

Theoretical Study on the Volume Expansion of Mixed Metals $Zn_xNi_{1-x}O$ at High Temperature for Different Concentration Value X

1. Dr. Madhulika Anand, 2. Prof. Jagdhar Mandal

*Tmb university, bhagalpur
University dept. Of physics, tmb university, bhagalpur*

Date of Submission: 01-11-2020

Date of Acceptance: 15-11-2020

ABSTRACT: The present work aims on the volume expansion of mixed metals under high temperature. The material of interest in the current study has been chosen as $Zn_xNi_{1-x}O$ for the concentration value $x=0.25$ and $x=0.50$. It has been the long desire of human-beings to have the exact knowledge of the properties of the minerals and solids under the influence of the pressure and high temperature [1-2]. The theory of thermal expansion has a central role in explaining the high temperature behavior of solids for their wide use in geophysical applications [3,4]. This concept gives a panoramic view in geochemical problems concerning with the study of upper mantle structure of the earth. This study is also essential to shed light on the thermo elastic and anharmonic properties of crystals, minerals and complex minerals.

KEY WORDS: Volume expansion, thermal expansion, anharmonic, bulk modulus.

I. INTRODUCTION:

It is well-understood that the knowledge of the properties of minerals and solid under the influence of high temperature and high pressure is of great significance for the proper understanding of the interior of the earth or any other planet, nature of the interatomic forces, thermal expansivity and high temperatures equation of state for minerals. These aspects generated lot of interest and drew the attention of theoretical as well as experimental workers [5-6]. Moreover, the study of elastic constants and their behaviour with temperature and pressure also provide important useful information and insight into the structural complexities of minerals. These insights proved to be useful in geophysical and geochemical problems related to the study of lower mantle compounds and mixed minerals and the interpretation of the structure of the mantle of the earth. For the purposes of acquiring concrete knowledge of the mantle structure and

seismic study. It is desirable to investigate the temperature variation of bulk modulus of minerals. This study is sufficient to shed light on the thermoelastic and anharmonic properties of crystals and minerals [9-12]. It is in the order of the systematic studied facts that pressure dependence of bulk modulus has also been studied from the concept of ionic potentials, but the methods employed for the determination of the temperature dependence of bulk modulus are not simple and straightforward in spite of the urgent need in geophysical applications [13]. Recently, Anderson [14-17] and co-workers have investigated the thermodynamic behavior of large number of minerals up to very high temperature nearly 2000K it was then realized that Suzuki equation must be modified. The difference in two methods leads to the different final forms for the expression of thermal expansivity at high temperature. All theoretical attempts mentioned above contain some weakness in the models adopted by several workers. These models involve some approximation and heavy computational work to get the results.

II. METHODOLOGY:

The expression for volume thermal expansion (V/V_0) is similarly obtained by making use of the fact as follows

$$dK_T = -\delta_T K_T \cdot \frac{dV}{V} \quad (1)$$

$$\frac{K_T}{K_0} = \left[1 - \frac{\alpha_0 K_0 \delta_T^0}{T_0^{k(k+1)}} \{ T^{k+1} - T_0^{k+1} \} \right]$$

(2)

Differentiating equation (2) with respect to temperature T, we get

$$dK_T = -\frac{\alpha_0 K_0 \delta_T^0}{T_0^k} T^k dT$$

$$(3) \quad \frac{dV}{V} = \frac{\alpha_0}{\left[1 - (\alpha_0 \delta_T^0) / (T_0^k (k+1)) (T^{k+1} - T_0^{k+1})\right]} dT.$$

(4) The integration of equation (3) provides us the expression known as Singh and Gupta's expression for volume thermal expansion given as

$$(5) \quad \frac{V}{V_0} = \exp \left[\int_{T_0}^T \frac{\alpha_0}{\left[1 - (\alpha_0 \delta_T^0) / (T_0^k (k+1)) (T^{k+1} - T_0^{k+1})\right]} dT. \right]$$

The above expression is known as Singh and Gupta's universal equation of state.

The value of thermoelastic constant, thermal expansion co-efficient α_0 at $T=T_0$ and the

value of Anderson- Grineisen parameter δ_T^0 at temperature $T=T_0$ usually T_0 is taken to be room temperature as the reference temperature for mixed crystal can be obtained by applying Vegard's law given as

$$\alpha_0^{mix} = x \alpha_0^{MgO} + (1-x) \alpha_0^{CaO}$$

$$(6) \quad K^{mix} = x K^{MgO} + (1-x) K^{CaO}$$

$$(7) \quad \delta_T^{0mix} = x \delta_T^{0MgO} + (1-x) \delta_T^{0CaO}$$

(8)

Here, x denotes the concentration of the dopant in the mixed minerals.

