Investigated optical and elastic properties of Porous silicon: Theoretical study

Abstract

Compatibility between experimental and theoretical works is achieved. Empirical Pseudopotential Method (EPM) is used to calculate the energy gap of Si which is found to be indirect. Features such as refractive index, optical dielectric constant, bulk modulus, elastic constants and short-range force constants have been investigated. In addition to the shear modulus, Young's modulus, Poisson's ratio and Lame's constants for both bulk Si (p = 0%) and Porous silicon (PS) are derived. The calculated results are found to be in good agreement with other experimental and theoretical ones. Also, the Debye temperature of PS is estimated from the average sound velocity. To our knowledge, the optical properties using specific models and elasticity of PS are reported for the first time.