THERMODYNAMIC PROPERTIES OF THE GRAY AND WHITE TIN

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Tin is commonly found in one of two allotropic forms: the stable phase at low temperature is alfa or gray tin which is a zero-gap semiconductor having the diamond structure; when the temperature is raised above T~13 °C, the crystal transforms into the beta-phase or white tin which is a body-centered tetragonal metal [1]. There is a lack of data for the enthalpy of alfaâ†'beta phase transformation. And there is a wide spread in the available results which do not very well converges between themselves [2], [3]. In this work we calculate mechanical and thermodynamic properties: equilibrium lattice parameters, bulk modulus, entropy and enthalpy of transformation, Gibbs free energy.

^{1.} Pavone P., Baroni S., Gironcoli S. // Phys.Rev.B. 1998. V. 57. No. 17.

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