Equation of State for Volume Thermal Expansion for Nanomaterials at high Temperature

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***Abstract*- The present work is based on the thermo-elastic properties of some nanomaterials under the effect of high temperature. There are various thermo-elastic properties out of them the volume thermal expansion(v/v_0) is calculated. We have derived a new integral form of equation of state (IFEOS) in which we have assumed that the Anderson-Gruneisen parameter (δ_T) varies with temperature. This equation of state has been applied to ten nanomaterials like 20nm-Ni and 15nm-(80Fe+20Ni), Ag, Zirconia, ZnO, TiO_2, NiO, Al, AlN/Al 39%, AlN/Al 11%. We have compared our results with the experimental data . The results obtained from our equation are in an excellent agreement with the experimental data. Our equation of sate is simpler and more compact than the equation of states which are published earlier and available in literature.**

***Keywords*- Nanomaterials, Equation of state, volume thermal expansion.**

I.INTRODUCTION-The study of volume thermal expansion of nanomaterials has been proved convenient for theoretical investigation as well as experimental works. This study is helpful in solving the various technological problems [1-3]. Thermodynamic and thermo-elastic properties are two main areas in scientific interest of nanocrystelline materials. We observe drastic change in physical and chemical properties of nanomaterials in comparison to bulk materials due to their small size [4]. Nanocrystals have large surface to volume ratio and surface effects take on a significance that is normally irrelevant for bulk materials. Since the atomic structure of materials, their stability and their atomic interactions are related in complex ways to their thermodynamic properties, it is of great fundamental interest to explore the thermodynamic consequences of the material system with interfacial regions. There are many equations of states have been derived for different class of solids within the Mie-Gruneisen approximation in terms of low pressure and temperature dependence. Very recently, volumetric thermal expansion behaviour of various nanofluids were measured experimentally by Nayak *et al.* [5]. They used the naofluids of Al_2O_3, CuO, SiO_2,TiO_2 nanoparticle suspending them in water by ultrasonication. Recently Bhagwat and Ramaswamy synthesized Nanocrystalline Zirconia powder with a fairly narrow particle size distribution using amorphous citrate route [6]. The crystalline size determined from XRD has been found 8nm and is close agreement with the particle size determined by TEM. The crystalline size has been found to increase with the increasing temperature. Xiang et al. studied the high pressure behaviour of two samples of ZnO nanorods with different grain sizes and compared with their corresponding bulk phase [7]. W.F. Zhang *et al.* prepared Titanium dioxide (TiO_2) nanocrystals by a hydrolysis process of tetrabutyl titanate . They obtained Nanocrystal samples with various sizes of 6.8-27.9 nm after annealing from 100 to 650 °C [8].A lot of experimental works have been done to understand the thermal properties of nanomaterials. Equally, there is a lacking of theoretical attempts. The idea of present study is to discuss a simple and straightforward method for evaluation of thermal expansion of nanomaterials. this method is applicable under the assumption that Anderson Gruneisen parameter(δ_T) is a temperature dependent parameter. Prasad *et al.*[9,10] studied these thermo-elastic properties of alkaline earth solids under the effect of high temperature and It has observed that the results on temperature dependent elastic properties get modify, if the linear dependence of δ_T with temperature is assumed. The main objective of present work is to investigate the validity of our newly established integral form of equation of state to determine the volume thermal expansion of nanomaterials taking eleven particular nanomaterials like Fullerene, 20nm-Ni and 15nm-(80Fe+20Ni), Ag, Zirconia, ZnO, TiO_2, NiO, Al, AlN/Al(39%), AlN/Al(11%).

II. METHOD OF ANALYSIS- Thermal expansion coefficient(CTE) for nanomaterials is defined as

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P$$

Which can be written as alternatively

$$\alpha = \left(\frac{\partial \ln V}{\partial T}\right)_P \qquad (1)$$

Or $$\int_{V_0}^{V} d(\ln V) = \int_{T_0}^{T} \alpha dT$$

Now since N.Prakash[11] derived an expression for CTE as $\alpha = \alpha_0[1- \alpha_0\delta_T(T-T_0)]^{-1}$, where δ_T is Anderson-Gruneisen parameter. Hence above expression can be written as

Or $$\int_{V_0}^{V} d(\ln V) = \int_{T_0}^{T} \frac{\alpha_0}{[1-\alpha_0\delta_T(T-T0)]} dT \quad (2)$$

The temperature dependency of δ_T may be written by following empirical relation[10],

$$\delta_T = \delta_T^0 (T/T_0)^k \quad (3)$$

Where k is a dimensionless thermo-elastic parameter and value of which can be calculated from the slope of the graph, $\log(\delta_T)$ versus $\log(T/T_0)$, which comes as a straight line.

