at zero pressure as a reference.
-A Calculated at pressures 0, 10, 20, 30, 40 and 50 GPa.
-B Calculated at pressures 50, 60, 70, 80, 90 and 100 GPa.

REFERENCE
1. Epperson, J. F. (2013). An introduction to numerical methods and analysis. John Wiley & Sons.
2. Hildebrand, F. B. (1987). Introduction to numerical analysis. Courier Corporation.
3. Chakraverty, S., Mahato, N., Karunakar, P., & Rao, T. D. (2019). Advanced numerical and semi-analytical methods for differential equations. John Wiley & Sons.
4. Ciarlet, P. G., & Lions, J. L. (Eds.). (2002). Handbook of numerical analysis (Vol. 8). Gulf Professional Publishing.
5. Deuflhard, P., &Hohmann, A. (2003). Numerical analysis in modern scientific computing: an introduction (Vol. 43). New York: Springer.
6. Hammer, P. C. (1958). The midpoint method of numerical integration. Mathematics Magazine, 31(4), 193-195.
7. You, P. (1967). Numerical Integration.
8. Kuncir, G. F. (1962). Algorithm 103: Simpson's rule integrator. Communications of the ACM, 5(6), 347.
9. Fox, L. (1967). Romberg integration for a class of singular integrands. The Computer Journal, 10(1), 87-93.

10. Barnes, C. E. (2003). Inorganic chemistry (catherine e. housecroft and alan g. sharpe). Journal of Chemical Education, 80(7), 747.
11. Huheey, J. E., Keiter, E. A., Keiter, R. L., &Medhi, O. K. (2006). Inorganic chemistry: principles of structure and reactivity. Pearson Education India.
12. Poirier, J. P. (2000). Introduction to the Physics of the Earth's Interior.CambridgeUniversityPress.
13. Noguchi, Y., Uchino, M., Hikosaka, H., Kusaba, K., Fukuoka, K., Mashimo, T., &Syono, Y. (1998). Shock compression of NiO to 130 GPa. The Review of High Pressure Science and Technology, 7, 832-834.
14. Shukla, A., Rueff, J. P., Badro, J., Vanko, G., Mattila, A., de Groot, F. F., &Sette, F. (2003). Charge transfer at very high pressure in NiO. Physical Review B, 67(8), 081101.
15. de PR Moreira, I., Illas, F., & Martin, R. L. (2002). Effect of Fock exchange on the electronic structure and magnetic coupling in NiO. Physical Review B, 65(15), 155102.
16. Zhang, W. B., Hu, Y. L., Han, K. L., & Tang, B. Y. (2006). Pressure dependence of exchange interactions in NiO. Physical Review B—Condensed Matter and Materials Physics, 74(5), 054421.
17. Kuneš, J., Anisimov, V. I., Skornyakov, S. L., Lukoyanov, A. V., &Vollhardt, D. (2007). NiO: correlated band structure of a charge-transfer insulator. Physical review letters, 99(15), 156404.
18. Liu, L., Li, X. D., Liu, J., Jiang, S., Li, Y. C., Shen, G. Y., ...& Xu, J. (2008). High pressure structural and elastic properties of NiO up to 67 GPa. Journal of Applied Physics, 104(11).
19. Chauhan, R., & Singh, S. (2008). Structural study of Novel (superhard) material: NiO. Pramana, 70, 307-311.
20. Nwanya, A. C., Offiah, S. U., Amaechi, I. C., Agbo, S., Ezugwu, S. C., Sone, B., ...&Ezema, F. I. (2015). Electrochromic and electrochemical supercapacitive properties of room temperature PVP capped Ni (OH) 2/NiO thin films. ElectrochimicaActa, 171, 128-141.
21. Potapkin, V., Dubrovinsky, L., Sergueev, I., Ekholm, M., Kantor, I., Bessas, D., ...&Abrikosov, I. A. (2016). Magnetic interactions in NiO at ultrahigh pressure. Physical Review B, 93(20), 201110.
22. Gavriliuk, A. G., Struzhkin, V. V., Ivanova, A. G., Prakapenka, V. B., Mironovich, A. A., Aksenov, S. N., ...&Morgenroth, W. (2023). The first-order structural transition in NiO at high pressure. Communications Physics, 6(1), 23.v
23. Achouri, A., Tlili, S., Kaddour, A., Nassiba, B., Nedjimi, M. S., Meddah, M. D., &Nassira, M. (2023). A study assessment of the thermodynamic properties of MgO and CaO at PREM pressures up to the outer core's limits of the Earth. NeuroQuantology, 21(7), 624.
24. Mahcene, Hocine. "Complementary Study to Determine the Thermodynamic Properties of Wüstite in Deep Earth Layers up to 140 GPa." Tobacco Regulatory Science (TRS) (2023): 2522-2542.
25. Lu, L. Y., Cheng, Y., Chen, X. R., & Zhu, J. (2005). Thermodynamic properties of MgO under high pressure from first-principles calculations. Physica B: Condensed Matter, 370(1-4), 236-24
26. Tuncel, E., Colakoglu, K., Deligoz, E., &Ciftci, Y. O. (2009). A first-principles study on the structural, elastic, vibrational, and thermodynamical properties of BaX (X= S, Se, and Te). Journal of Physics and Chemistry of Solids, 70(2), 371-378.
27. Hai-jun, H., & Fan-jie, K. (2011). The structural, elastic and thermodynamical properties of zinc-blendeBeTe from first-principles. ComputationalMaterials Science, 50(4), 1437-1441.
28. Segall, M. D., Lindan, P. J., Probert, M. A., Pickard, C. J., Hasnip, P. J., Clark, S. J., & Payne, M. C. (2002). First-principles simulation: ideas, illustrations and the CASTEP code. Journal of physics: condensed matter, 14(11), 2717.
29. Hohenberg, P., & Kohn, W. J. P. R. (1964). Density functional theory (DFT). Phys. Rev, 136(1964), B864.
30. Perdew, J. P., &Zunger, A. (1981). Self-interaction correction to density-functional approximations for many-electron systems. Physical review B, 23(10), 5048.
31. Perdew, J. P., Burke, K., &Ernzerhof, M. (1996). Generalized gradient approximation made simple. Physical review letters, 77(18), 3865.
32. Perdew, J. P., Ruzsinszky, A., Csonka, G. I., Vydrov, O. A., Scuseria, G. E., Constantin, L. A., ... & Burke, K. (2008). Restoring the density-gradient expansion for exchange in solids and surfaces. Physical review letters, 100(13), 136406.