Equation of state for Coefficient of Thermal Expansion comprising temperature dependent Anderson-Gruneisen parameter for nanomaterials

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***Abstract*-There are many Equation of states(EOSs) for the coefficient of thermal expansion(CTE) but almost all EOSs consider that Anderson-Gruneisen parameter is independent of temperature so the result does not match with experimental data so nicely. Since there are strong evidences that parameter varies with temperature. So we have derived a new EOS for the CTE which comprises of temperature dependent Anderson-Gruneisen parameter(δ_T) and through which we can investigate how the CTE varies with temeperature. We have applied this EOS to some of the nanomaterials like 20nm-Ni, Fullerene, 15nm-(80Fe+20Ni), and nm-NiO. We found a nice matching of our results with experimental data. Our work may provide a new insights to theoretical as we as experimental workers of nanomaterials.**

***Keywords*- Nanomaterials, CTE. Anderson-Gruneisen parameter.**

I.INTRODUCTION-Many potential applications of nanomaterials in nanotechnology depend on its thermo-elastic properties. Nanomaterials possess a high surface to volume ratio and surface plays an essential role in size-dependent and temperature-dependent properties of material. various models have been developed to study the CTE. A simple theoretical model was developed by Raghuvesh Kumar *et al*. in 2013 to study the effect of size and temperature on the coefficient of thermal expansion and lattice parameter of nanomaterials. They studied the size dependence of thermal expansion coefficient of Pb, Ag and Zn in different shape viz. spherical, nanowire and nanofilm. A good agreement between theory and available experimental data confirmed the model predictions. They used these results to study the temperature dependence of lattice parameter [1]. M Dubiel *et al.* studied the thermal expansion behaviour of silver fcc using EXAFS data in the temperature range between 10 and 300 K. The linear expansion coefficient of a bulk silver foil agrees well with X-ray diffraction data [2]. In 2017, Krishna Chandra *et al.* developed a simple theoretical model to explore the size and shape dependence of thermal expansion and Debye temperature of nanomaterials. The theory of that model theory was based on cohesive energy and surface area change of the nanocrystals compared to the bulk crystals. It was found that the Debye temperature decreases with the decrease in particle size whereas, the thermal expansion increases as the particle size decreases. The model predictions were consistent with the available experiment data[3]. In 2016 Xiao -Ye Zhou *et al*. studied the surface-induced size- and temperature-dependent Young's modulus and size-dependent thermal expansion coefficient in nanometre-thick films [4]. Vladimir Kochergin *et al.* did a systematic study of the thermal expansion of copper oxide(CuO) nanoparticles and copper oxide based composites, prepared by a range of techniques, at cryogenic temperatures[5]. Neetu Sorot *et al.* have calculated the temperature dependent properties such as the volume thermal expansion, and thermal expansion coefficient of the graphene using the equation of state (EOS) based on thermodynamic variables. They applied a simple theoretical method determine the thermal expansion and thermal expansion properties of graphene [6]. Recently Deepika Joshi *et al*. presented a theory which explains the behaviour of nanomaterials such as AlN, CdSe, Ge, WC, and Fe-filled-MWCNT under high pressure[7]. In 2006, Chen X *et al*. worked on the various properties of nm-TiO_2 which has been proven a promising material for many emerging applications. Their study included the synthesis of TiO_2 nanoparticles, nanorods, nanowires, nanotubes, and nanoporous materials using different preparation approaches[8]. In our present work we are going to develop a simple model which investigates how the CTE varies with the temperature. We seek a model which requires the less number of input parameter.

II.METHOD OF ANALYSIS- Coefficient of thermal expansion(CTE) is defined as

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

Where V is the volume and T is the temperature. N.Prakash[9] determined α of SWCNT using molecular dynamics simulations. During these studies, N.Prakash expressed the temperature dependency of α(CTE) as follows

$$\alpha = a + bT + cT^2 \qquad (2)$$

Where a, b and c are constants. Since this equation is not consistent with the initial boundary conditions, viz. $\alpha = \alpha_0$ at $T = T_0$. Hence, in order to satisfy this condition, he expressed the equation (2) in following way

$$\alpha = \alpha_0 + b(T - T_0) + c(T - T_0) \qquad (3)$$

By the use of simple algebraic expressions and identities he reached at the final expresion for coefficient of thermal expansion which is written as follows

$$\alpha = \alpha_0[1 - \alpha_0\delta_T(T - T_0)]^{-1} \quad (4)$$

The equation derived by N.Prakash is nice equation one but doesn't consider temperature dependency of the Anderson-gruneisen parameter. Recently there are strong evidences that Anderson-Gruneisen parameter is a temperature dependent parameter hence we have to modify this expression for CTE. The temperature dependency of δ_T may be written by following empirical relation[10],