Now combining equations (2) and (3) we get

$$V/V_0 = \exp \int_{T_0}^{T} \frac{\alpha_0}{[1-\alpha_0\delta_T^0(\frac{T}{T_0})(T-T0)]} dT \quad (4)$$

or $$\frac{V}{V_0} = \mathrm{Exp}[\int_{T_0}^{T} \frac{\alpha_0}{[1-\alpha_0\delta_T^0 T^k T_0^{-k}(T-T_0)]} dT] \quad (5)$$

This new equation can be introduced as KM2SEOS(Krishna-Mahipal-Madan-Harish equation of state) for variation of volume thermal expansion for nanomaterials by considering the fact that Anderson-Gruneisen parameter varies with temperature, which looks much simpler than those of which are published earlier and available in literature and which are very few in numbers.

III. RESULTS AND DISCUSSION:

We have computed, using KM2EOS, the values of relative volume thermal expansion V/V_0 under the effect of high temperature and the atmospheric pressure of 20nm-Ni, 15nm-(80Ni+20Fe), nm-Ag, Zirconia, nm-ZnO, nm-TiO_2, nm-NiO, nm-Al, 11%AlN/Al and 39%AlN/Al nanomaterials. It has been observed that the volume thermal expansion increases linearly with temperature. The input parameter required to compute the value of V/V_0 has been tabulated as follows

TABLE.1. INPUT PARAMETER USED IN PRESENT WORK-

Nanomaterials	(α_0x10^{-6} K^{-1})	δ_T^0	Reference temperature(K)	Reference
20nm-Ni	33	26.34	300	[14]
15nm-(80Ni+20Fe)	33.36	20.81	300	[14]
nm-Ag	18	4	300	[15]
Zirconia	34.6	4	300	[15]
nm-ZnO	10.4	4	300	[15]
nm-TiO2	15.2	4	200	[15]
nm-NiO	37.7	4	400	[15]
nm-Al	78	4	300	[15]
AlN/Al 39%	42	4	300	[15]
AlN/Al 11%	58.8	4	300	[15]

This equation needs only three input parameters such as Anderson-Gruneisen parameter(δ_T^0), volume thermal expansion coefficient(α_0) along with reference temperature. Volume expansion is computed by KM2EOS i.e., equation(5) as a function of temperature in the range of 300-750K for 20nmNi, 15nm-(80Ni+20Fe), AlN/Al(11%) and AlN/Al(39%) nanomaterials respectively, The results obtained are reported in figs.1,2,3, and10 respectively. For nanomaterials Ag, zirconia, ZnO_2, TiO_2, NiO, Al, the temperature range has taken as 300-1000K, 300-1600K, 300-1400K, 200-1100K, 400-1600K and 250-750K respectively. The results obtained are reported in figs.4, 5, 6, 7, 8 and 9 respectively. The reason for categories these nanomaterials in two parts are accessibility of experimental data at particular temperatures. There are no experimental data available regarding our work for 20nm-Ni and 15nm-(80Ni+20Fe) so we could not compare our result with experimental one.

