



Theoretical model for size, dimension and shape effect on electrical behavior of semiconductor nanomaterials

Uma Pachauri¹ · Deepika P. Joshi¹ · Neha Arora¹

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Abstract

The present study is an effort to develop a simple analytical model without any adjustable parameter for observing the collective effect of size, dimension and shape on electrical susceptibility and dielectric constant of nanomaterials. The size dependence of electrical susceptibility and dielectric constant has been observed for some pure as well as binary semiconductor nanomaterials, in three different dimensions (i.e., nanoparticles, nanowires and nanofilms). It has been observed that the electrical susceptibility and dielectric constant both show reduction with the decrement in size, due to the increased surface-to-volume ratio and lower coordination number. The present study reveals that the difference between the values of electrical susceptibility of nanoparticles and nanowires (5–50%) is less in comparison with nanofilms (10–90%). This difference diminishes on moving toward the higher size range. The decrement in the value of dielectric constant with size is found, maximum for nanoparticles (10–80%) followed by nanowires (10–70%) and minimum in nanofilms (5–60%). The outcomes for the size-dependent dielectric constant have been compared with the available experimental and other theoretical data and found consistency in calculated results with experimental data. The model has been extended to investigate the cross-sectional shape effect along with size on the electrical susceptibility and dielectric constant of nanowires due to large applications by incorporating shape factor. Four different cross-sectional shapes: spherical, square, rectangular and hexagonal nanowires, have been taken for the present study. The calculated results of dielectric constant have been compared with the available experimental data, and close agreement was found. It has been observed that the electrical susceptibility and dielectric constant have the highest value for spherical cross-sectional-shaped nanowires and the lowest for rectangular cross-sectional-shaped nanowires. Deviation graphs show that the values of electrical susceptibility and dielectric constant for rectangular, square and hexagonal cross-sectional-shaped nanowires deviate from spherical nanowires as 2–14%, 2–4% and 1–2%, respectively. The present study confirms the importance of shape effect along with size and dimension for electrical properties of semiconductor nanomaterials.

Keywords Electrical susceptibility · Dielectric constant · Nanowires · Shape factor

1 Introduction

Nanoscience is concerned with creating new or enhanced materials, which have special characteristics that differ from those of bulk solids and have an influence on the nanoscale devices in electronics. Nanomaterials are considered as agglomerate of nanocrystals with interfaces or grain boundaries and classified into three categories on the basis of dimensions: 0 dimension (nanoparticles), 1 dimension

(nanowires) and 2 dimension (nanofilms). The unique properties of these materials result from the high surface-to-volume ratio and quantum effect. At nano-level, more atoms are located on the surface and quantum confinement effects dominate the electrical and optical properties of systems. Semiconductor nanomaterials exhibit size-dependent electrical and optical properties due to the quantum confinement effects [1]. The quantum confinement modifies the band gap in semiconductor nanomaterials [2–4]; therefore, properties can be tuned by changing the nanomaterial's size, which are of great importance for potential applications, such as light emitting diodes [5], solar cells [6], optoelectronic devices [7] and biological labels [8, 9].

✉ Uma Pachauri
umapachauri21@gmail.com

¹ Department of Physics, G. B. Pant University of Agriculture and Technology, Pantnagar, Uttarakhand 263145, India

Dielectric properties are becoming increasingly important for the materials, which are designed for nano-devices. Dielectric constants specify the response to the dipole displacement in an externally applied field in terms of ion and electron motion and closely relate to the conductivity and optical properties of materials. The modification of dielectric constant affects the Coulomb interaction among electrons, which leads to the variation in the activation (electron–hole pair) energies and thus would significantly change the optical absorption and transport properties of semiconductor devices [10]. The modified dielectric properties have been used as capacitors, electronic memories and optical filters. In the literature, many studies have shown the size dependence of dielectric constant experimentally and theoretically [11–14]. Among these models, some involve the adjustable parameters being lack of physical meanings [15] and some models are complicated for being utilized [16].

One-dimensional nanocrystals are envisioned as fundamental building blocks of future electronic, sensing, electro-mechanical and nanogenerator system. Researchers have exhibit unique and novel nanostructures with extraordinary functionalities in the last two decades. The study of size and shape effects on material properties has attracted enormous attention due to their scientific and industrial importance. Over the past many years, there have been many studies on the size-dependent properties of cylindrical nanowires and non-cylindrical nanowires with distinct types of cross-sectional shapes, like rectangular, square, triangular, tetrahedral, etc. [17–19]. It was observed that the properties strongly depend on their size and shape. Lu and Meng [14] also considered the size and shape effect on dielectric constant of GaN nanowires using Lu’s model. In the present work, a simple analytical model for the study of size, dimension and shape effect on dielectric constant for nanomaterials has been proposed and the beauty of the model is that it is free from any adjustable parameter.