III. OBSERVATION AND CALCULATION:

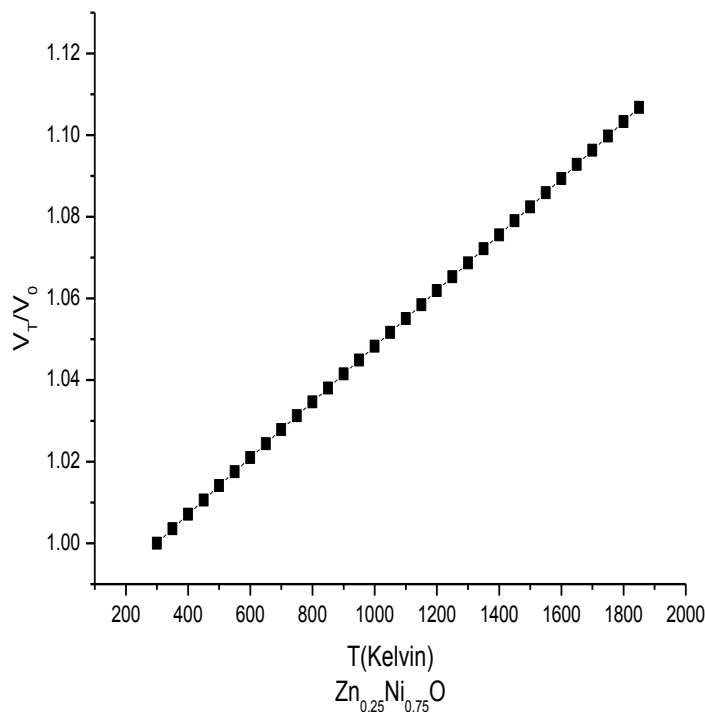
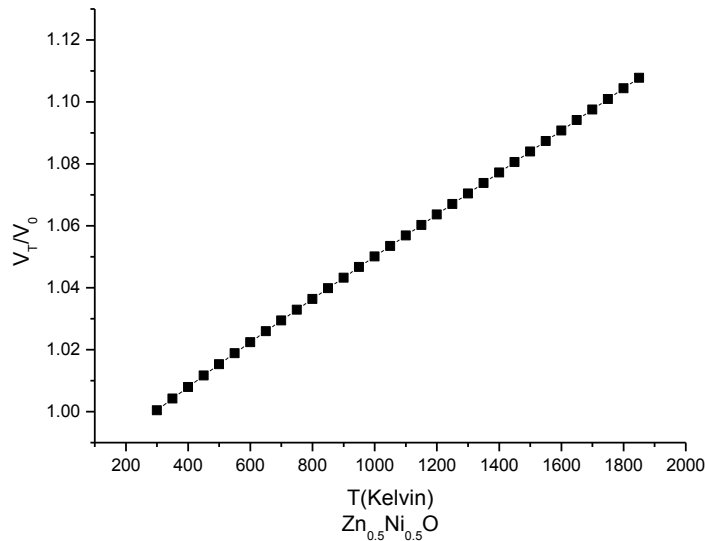


Fig.(1) . Variation of V_T/V_0 with temperature for $Zn_{0.25}Ni_{0.75}O$



Fig(2). Variation of V_T/V_0 with temperature for $Zn_{0.5}Ni_{0.5}O$

IV. CONCLUSION:

We have calculated the values of the volume expansion for mixed crystals under consideration as a function of temperature in the range 300-1800K. The close agreement of calculated values of volume expansion for pure minerals and similar pattern of variation of these composite minerals for different do pant concentration with temperature establishes correctness and the validity of the procedure used in our study.

REFERENCES:

- [1]. O.L.Anderson, Phys. Rev. 144(1961)553.
- [2]. O.L.Anderson, D.G.Isaak, H.Oda, Rev.Geophys.30(1992)57.
- [3]. S.S.Bedi, and M.S.Bhangoo, Modern Physics. Lett.10(15)(1996).697.
- [4]. D.G.Isaak, O.L.Anderson, T.Goto, phys. chem. Minerals 16(1989)704.
- [5]. M.Kumar, Physica B 222(1996)229
- [6]. E. R. Cowley, Z. Gong and G. K. Hortan Phys. Rev. B, Condensed matter 41, 2150 (1990)
- [7]. O. L. Anderson and D. G. Issak, Mineral Physics and Crystallography. Habdbook of constants, American Geophysical Union OCL. A Press Los Angles 2, 64(1995).
- [8]. M. Kumar & S. S. Bedi Phys. State Sol(b) 188 645 (1995) High temp. High press. 27,595 (1996).
- [9]. F. F. Voronov, E. V. Chernysheva, V. A. Goncharova-High pressure Science & Technology, proceeding of the VIIth International AIRAPS Confever et.al,1980.
- [10]. D.C.Wallace, Thermodynamic of crystals (Woley New York,1972)
- [11]. R.Jeanloz, J.Geophys. Res. 84(1979)6059.
- [12]. R.M.Hazen and L.W.Finger, Comprative crystals chemistry (Wiley,New York, 1982)
- [13]. O.L.Anderson,Int.J.Thermophys.12,757. (1991)
- [14]. R.BoechleandG.C.Kennedy.J.phys.chem.Sol .41, 517,1019(1980)
- [15]. T.G.phymate and J.H.stait, J.Geophys.Res1394, 9477. (1989)
- [16]. F. F. Voronov, E. V. Chernysheva, V. A. Goncharova-High pressure Science & Technology, proceeding of the VIIth International AIRAPS Confever et.al,1980. 17.D.C.Wallace, Thermodynamic of crystals (Woley New York,1972)