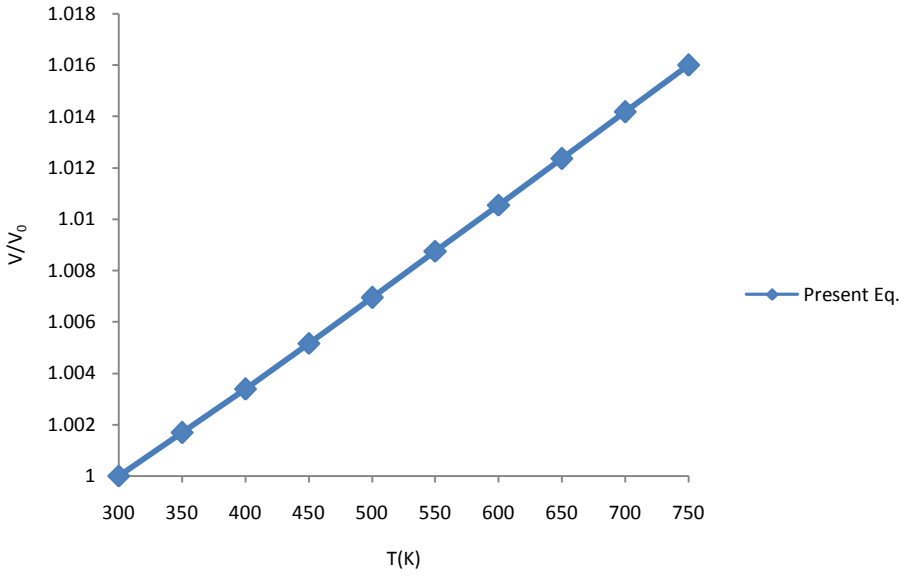

Fig.1.Temperature dependence of V/V_0 of 20nm-Ni

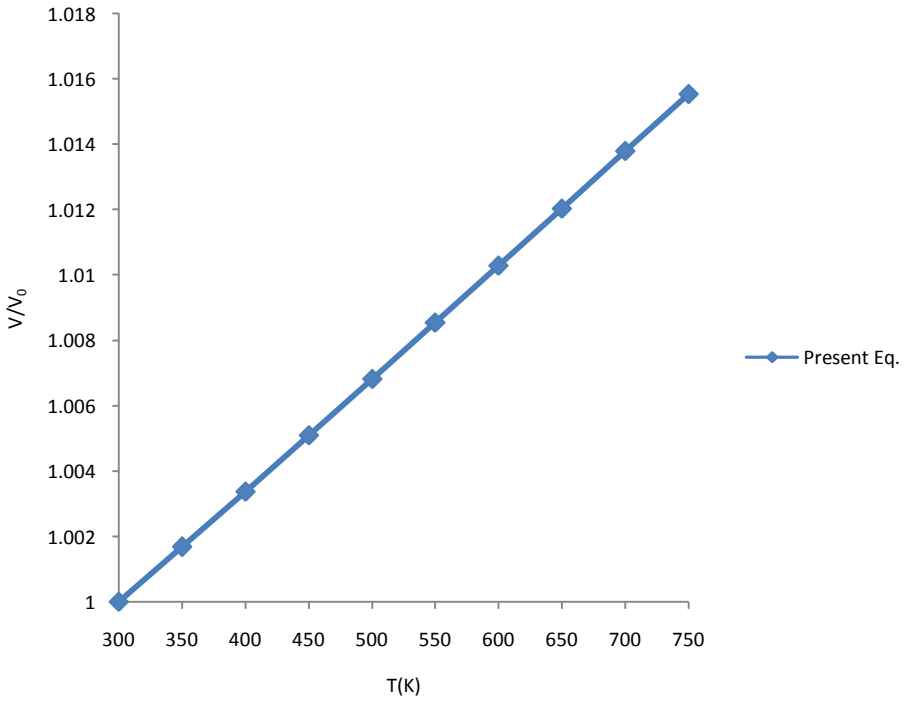

Fig.2. Temperature dependence of V/V_0 of 15nm (80Ni+20Fe)