2 Methods

The dielectric constant (ϵ) of a semiconductor is directly related to electrical susceptibility (χ) as:

$$\chi = \epsilon - 1 \tag{1}$$

Electrical susceptibility is a dimensionless quantity that indicates the degree of polarization of a dielectric material and hence related to the band gap of material. Sun et al. [20] presented the approximation relation of electrical susceptibility (χ) with the band gap (E_g) as:

$$\chi(\infty) \propto [E_g(\infty)]^{-2} \tag{2}$$

$\chi(\infty)$ and $E_g(\infty)$ are electrical susceptibility and band gap for bulk materials, respectively. Equation (2) can be written for nanomaterials as:

$$\frac{\chi(D)}{\chi(\infty)} = \left[\frac{E_g(D)}{E_g(\infty)} \right]^{-2} \tag{3}$$

where $\chi(D)$ and $E_g(D)$ are electrical susceptibility and band gap for nanomaterials, respectively, with diametric size ‘D’. Dielectric constant consequent from the electronic polarization or electron migration from the lower valence band to the upper conduction band therefore dielectric constant can also be related to the band gap of material:

$$\frac{\epsilon(D) - 1}{\epsilon(\infty) - 1} = \left[\frac{E_g(D)}{E_g(\infty)} \right]^{-2} \tag{4}$$

$\epsilon(D)$ and $\epsilon(\infty)$ represent the dielectric constant for nano- and bulk materials, respectively. Now to proceed further, it is required to give the size dependence of band gap for nanomaterials.

According to the nearly free-electron approach, $E_g = 2|V_1|$. Here, V_1 is the crystalline field depending on the interatomic interaction of solids (V) and total number of atoms [21]. Generalizing this relationship for nanomaterials:

$$\frac{\Delta E_g(D)}{E_g(\infty)} = \left| \frac{\Delta V(D)}{V(\infty)} \right| \tag{5}$$

Here, Δ represent the change in properties. $V(D)$ and $V(\infty)$ are interatomic interaction for nano- and bulk solids, respectively.

Lang et al. [21] showed $V \propto E_c$, where E_c is the atomic cohesive energy [21], therefore

$$\frac{\Delta E_g(D)}{E_g(\infty)} = \frac{\Delta V(D)}{V(\infty)} = \left| \frac{E_c(D) - E_c(\infty)}{E_c(\infty)} \right| = 1 - \frac{E_c(D)}{E_c(\infty)}. \tag{6}$$

The cohesive energy and melting temperature (T_m) are linearly related and have been given as [22]:

$$\frac{E_c(D)}{E_c(\infty)} = \frac{T_m(D)}{T_m(\infty)} \tag{7}$$

$E_c(D)$, $E_c(\infty)$ and $T_m(D)$, $T_m(\infty)$ are cohesive energies and melting temperatures for nano- and bulk materials, respectively.

Numerous theoretical models have been reported in the literature to enlighten the change in electronic structures of nanocrystallites as a function of its size [23, 24]. Efros and Efros [25] were the first to report the size-dependent behavior

of electronic properties based on the effective mass of holes and electron in nanocrystals. Arora and Joshi [26] gave a quantitative model for the size as well as shape effect on the band gap for semiconductor nanomaterials. They compared different classical as well as quantum models and found that the Jiang's model is well suited for the size and shape-dependent band gap study for nanomaterials. Therefore, in the present work, Jiang's model has been used for the size-dependent study of electrical susceptibility and dielectric constant for semiconductor nanomaterials.

According to Jiang et al. [27], size-dependent melting temperature can be given as:

$$\frac{T_m(D, d)}{T_m(\infty)} = \exp\left[-\frac{2S_{\text{vib}}}{3R} \frac{1}{D/D_0 - 1}\right] \quad (8)$$

where S_{vib} and R are the bulk vibrational melting entropy and the gas constant, respectively. For semiconductors, $S_{\text{vib}} = S_m - R$, $'S'_m$ is the solid-to-liquid transition entropy. $D_0 = 2(3-f) \times h$, is the critical diameter at which all the atoms of the crystal are located at the surface. $'f'$ and $'h'$ represent the degree of freedom and atomic diameter, respectively. $f=0, 1$ and 2 for nanoparticles, nanowires and nanofilms, respectively.

Now, the expression for size-dependent electrical susceptibility and dielectric constant for nanomaterials in different dimensions can be written as:

For nanoparticles,

$$\frac{\chi(D)}{\chi(\infty)} = \left[2 - \left\{\exp\left(-\frac{2S_{\text{vib}}}{3R} \frac{1}{D/6h - 1}\right)\right\}\right]^{-2} \quad (9)$$

$$\varepsilon(D) = 1 + (\varepsilon(\infty) - 1) \times \left[2 - \left\{\exp\left(-\frac{2S_{\text{vib}}}{3R} \frac{1}{D/6h - 1}\right)\right\}\right]^{-2} \quad (10)$$

Equations (9) and (10) can be used to see the size effect on electrical susceptibility and dielectric constant of nanoparticles, respectively.

For nanowires

$$\frac{\chi(D)}{\chi(\infty)} = \left[2 - \left\{\exp\left(-\frac{2S_{\text{vib}}}{3R} \frac{1}{D/4h - 1}\right)\right\}\right]^{-2} \quad (11)$$

$$\varepsilon(D) = 1 + (\varepsilon(\infty) - 1) \times \left[2 - \left\{\exp\left(-\frac{2S_{\text{vib}}}{3R} \frac{1}{D/4h - 1}\right)\right\}\right]^{-2} \quad (12)$$

Equations (11) and (12) can be used to see the size effect on electrical susceptibility and dielectric constant of nanowires, respectively.

