World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:14, No:04, 2020

Models to Calculate Lattice Spacing, Melting Point and Lattice Thermal Expansion of Ga_2Se_3 Nanoparticles

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Abstract : The formula which contains the maximum increase of mean bond length, melting entropy and critical particle radius is used to calculate lattice volume in nanoscale size crystals of Ga_2Se_3. This compound belongs to the binary group of III_2VI_3. The critical radius is calculated from the values of the first surface atomic layer height which is equal to 0.336nm. The size-dependent mean bond length is calculated by using an equation-free from fitting parameters. The size-dependent lattice parameter then is accordingly used to calculate the size-dependent lattice volume. The lattice size in the nanoscale region increases to about 77.6 A^3, which is up to four times of its bulk state value 19.97 A^3. From the values of the nanosize scale dependence of lattice volume, the nanoscale size dependence of melting temperatures is calculated. The melting temperature decreases with the nanoparticles size reduction, it becomes zero when the radius reaches to its critical value. Bulk melting temperature for Ga_2Se_3, for example, has values of 1293 K. From the size-dependent melting temperature and mean bond length, the size-dependent lattice thermal expansion is calculated. Lattice thermal expansion decreases with the decrease of nanoparticles size and reaches to its minimum value as the radius drops down to about 5nm.

Keywords : Ga_2Se_3, lattice volume, lattice thermal expansion, melting point, nanoparticles
Conference Title : ICCMPN 2020 : International Conference on Condensed Matter Physics and Nanotechnology
Conference Location : New York, United States
Conference Dates : April 23-24, 2020