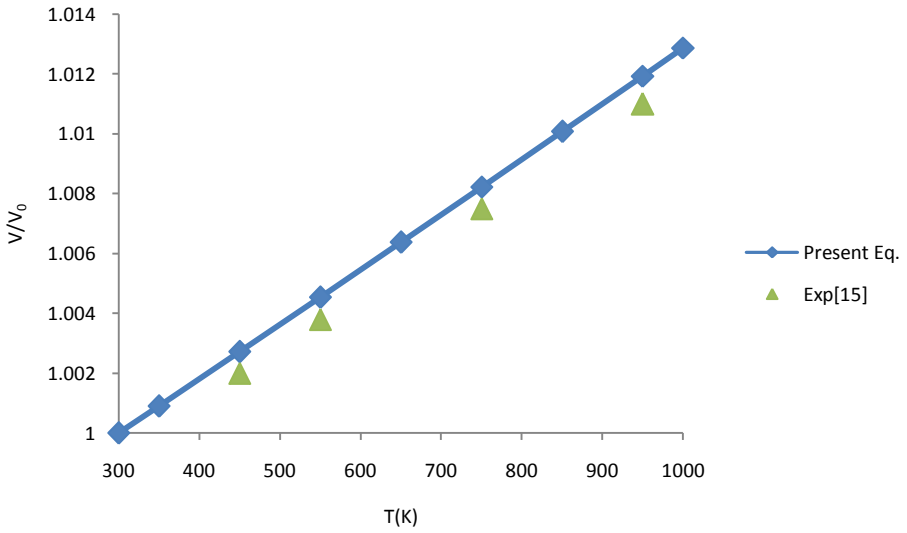

Fig.3.Temperature dependence of V/V_0 of nm-Ag

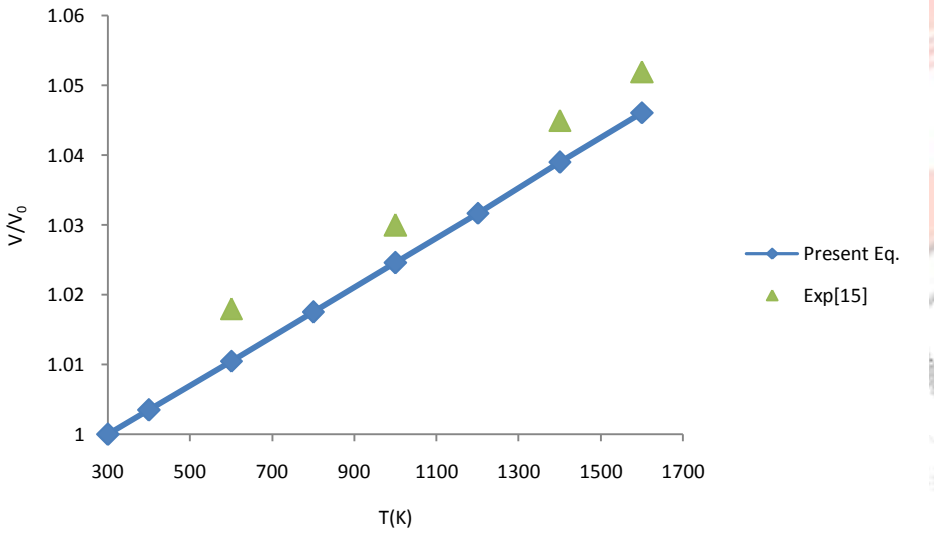

Fig.4.Temperature dependence of V/V_0 of nm-ZrO_2

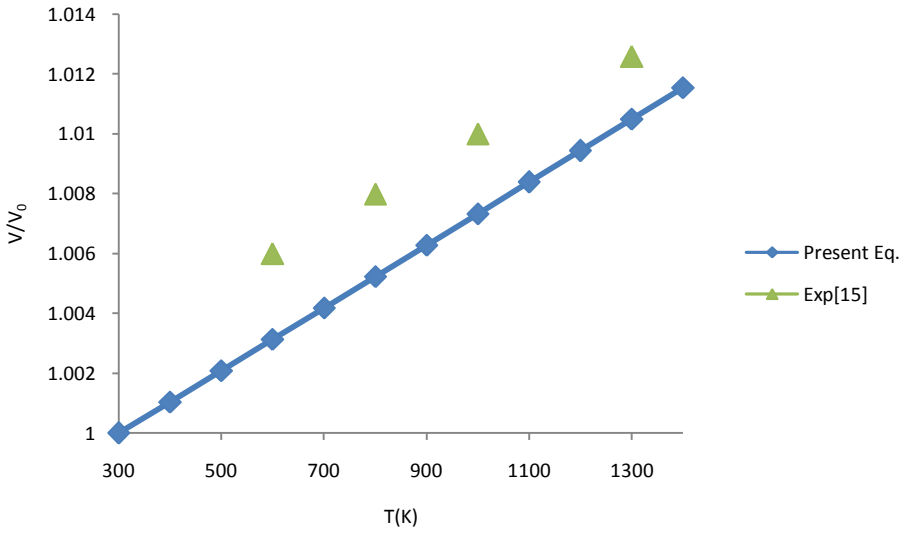

Fig.5. Temperature dependence of V/V_0 of nm-ZnO

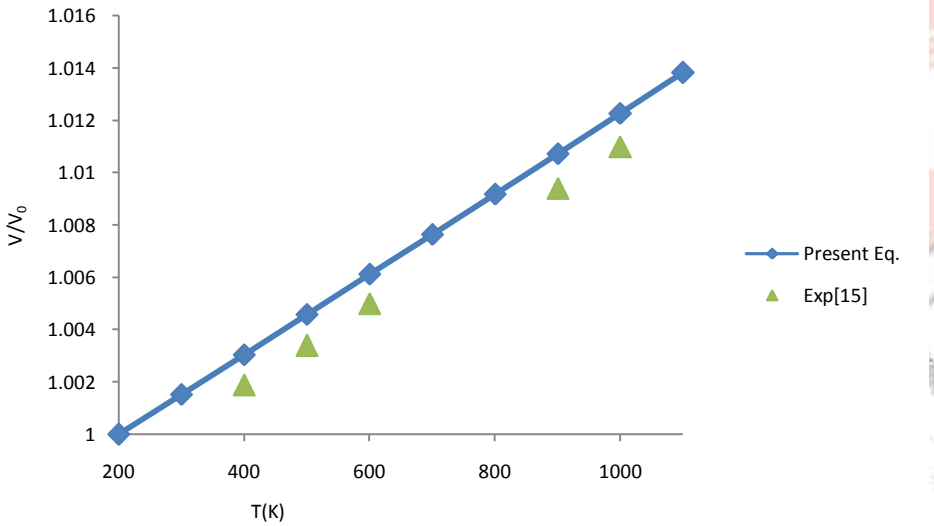

Fig.6. Temperature dependence of V/V_0 of $nmTiO_2$

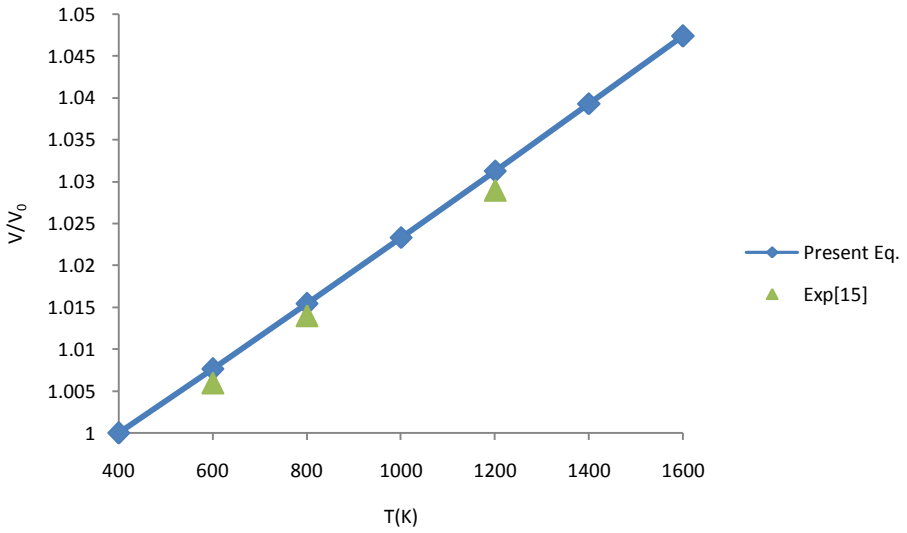

Fig.7.Temperature dependence of V/V_0 of nm-NiO

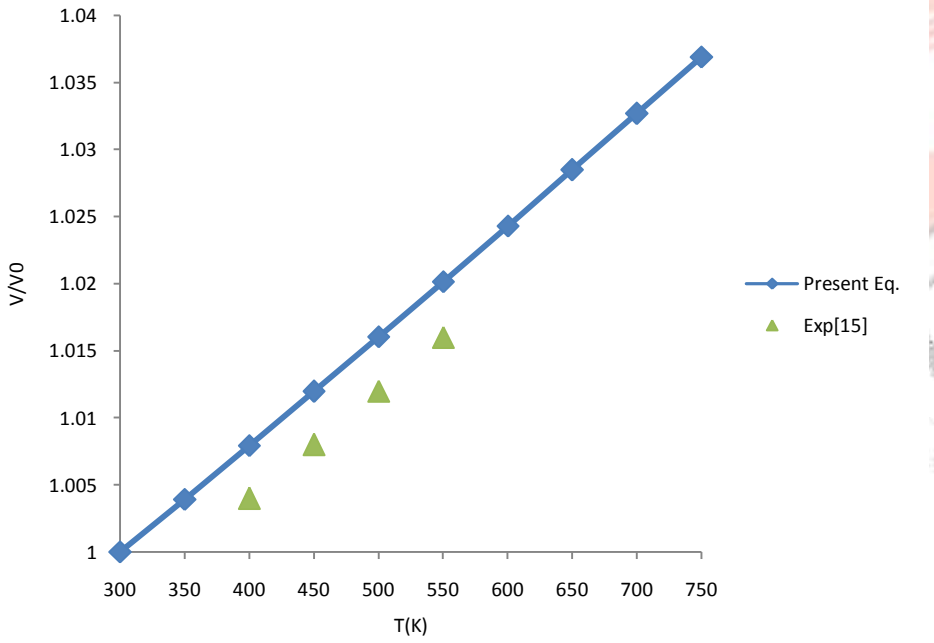

Fig.8. Temperature dependence of V/V_0 of nm-Al

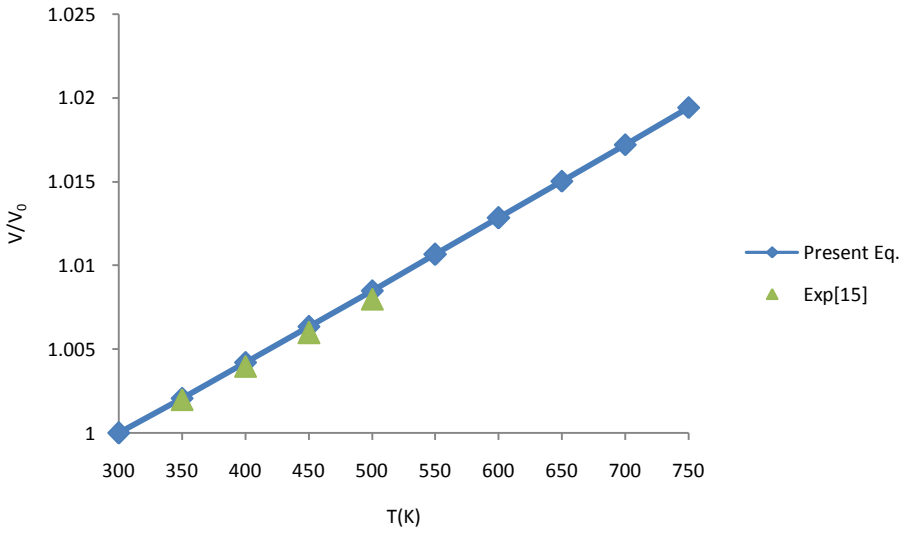

Fig.9. Temperature dependence of V/V_0 of nm- AlN/Al 39%

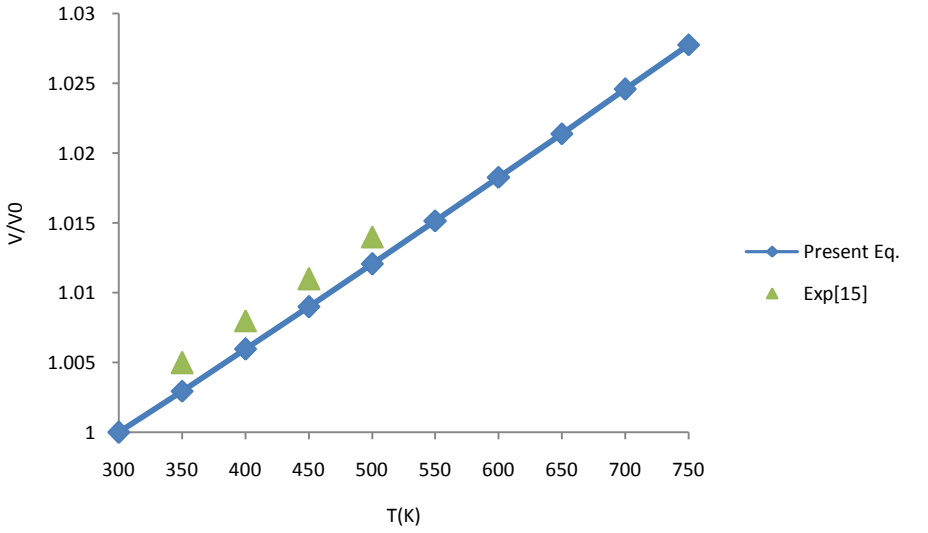

Fig.10. Temperature dependence of V/V of nm-AlN/Al 11%

IV. CONCLUSION- A new integral form of equation of state for relative volume thermal expansion has been developed. The values of relative volume thermal expansion (V/V_0) at different temperatures for nanomaterials 20nm-Ni, 15nm-(80Ni+20Fe), nm-Ag, nm-ZrO_2, nm-ZnO, nm-TiO_2, nm-NiO, nm-Al, nm-39%AlN/Al, nm-11%AlN/Al is calculated by using this