For nanofilms

$$\frac{\chi(D)}{\chi(\infty)} = \left[2 - \left\{\exp\left(-\frac{2S_{\text{vib}}}{3R} \frac{1}{D/2h - 1}\right)\right\}\right]^{-2} \quad (13)$$

$$\varepsilon(D) = 1 + (\varepsilon(\infty) - 1) \times \left[2 - \left\{\exp\left(-\frac{2S_{\text{vib}}}{3R} \frac{1}{D/2h - 1}\right)\right\}\right]^{-2} \quad (14)$$

Equations (13) and (14) can be used to see the size effect on electrical susceptibility and dielectric constant of nanofilms, respectively.

The expression for size and shape-dependent electrical susceptibility and dielectric constant can be given by incorporating the shape factor (δ) [17] in Eqs. (11) and (12) for nanowires as:

$$\frac{\chi(D)}{\chi(\infty)} = \left[2 - \left\{\exp\left(-\frac{2\delta S_{\text{vib}}}{3R} \frac{1}{D/4h - 1}\right)\right\}\right]^{-2} \quad (15)$$

$$\varepsilon(D) = 1 + (\varepsilon(\infty) - 1) \times \left[2 - \left\{\exp\left(-\frac{2\delta S_{\text{vib}}}{3R} \frac{1}{D/4h - 1}\right)\right\}\right]^{-2} \quad (16)$$

3 Results and discussion

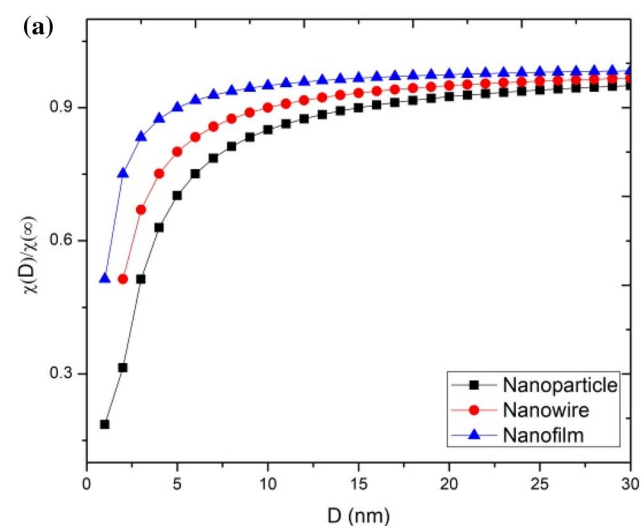
Semiconductor nanomaterials have gained a lot of attention recently due to drastic change in their physical (structural, optical, magnetic, thermal, dielectric, etc.) and chemical properties resulting from surface effects and quantum size effects [28, 29]. Semiconducting nanomaterials have been used in optoelectronic devices, memory devices, single electron devices, magnetic sensors, etc., because of their unique properties. Dielectric constant is one of the most important parameters for physical and optoelectrical properties of semiconducting nanomaterials and has been studied intensively both theoretically and experimentally [11, 12, 30–32]. The understanding of dielectric properties is needed for designing the devices of desired performance therefore; first principal calculations and other theoretical models have reported the size effects on dielectric constant [10, 33, 34]. These studies have shown good consistence with experimental results but due to complexity in calculation

and reliability on adjustable parameters put limits to the direct use of these models. In present work, an effort has been made to develop a simple model which is free from any adjustable parameter, for investigating the effect of size, shape and dimension on electrical properties like electrical susceptibility and dielectric constant of semiconducting nanomaterials. The dielectric constant determines the optical response of semiconductors, hence related to its band gap so in the present formulation electrical susceptibility has been used as a mediator which, directly relates to the band gap. First, the calculations have been done for the size dependence of electrical susceptibility and then the size dependence of dielectric constant for semiconductor nanomaterials has been observed.

The calculations of the size dependence of electrical susceptibility and dielectric constant have been done for some pure as well as binary semiconductor nanomaterials like CdS, InAs and Si for three different dimensions, i.e., 0 dimension as nanoparticles (using Eqs. 9 and 10), 1 dimension as nanowires (using Eqs. 11 and 12) and 2 dimension as nanofilms (using Eqs. 13 and 14), respectively. The related parameters used for the calculations are listed in Table 1.

Table 1 Input parameters used for the present study

S. No.	Materials	h (nm)	S_m (J/g atom K)	$\epsilon(\infty)$
1	CdS	0.252 [36]	6.18 [36]	8.7 [36]
2	GaN	0.162 [14]	108.082 [14]	8.63 [14]
3	InAs	0.262 [36]	10.56 [36]	15.2 [36]
4	InP	0.254 [36]	15.63 [36]	12.5 [36]
5	Si	0.234 [36]	6.72 [36]	11.7 [36]



The calculated results for the size and dimension dependence of electrical susceptibility of above said materials are graphically represented in Figs. 1a, 2a, 3a. The deviation in values of susceptibility for nanowires and nanofilms from nanoparticle has been shown in deviation curves from Figs. 1b, 2b, 3b, respectively. The calculated results for size- and dimension-dependent dielectric constant are plotted in Figs. 4a, 5a, 6a, respectively, along with the data available from experiments and other theories [11–13, 35]. The deviation in dielectric constant from the bulk value is also shown graphically in Figs. 4b, 5b, 6b for semiconductor nanomaterials.

