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A bond energy model to study the melting point and Debye temperature of nanomaterials

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The physical properties of materials change when the size of the material approaches from bulk to nanoscale. The size effect is taken by increasing the fraction of the surface atoms with lower coordination numbers, therefore increasing number of dangling bonds, which results in causing the thermodynamical properties as cohesive energy at nanoscale. The cohesive energy of nanoparticles decreases due to the dangling chemical bonds. On considering the surface effect, using bond energy model, a size dependent theory is discussed to study the melting point and Debye temperature of nanoscale materials. The number of atoms on the surface to the total number of atoms in nanosolid is analysed in terms of shape factor and the size of nanomaterials. The variation of melting point and Debye temperature is reported for spherical, regular tetrahedral, regular hexahedral and regular octahedral nanomaterials. It is found that the melting temperature and Debye temperature decrease as the particle size is reduced. The result reported is compared with the available experimental and simulation data. A good agreement between the present calculated results and the results reported by earlier researcher confirms the validity of the existing theory. Due to the simplicity and applicability, this model can be extended to the other nanomaterials and may be the recent consideration of the scholars engaged in the study of thermodynamical properties of nanosolids.

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