equation. The results are compared along with experimental data. It is found that for most of the materials, the results are very close and are agreeable with experimental data. By study of literature we have observed that very less number of equations of state are available which comprises the temperature dependent Anderson-Gruneisen parameter. KCEOS is simpler and compact with including the temperature dependent nature of Anderson-Gruneisen parameter, as very few equations are available in literatures which consider this type of temperature dependency of this parameter. This equation will provide a new insight for theoretical and experimental workers of relative volume thermal expansion of nanomaterials.

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References-

[1] S.C. Kim, T.H. Kwon, Temperature dependence of the elastic constants of KCl. Journal of Physics and Chemistry of Solids, vol.53, pp.539-548, (1992)

[2] Y. Kuru, M. Wohlschlogel, U. Welzel, E.J. Mittemeijer, Crystallite size dependence of the coefficient of thermal expansion of metals. Appl. Phys. Lett. Vol.90, pp.243113, (2007)

[3] R. Seelabouina, N. Phatak, R.P. Gulve, H.P. Leirmann, S.K. Saxena, Thermal Expansion of Nanocrystalline titanium dioxide (TiO_2), zinc oxide (ZnO), nickel oxide (NiO). Thermal Conduct. Vol.27 pp.647-666, (2005)

[4] V. Pischedda, G.R.Hearne, A.M. Dawe, and J.E.Lowther, Ultrastability and Enhanced Stiffness of ~6 nm TiO2 Nanoanatase and Eventual Pressure-Induced Disorder on the Nanometer Scale Phys. Rev. Lett. Vol.96, pp.3-6, (2006)

[5] A. K. Nayak, R. K. Singh, P. P. Kulkarni, Measurement of volumetric thermal expansion coefficient of various nanofluids,Technical Physics Letters. Vol.36, pp. 696- 698, (2010)

[6] M.Bhagwat and V.Ramaswamy, Synthesis of nanocrystalline zirconia by amorphous citrate route: structural and thermal (HTXRD) studies, Mater. Res. Bull. Vol.39, pp.1627- 1640, (2004)

[7] Wu X, Wu Z, Guo L, Liu J, Li X, Xu H, Pressure-induced phase transformation in controlled shape ZnO nanorods, solid state Commun. 135, pp.780-784, (2005)

[8] W.F. Zhang, Y.He, M.S. Zhang, Z.Yin and Q. Chen, Raman scattering study on anatase TiO_2 nanocrystals , J Phys D. vol.33, pp.912, (2000)

[9] R K Kumar, G Sharma, M Kumar, Size and Temperature Effect on Thermal Expansion efficient and Lattice Parameter of Nanomaterials, Modern Physics Letters B, vol.27, pp. 135018, (2013)

[10] A. Prasad, M.Singh, B.R.K. Gupta, "Study of Elastic constants and bulk modulus of alkaline earth solids under the effect of high temperature" Indian J Phys. Vol.76A, pp.291, (2002)

[11 N.Prakash, Master of Science Thesis, The Florida state of University (2005)

[12] Isao Suzuki, Thermal Expansion of Periclase and Olivine, and their Anharmonic Properties, J. Phys. Earth, vol.23, pp.145-159, (1975)

[13] K.Y.Singh, B.R.K. Gupta, A simple approach to analyse the thermal expansion in minerals under the effect of high temperature, Physica B, vol.334 pp.266-271, (2003)

[14] Jeewan Chandra, Deepika Kandpal, B.R.K. Gupta, Study of thermo-elastic properties of nanomaterials under high temperature, Physica B, vol.404, pp.1087-1091, (2009)

[15] Madan Singh, B.R.K. Gupta, Study of thermoelastic properties of nanomaterials under high temperature, IJAET, vol.6 , pp.2514-2523, (2014)