It has been observed from the graphs that the electrical susceptibility decreases with the decrement in size. Deviation graphs of electrical susceptibility showed that the difference between the values of electrical susceptibility of nanoparticles from nanowires (5–50%) is less in comparison with nanofilms (10–90%). This difference diminishes on moving toward the higher size range. Similar declining trend with the reduction in size has been observed for dielectric constant, and the computed results for the size-dependent dielectric constant have been compared with the available experimental and other theoretical data and found good agreement between both the data. Deviation graphs showed that the decrement in the value of dielectric constant with respect to bulk materials is the highest for nanoparticles (10–80%) then followed by nanowires (10–70%) and the lowest for nanofilms (5–60%).

The reduction in the values of electrical susceptibility and dielectric constant is due to the size effects. The increased, surface-to-volume ratio and lower coordination number result the decrement in cohesive energy which encourages

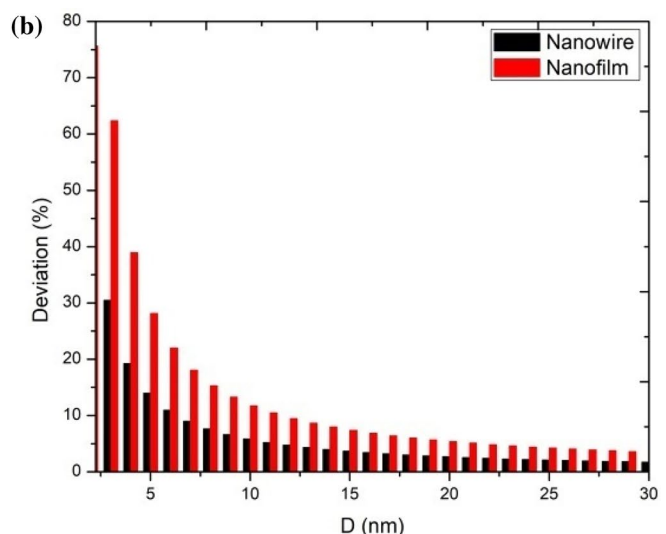


Fig. 1 **a** Variation in relative electrical susceptibility with size for different dimensions of CdS semiconductor nanomaterials. **b** % deviation in electrical susceptibility of CdS nanowire and nanofilm from nanoparticle with size

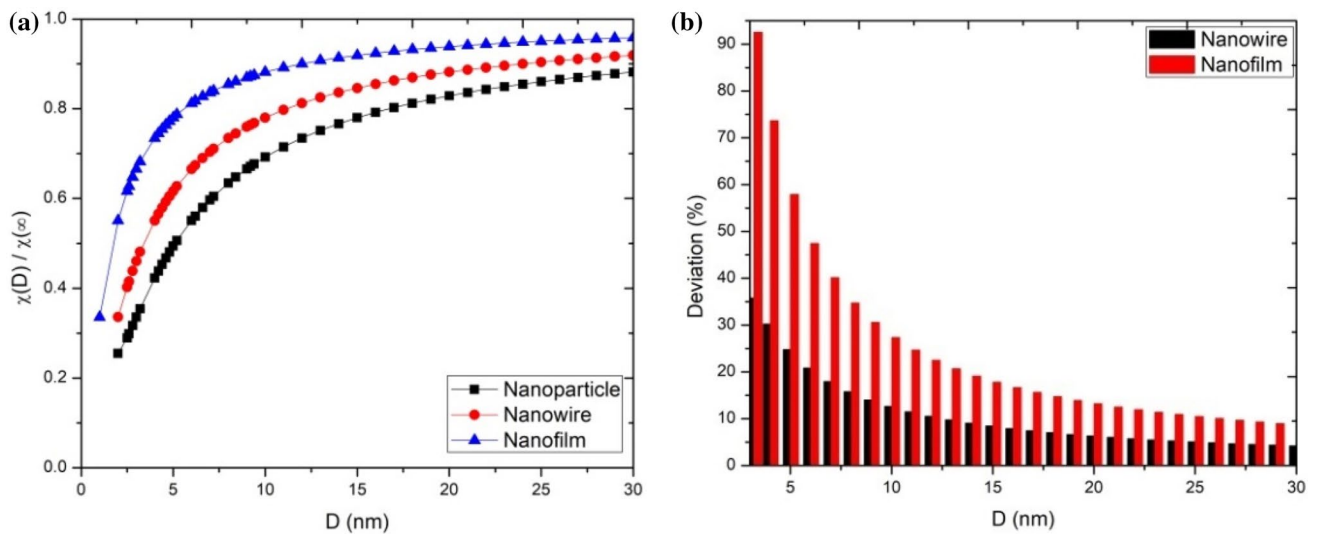


Fig. 2 **a** Variation in relative electrical susceptibility with size for different dimensions of InAs semiconductor nanomaterials. **b** % deviation in electrical susceptibility of InAs nanowire and nanofilm from nanoparticle with size

