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Size and shape impact on thermal expansion coefficient of nanowires

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The properties of bulk crystals depend upon their structure but in case of nanocrystal, in addition to the structure, size and shape are the significant factor, which affect their properties. The shape factor has been introduced in the bond energy model. The basic idea is that the atomic cohesive energy decides the thermodynamical properties of the crystals. Also, cohesive energy changes with the atomic coordination background. The bond energy model justifies that how the surface dangling bonds depress the melting temperature of the nanomaterials and how the order disorder transition of the nanoparticles varies upon the particle size. The cohesive energy associated with these surface atoms will be unlike from their bulk materials. The excess energy associated with these surface atoms is defined as the surface free energy. On examining the surface effect, a simple model is debated to study the size and shape dependence of thermal expansion coefficient of Se and Si nanowires with different cross sectional shapes. It is projected that the thermal expansion increases with decrease in particle size. Also, it is recognized that the particle shape can impact the thermal expansion of nanoparticles and this effect on the thermal expansion becomes more with decreasing of particle size. Our theoretical predictions approve fairly well with the existing experimental and simulation results for nanowires in different shapes. Due to the modesty and applicability, this model can be stretched to the other nanomaterials and may be the recent attention of the researches engaged in the study of physical properties of nanomaterials.

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Primary author: Prof. SINGH, Madan (National University of Lesotho)

Co-author: Dr DEVLAL, Kamal (Department of Physics, Utrakhand Open University, India)

Presenter: Prof. SINGH, Madan (National University of Lesotho)

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