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Shape- and dimension-dependent study of volume thermal expansion of nanomaterials

ABSTRACT. Nanomaterials are the foundation of nanotechnology and they exist in different dimensions, shapes and sizes in nature. A simple theoretical method has been developed to study the thermal behaviour of nanomaterials by modifying the He and Yan (2001) model. This behaviour give vital information about their intrinsic structural characteristics. As external parameters like temperature, pressure, shape, size and dimensionality of nanomaterials change, their behaviour changes. He and Yan proposed an equation of state (assuming the Anderson–Grüneisen parameter (δ_T) to be independent of temperature) for the study of temperature effects on interatomic separation and bulk modulus of the bulk materials. In the present study, the He–Yan model has been modified by introducing the volume thermal expansion coefficient for nanomaterials (α_{0n}) in place of its bulk equivalent (α_0). The modified equation of state has been applied to four nanomaterials: silver (20 nm), aluminium (40 nm), nickel oxide (25 nm), and titanium dioxide (35 nm). The calculated results are compared with available experimental data and their bulk counterparts. It was found that the size-dependent properties of nanomaterials changes with the relative number of atoms present at the surface. Hence the energy linked with the atoms also changes. Consistency with experimental data supports the validity of the proposed model. Further, the effect of different shapes, viz. spherical nanomaterials (0D), nanowires (1D) and nanofilms (2D) on volume thermal expansion has also been studied: it varies with dimension due to the variation in surface-to-volume ratio.

Keywords: Anderson–Grüneisen parameter, equation of state, nanoparticles, nanotechnology, thermal properties

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