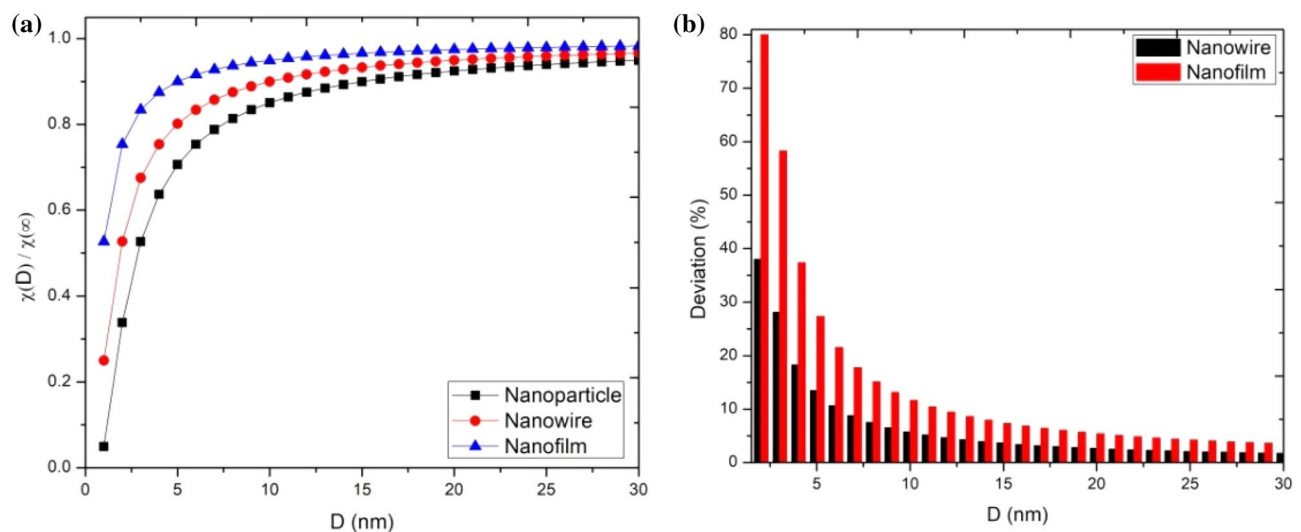


Fig. 3 **a** Variation in relative electrical susceptibility with size for different dimensions of Si semiconductor nanomaterials. **b** % deviation in electrical susceptibility of Si nanowire and nanofilm from nanoparticle with size

local quantum entrapment, leading to perturbed Hamiltonian that limits the band gap [13]. Band gap expansion modifies the process of electron polarization and consequently suppresses electrical susceptibility and hence decrement in dielectric constant. The reduction in the value of dielectric constant can improve the Coulomb interactions among charge carriers (electrons and holes) and ionized shallow impurities in nano-devices, which modify the optical and transport properties [10].

To investigate the cross-sectional shape effect along with size and dimension effect on the electrical susceptibility and

dielectric constant of semiconductor nanowires, Eqs. (15) and (16) have been used. Four different cross-sectional shapes such as spherical, square, rectangular and hexagonal nanowires have been considered for the study. The values of shape factor used for the computation are given in Table 2. The variation in electrical susceptibility and dielectric constant for different cross-sectional shape with size has been plotted along with available experimental data for CdS, GaN and InP semiconductor nanowires in Figs. 7a, 8a, 9a, 10a, 11a, 12a, respectively.

