Calculation of lattice vibrational and thermal properties of CdS nanocrystal and growth preference of CdS power during microwave-hydrothermal process

Jia Fu[1] and Xing Liu[1]

[1]Xi'an Shiyou University

June 8, 2021

Abstract

The lattice vibration and thermal properties of CdS by first-principles calculations based on density functional theory are especially investigated. The results of phonon spectra show that CdS is thermodynamically stable. Combined with the concept of irreducible representation, the contribution of atoms in CdS to Raman and infrared is analyzed, that is: A1 and E1 participate in Raman vibration, and A1, E1 and E2 participate in infrared vibration. The electronic band structure and optical properties such as dielectric constant, refractive index, reflectivity are determined theoretically using DFT method. The thermal properties of CdS show that Debye temperature, isochoric specific heat capacity and coefficient of thermal expansion increase with the increase of temperature, and then tend to equilibrium. The equilibrium values are 353.13 K, 23.86 cal/cell.K and 1.04×10-4 K-1, respectively. For comparison. piezoelectric semiconductor material CdS power is synthesized by microwave hydrothermal process (temperature at 140°C + time about 15min), with particle size ranges from 50nm to 1000nm. The HRTEM imagine of CdS are experimentally studied to understand the crystal structure, with the growth preference along the plane (1000) and nanocrystal distance of 6.76 Å. This study is of great significance and provides theoretical guidance for further designing CdS matrix composite materials and to improve photoanode performance through doping of CdS and quantum dots co-sensitization.

Hosted file

`CdS-Jia.doc` available at https://authorea.com/users/418676/articles/525344-calculation-of-lattice-vibrational-and-thermal-properties-of-cds-nanocrystal-and-growth-preference-of-cds-power-during-microwave-hydrothermal-process