$$\delta_T = \delta_T^0(T/T_0)^k \quad (5)$$

Now substituting the expression of δ_T in equation (4) then we get;

$$\alpha = \alpha_0[1 - \alpha_0\delta_T^0(T/T_0)^k(T - T_0)]^{-1} \quad (6)$$

Where T_0 is the reference temperature and δ_T^0 is the value of Anderson-Gruneisen parameter at $T=T_0$ and k is a dimensionless thermo elastic parameter whose value is calculated by following way; taking the logarithmic of equation (5), we have,

$$\ln\delta_T = \ln\delta_T^0 + k\ln\left(\frac{T}{T_0}\right)$$

Now applying partial differential operator on both sides, we have

$$\partial(\ln\delta_T) = \partial\left(\ln\delta_T^0\right) + k\,\partial\left\{\ln\left(\frac{T}{T_0}\right)\right.$$

Since δ_T^0 is constant, therefore the first term on r.h.s. becomes zero and the remaining part provides us the expression for k as follows,

$$k = \left(\frac{\partial \ln \delta_T}{\partial \ln(T/T_0)}\right) \quad (7)$$

Hence the value of k can be calculated by the slope of the graph plotted between $\log(\delta_T)$ and $\log(T/T_0)$. Hence Eq.(6) represents a new EOS for variation of CTE for nanomaterials. This new equation of state considers the temperature dependency of the Anderson-Gruneisen parameter. Now our next task is to justify this equation of state by applying this equation to some nanomaterials and compare our results with experimental data .

III.RESULTS AND DISCUSSION- This equation needs only three input parameters such as δ_T^0, , α_0 along with T_0. The dimensionless thermo-elastic parameter (k) is calculated from the slope of the graph, i.e. $\log(\delta_T)$ versus $\log(T/T_0)$, which comes out in the form of a straight line.

TABLE.1.INPUT PARAMETERS-

Nanomaterials	δ_T^0	α_0(x10^{-6} K^{-1})	Ref. Temp. (K)
20nm-Ni	26.34	26.34	300
Fullerene	122	122	300
15nm(80Fe+20Ni)	20.81	20.81	300
nm-NiO	1.528	1.528	500

CTE is calculated by Eq. (6) as function of temperature in the range of 300-750K for 20nmNi, Fullerene and15nm-(80Ni+20Fe), respectively. While for nm- NiO we took temperature in range 500K to 950K respectively. The results obtained are reported in figs.1, 2, 3, and 4 respectively. There are no experimental data available regarding nm-NiO so we could not compare our result with experimental one.