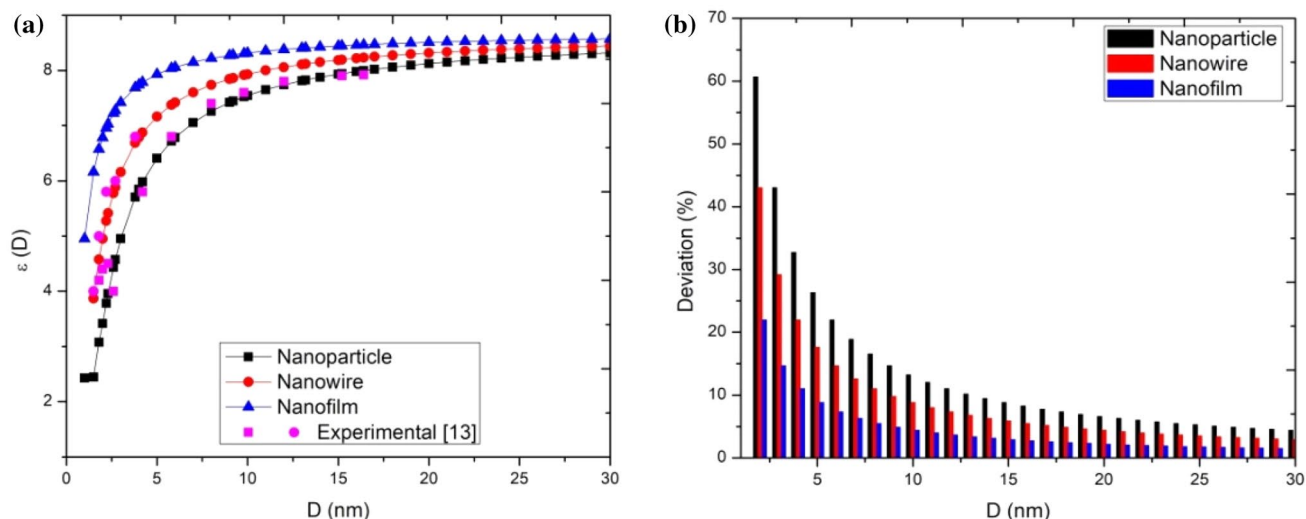


Fig. 4 **a** Variation of dielectric constant with size for different dimensions of CdS semiconductor nanomaterials. **b** % deviation in the values of dielectric constant from bulk for CdS with size

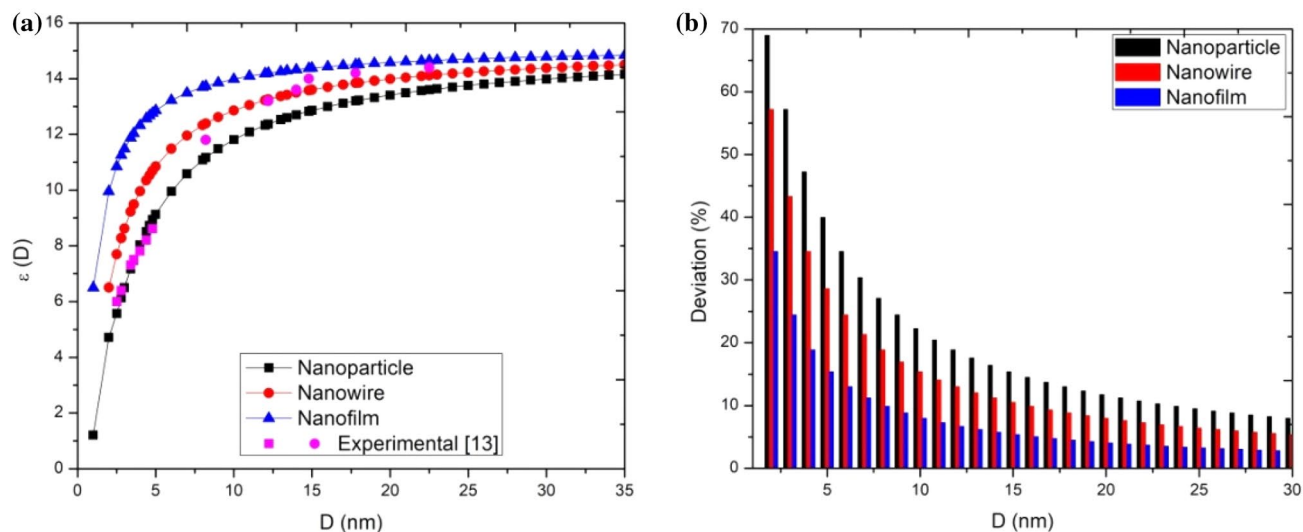


Fig. 5 **a** Variation of dielectric constant with size for different dimensions of InAs semiconductor nanomaterials. **b** % deviation in the values of dielectric constant from bulk for InAs with size

Figures 7b, 8b, 9b, 10b, 11b, 12b graphically represent the deviation of electrical susceptibility and dielectric constant on moving from spherical-shaped cross-sectional nanowires to non-spherical-shaped cross-sectional nanowires.

From graphs, it has been observed that as the size of the nanowires decreases electrical susceptibility and dielectric constant both decrease due to the surface effects. The calculated results of dielectric constant have been compared with the available experimental and theoretical data [13, 35], and close agreement has been found. It has been observed that electrical susceptibility and dielectric constant are the highest for spherical cross-sectional-shaped

nanowires and the lowest for rectangular cross-sectional-shaped nanowires. The deviation in the values of electrical susceptibility and dielectric constant for rectangular, square and hexagonal cross-sectional-shaped nanowires from spherical nanowires has been found approximately 2–14%, 2–4% and 1–2%, respectively. Previously, Jiang et al. have also shown for GaN semiconductor nanowire that dielectric constant is higher for low shape factor value [35]. The importance of shape effect with size and dimension has been confirmed in the present study. This study can be helpful to study the combined effect of shape and

