Structure and Thermal Properties of Binary Group III-V Nanoparticles

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A formula to calculate lattice volume in nanoscale size crystals free of fitting parameters is derived depending on the maximum increase of mean bond length d_{mean}, melting entropy S_m and critical particles radius. The particle critical radius (r_c) is calculated from the values of the first surface atomic layer height symboled by (h).The surface first layer height of atoms h is calculated according to the fitting relation, h=1.429 d(mean, for bulk state) . For InP values of (h) and melting entropy (Sm) are 0.3775nm 30.28(Jg-atom^{-1}K^{-1}) respectively. Size dependent mean bond length can be calculated using the relation [d_{mean}(r)=h-(increase of d(r)]. Knowing d_{mean}(r), the size dependent lattice parameter *a*(r) can be calculated according to the relation $d_{mean}(r)=[a(r)/4].3^{1/2}$ and then the lattice volume V(r), ris the nanoparticles radius. The bulk state for this relation as (r go to infinity) give values of d_{mean}(infinity) for seven of binary III-V compounds including AlSb, GaAs, GaP, GaSb, InAs, InP and InSb as interested in this work. The increase of lattice size reaches to about three times of its bulk state when r reaches r_c as V(r_c) for example for InP it reaches to 83 A^3 from its bulk value of 25 A^3. From the values of V(r) calculated according to the information above, the nanoscale size dependence of melting temperature T_m(r)for all compounds are calculated according to the modified model (Omar 2012), depending on the increase of lattice volume V(r), melting entropy, nanoparticles critical radius and the materials bulk melting temperature. The melting temperature decreases with the decrease of nanoparticles size and reaches zero when its radius reaches its critical value (r_c). Bulk melting temperature and lattice volume, for InP for example, have values of 1333 K and 25 respectively. From the size dependent melting temperature T(r) and mean bond length d_{mean}(r) , the size dependent lattice thermal expansion LTE(r) are calculated according to the modified relation reported by (Omar 2012). For all compounds investigated in this work, LTE decreases with the decrease of nanoparticles radius and reaches down to zero for r approaches about 3nm for InP as an example. For other compounds their minimum values higher than zero still they are occurred at the same radius

References

[1]. M. S. Omar**,** Materials Research Bulletin 47, 3518(2012**)**