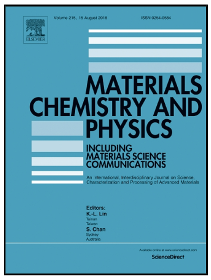
Accepted Manuscript



Effect of Size and Dimension dependent Specific Heat on Thermal Conductivity of Nanostructured Semiconductors

Neha Arora, Deepika P. Joshi, Uma Pachauri

PII: S0254-0584(18)30476-0

DOI: 10.1016/j.matchemphys.2018.05.071

Reference: MAC 20686

To appear in: *Materials Chemistry and Physics*

Received Date: 22 May 2017

Accepted Date: 28 May 2018

Effect of Size and Dimension dependent Specific Heat on Thermal Conductivity of Nanostructured Semiconductors

Neha Arora*, Deepika P. Joshi and Uma Pachauri
Department of Physics, G.B.P.U.A. &T., Pantnagar, Uttarakhand -263145, INDIA
*E-mail address: *arora.neha1287@gmail.com*

Abstract

A thermodynamic model is proposed to study the collective effect of size and dimension dependent specific heat capacity along with phonon surface scattering on thermal conductivity as well as on diffusivity of nanostructured semiconductors. Thermal conductivity and diffusivity of pure and compound semiconducting nanomaterials for partially smooth and rough surfaces at different sizes and dimensions have been calculated. Thermal conductivity and diffusivity decreases with size and increases while moving towards the specular surfaces. Incorporation of size and dimension effect of specific heat capacity with phonon interface scattering gives the better explanation of thermal conductivity, whereas classical approach alone is inadequate. To validate the obtained results, we have compared our results with the experimental data and other model reported in literature.

Keywords: Thermal conductivity; Diffusivity; Semiconductors; Size effect

Introduction

There has been a great deal of interest to study the electrical, optical, mechanical properties as well as thermal transport in semiconducting nanomaterials due to the size quantization effect. Due to the confinement of electrons and holes with the diminishing size of the material, consequent change in the electronic structure will take place. Size-dependent luminescence, the blue shift in the optical absorption spectrum, enhanced band gap all are the examples of the profound modifications of the physical properties of the Nanostructured semiconductors. They are used in sensors, transistors, field emitters and in exceptionally small electronic circuits with enhanced properties and new functions in different areas of technology. These materials behave as the building blocks or like the tools for nanoelectronics [1-3]. Melting temperature, thermal conductivity and other physical parameters of semiconductor play important role in manufacturing and processing of electronic devices. Thermal conductivity is highly sensitive for size, thickness and interface of the material. Moreover, temperature, surface roughness, shape and dimension of the nanomaterials are observed to affect the thermal transport. Therefore, it is necessary to comprehend the effect of size, dimension and surface scattering of phonons on thermal and electrical properties of semiconducting nanomaterials. Semiconducting nanomaterials exhibit novel optical and electronic properties due to their unique electronic structure and wide band gap. In recent years materials with desired thermal properties are drawing more attention. The efficiency of any material is defined by the dimensionless parameter, known as Figure of merit. Low thermal conductive materials are desired for improving the efficiency of any material or enhancing the figure of merit of materials (FOM) which is given by [4]

$$FOM(ZT) = S^2 T / \rho K$$

S, ρ, T and K represents Seebeck coefficient (or thermoelectric power), electronic resistivity, temperature and total thermal conductivity respectively. Hence, the performance of a thermoelectric material depends on three quantities: electrical conductivity, Seebeck coefficient and thermal conductivity. For highest electrical conversion any material should have high Seebeck coefficient and low thermal conductivity [5]. Inverse effect of electrical conductivity and Seebeck coefficient is a hurdle for achieving high quality performance of materials. It's a challenge