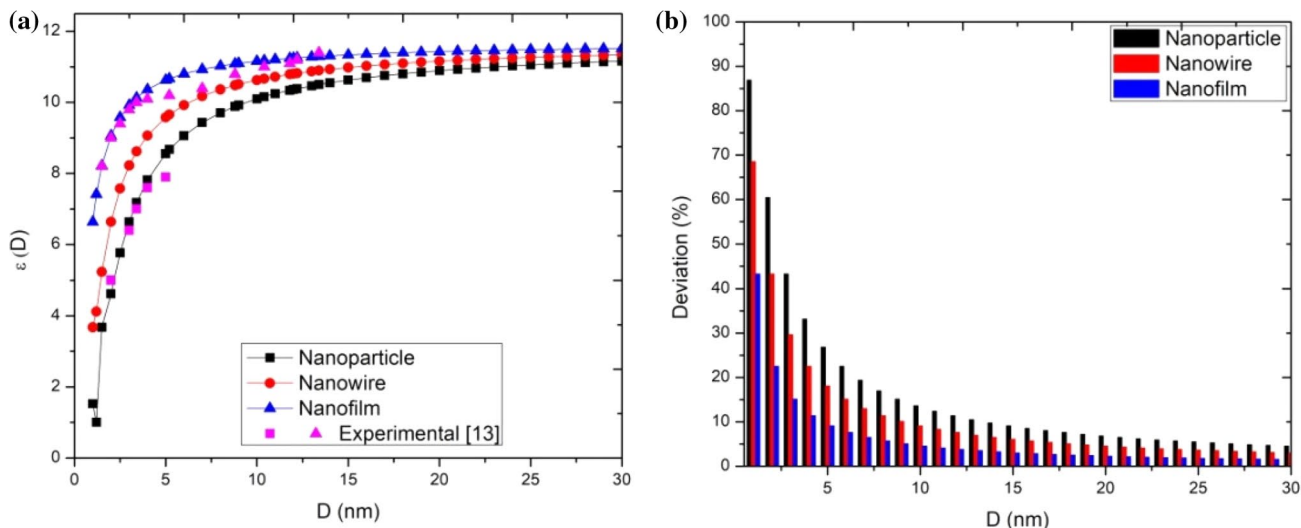


Fig. 6 a Variation of dielectric constant with size for different dimensions of Si semiconductor nanomaterials. b % deviation in the values of dielectric constant from bulk for Si with size

Table 2 Shape factor for different cross-sectional shapes of nanowire

Shape	Value of shape factor (δ) [17]
Rectangular	$\frac{n+1}{\sqrt[n]{\pi n}}$, ($t = nb$); t, b are thickness and width of rectangular nanowires and n is real integer
Square	1.128
Hexagonal	1.050
Spherical	1

grain boundaries on electrical behavior of semiconductor nanomaterials.

4 Conclusion

The present work includes the electrical study of semiconductor nanomaterials. The size and dimension effect on electrical susceptibility and dielectric constant have

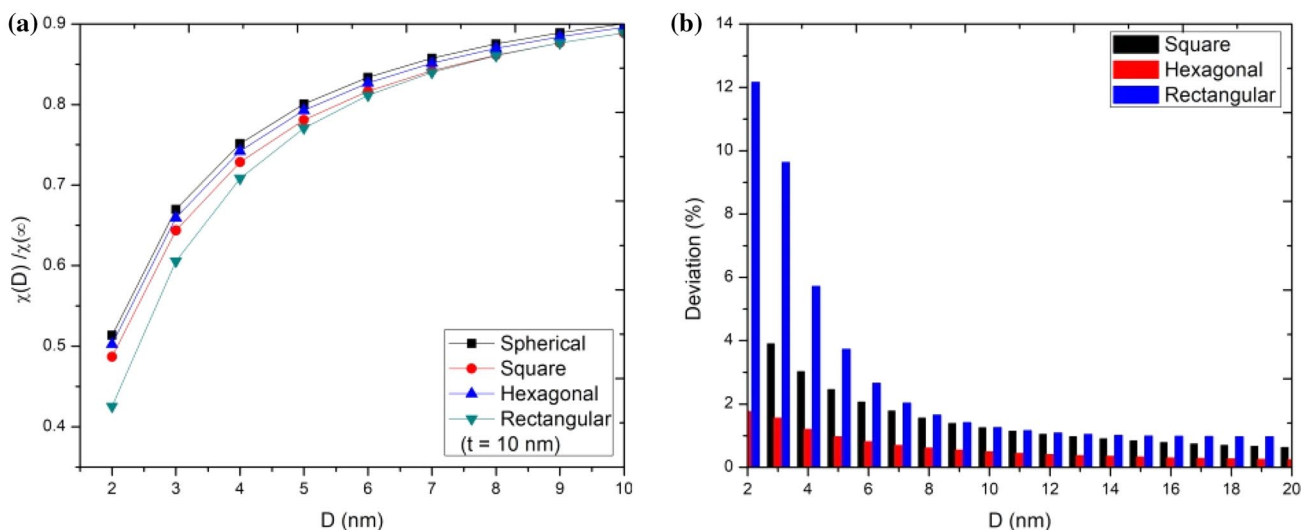


Fig. 7 a Variation of electrical susceptibility with size for different cross-sectional shapes of CdS semiconductor nanowires. b % deviation in electrical susceptibility of different cross-sectional shapes from spherical CdS semiconductor nanowires

