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Behaviour of Isothermal Bulk Modulus of Nanomaterials under the Effect of Temperature

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In the present work, the behaviour of isothermal bulk modulus of nanomaterials under the effect has been studied. Using the theoretical model, the relative isothermal bulk modulus of Fullerene (C_{60}), 20 nm-Ni and 15 nm (80 Ni+20 Fe) nanomaterials with temperature have been calculated in the temperature range of 300 K (room temperature)- 700 K. It is found that the relative isothermal bulk modulus of these nanomaterials decreases with increase in temperature.

1. Introduction

Over the past decade, the nanomaterials have been the subject of enormous interest. These materials, remarkable for their extremely small size, have the potential for wide ranging industrial, biomedical, electronic and engineering applications. Therefore, it is not just a matter of great interest but also a necessity to study various thermo-elastic properties like isothermal bulk modulus of nanomaterials. Nanomaterials are usually very sensitive to external parameters such as temperature etc. Investigation of the behaviour of nanomaterials under high temperature can provide valuable information about their intrinsic micro-structural characteristics. The physical properties of these materials depend on structures and inter-atomic separations. Due to the possibilities of substantially different behaviour compared to the bulk, the study of Nano crystalline materials under high temperature are of current interest.

Some experimental scientists have estimated bulk modulus of ZnO nano at room temperature [1, 2]. The bulk modulus for ZnO nanomaterial has been calculated in the temperature range from 300 K to 1200 K from the data on the propagation velocities of ultrasonic waves [3]. The analysis of the experimental data reveals that with rising temperature, the magnitude of bulk modulus decreases almost linearly. Recently, using powder X-ray diffraction, the bulk modulus of ZnO nanomaterials has been determined [4] and found to decrease with increase in temperature.

There are few theoretical work on temperature dependence of bulk modulus of nanomaterials. Relative bulk modulus of various nanomaterials with temperature has been studied theoretically [5] and a decrease in bulk modulus with increase in temperature has been reported. Using pseudo potential and plane wave basis based on the density functional theory, the effect of temperatures on isothermal bulk modulus for both two structures of ZnO has been investigated [6]. It is found that the wurtzite structure phase of ZnO is with the smaller isothermal bulk modulus comparing with the rock salt structure phase of ZnO under the same conditions and for both forms of ZnO, the isothermal bulk modulus decreases almost linearly with temperature. Simple model has been developed to study the effect of temperature on bulk modulus of C_{60} solid [7]. Recently, variation of bulk modulus of 20 nm-Ni and carbon fullerene at different temperatures has been studied [8] and found that bulk modulus decreases with increase in temperature. Temperature dependence of isothermal bulk modulus of ZnO nanomaterials has been studied [9]. For this purpose, a linear relationship to show the variation of isothermal bulk modulus with respect to temperature has been modified to preset a non-linear model of isothermal bulk modulus with the change in temperature. Although, a few work on temperature dependence of bulk modulus of nanomaterials has been done while sufficient studies on the behaviour of isothermal bulk modulus of these materials are required. Therefore, in the present work, we have planned to study and analyze the behaviour of isothermal bulk modulus of nanomaterials under the effect of temperature.

2. Analysis Methods

A linear relationship between bulk modulus (K) and temperature (T) has been reported by many workers [9, 10] in the following way:

$$K = K_0[1 - \alpha_0 \delta_T^0 (T - T_0)] \qquad (1)$$

Where, K, K_0 , α_0 and δ_T^0 are isothermal bulk modulus at temperature T, bulk modulus at T = T_0 (room temperature or reference temperature), volume thermal expansivity at room temperature and Anderson-Gruneisen parameter at T = T_0.

The Eq. (1) can be written as:

$$\frac{K}{K_0} = [1 - \alpha_0 \delta_T^0 (T - T_0)] \qquad (2)$$

Eq. (2) shows the variation of relative isothermal bulk modulus($\frac{K}{K_0}$) with temperature (T). Using Eq. (2), the value of relative isothermal bulk modulus can be calculated and the behaviour of isothermal bulk modulus of nanomaterials under the effect of temperature can be studied and analyzed.

3. Results and Discussion

Using relation Eq. (2), the value of relative isothermal bulk modulus($\frac{K}{K_0}$) of Fullerene (C_{60}) 20 nm-Ni and 15 nm (80Ni + 20 Fe) nanomaterials with various temperatures have been calculated in the temperature range of 300 K (room temperature) to 700 K. The input parameters used in the present work have been shown in Table 1.

Fig. 1 represents the variation of relative isothermal bulk modulus($\frac{K}{K_0}$) with temperature (T) for Fullerene (C_{60}), 20 nm-Ni and 15 nm (80 Ni + 20 Fe) nanomaterials. It is obvious that the relative isothermal bulk modulus($\frac{K}{K_0}$) of these nanomaterials decreases with increase in

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temperature (T). The relative isothermal bulk modulus decreases sharply in case of C_{60}. The variation of bulk modulus with temperature could not be compared to the experimental values.

Table 1 Input parameters used in the present work [11]

Nanomaterial	α_0 (K^{-1})	δ_T^0
Fullerene (C_{60})	17.27	122
20 nm-Ni	33.0	26.34
15 nm (80 Ni + 20 Fe)	33.36	20.81

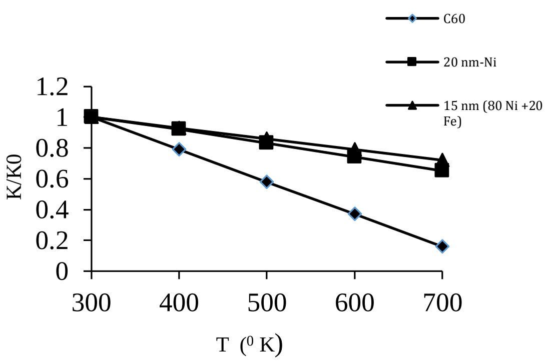

Fig. 1 Variation of relative isothermal bulk modulus (K/K_0) with temperature (T)

Since, the experimental data on isothermal bulk modulus with variation of temperature are not available. However, the calculated values may counter feed the experimental investigation in future.

4. Conclusion

In the present work, the behaviour of isothermal bulk modulus of C_{60}, 20 nm-Ni and 15 nm (80 Ni + 20 Fe) nanomaterials with temperature has been studied in the temperature range of 300 K (room temperature) to 700 K. The study shows a decrement in relative isothermal bulk modulus with increase in temperature.

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