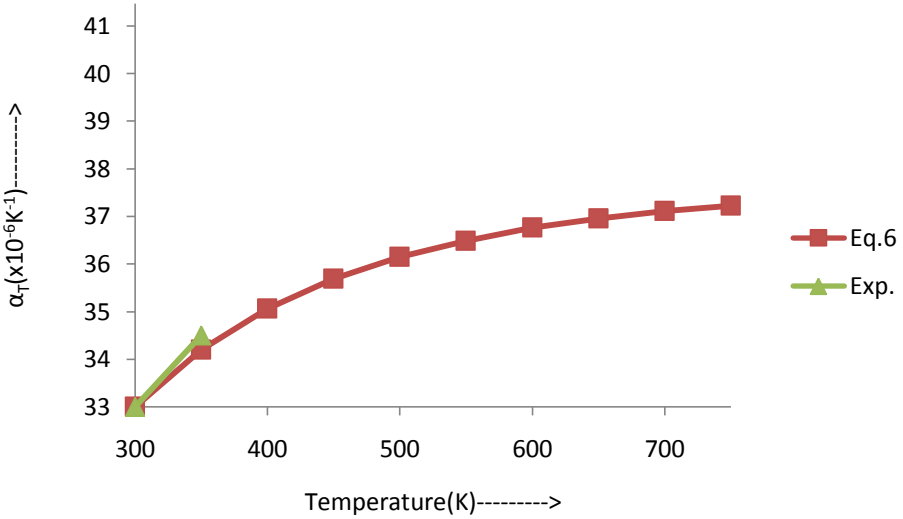

Fig.1. CTE variation of 20nm-Ni with temperature

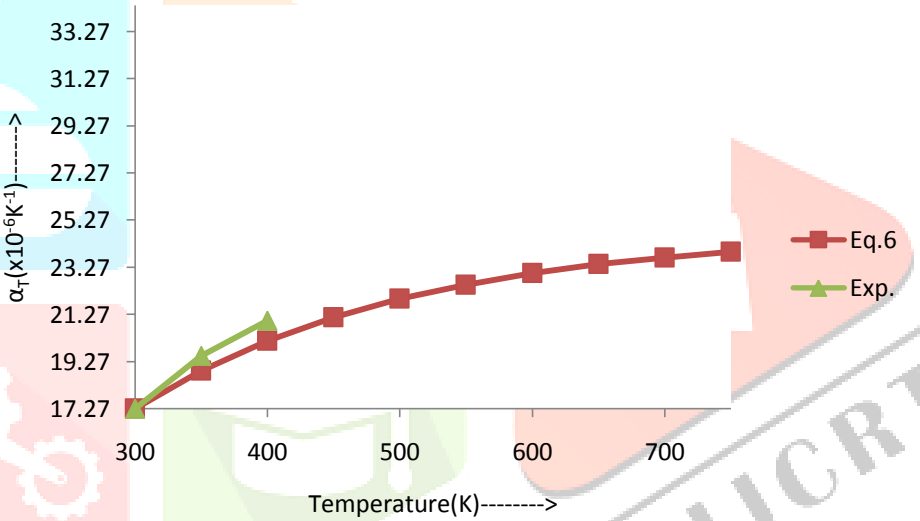

Fig.2. CTE variation of Fullerene with temperature

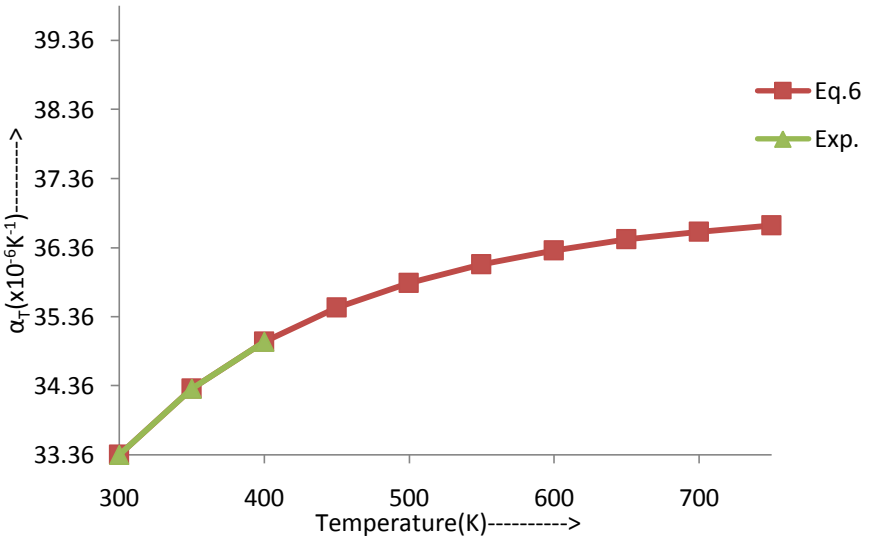

Fig.3. CTE variation of 15nm(80Fe+20Ni) with temperature

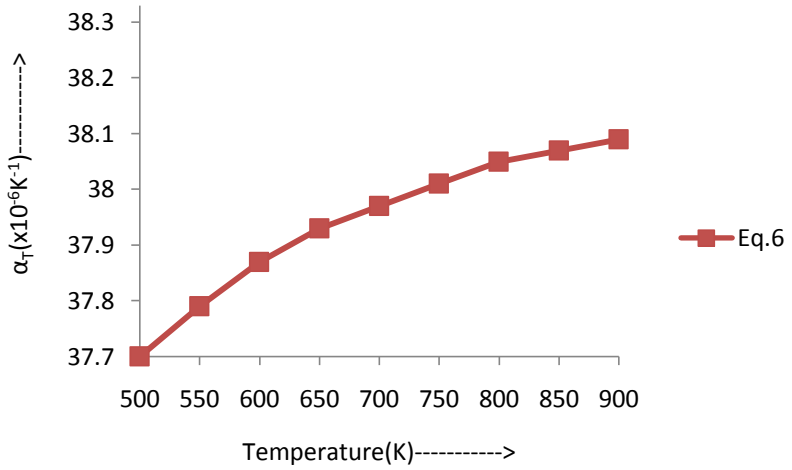

Fig.4.CTE variation of nm-NiO with temperature

CONCLUSION- A new equation of state for coefficient of thermal expansion(CTE) for nanomaterials has established. The values of CTE are calculated at different temperatures for different materials like 20nm-Ni, Fullerene, 15nm-(80Ni+20Fe) and nm-NiO, using this equation. The trend followed by this equation is same as experimental data. The Present EOS is straightforward and simpler. Present EOS needs only three input parameter. Present EOS gives the result very close to experimental one. Very fewer of the EOS are available in literature, which consider the temperature dependency of the Anderson-Gruneisen parameter. Therefore this EOS may help to provide a new insight for theoretical as well as experimental workers of nanomaterials.

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