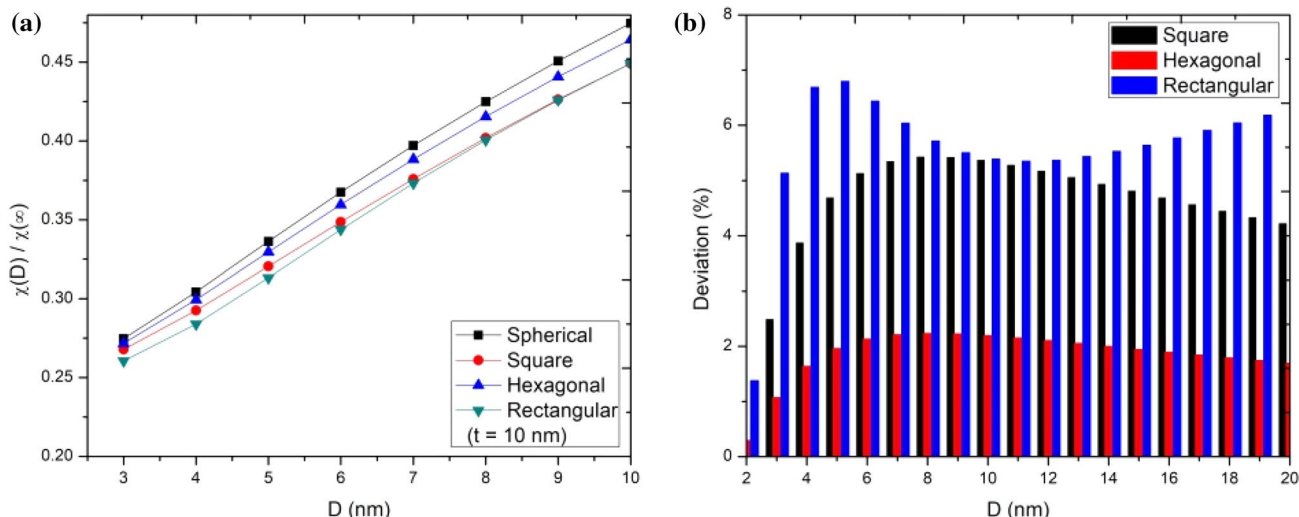


Fig. 8 **a** Variation of electrical susceptibility with size for different cross-sectional shapes of GaN semiconductor nanowires. **b** % deviation in electrical susceptibility of different cross-sectional shapes from spherical GaN semiconductor nanowires

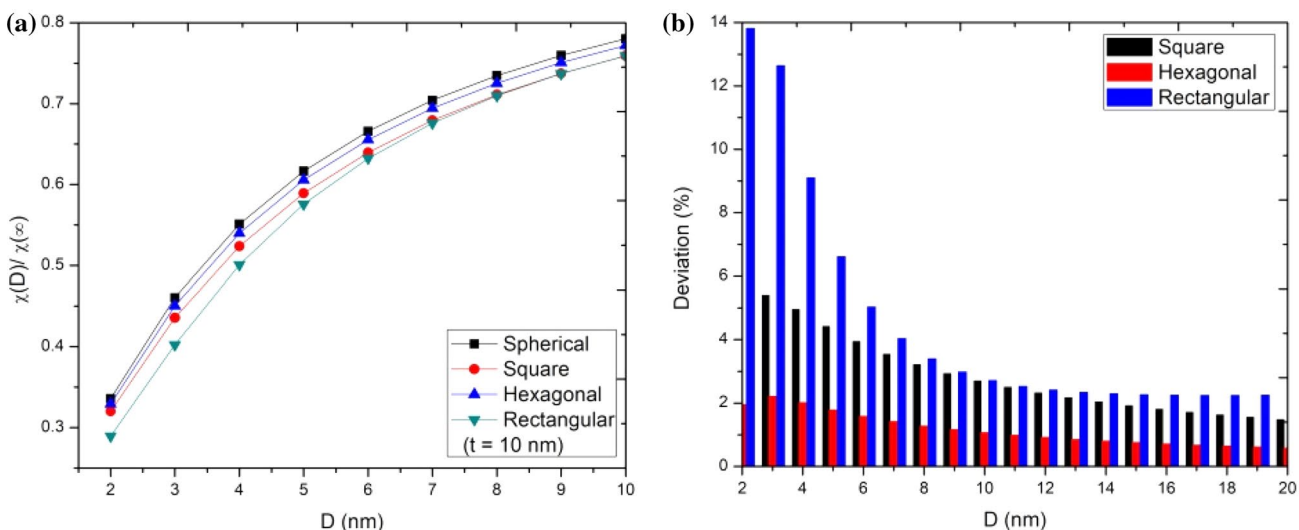


Fig. 9 **a** Variation of electrical susceptibility with size for different cross-sectional shapes of InP semiconductor nanowires. **b** % deviation in electrical susceptibility of different cross-sectional shapes from spherical InP semiconductor nanowires

been observed. It was found that electrical susceptibility and dielectric constant both decrease with decreasing size of nanomaterials. It was also observed that the electrical susceptibility and dielectric constant depend on the dimension of nanomaterials; the largest decrement was found in nanoparticles and the least for nanofilms. Shape effect has also been incorporated for semiconductor nanowires, and the results showed that non-cylindrical nanowires have less value of electrical susceptibility and dielectric

constant in comparison with cylindrical nanowires. The obtained results have been compared with the available simulated and experimental data. Consistency in results of proposed model and available experimental data supports the validity of the present work. The reduction in the value of dielectric constant can improve the Coulomb interactions among charge carriers (electrons and holes) and ionized shallow impurities in nano-devices, which helps to modify the optical and transport properties.

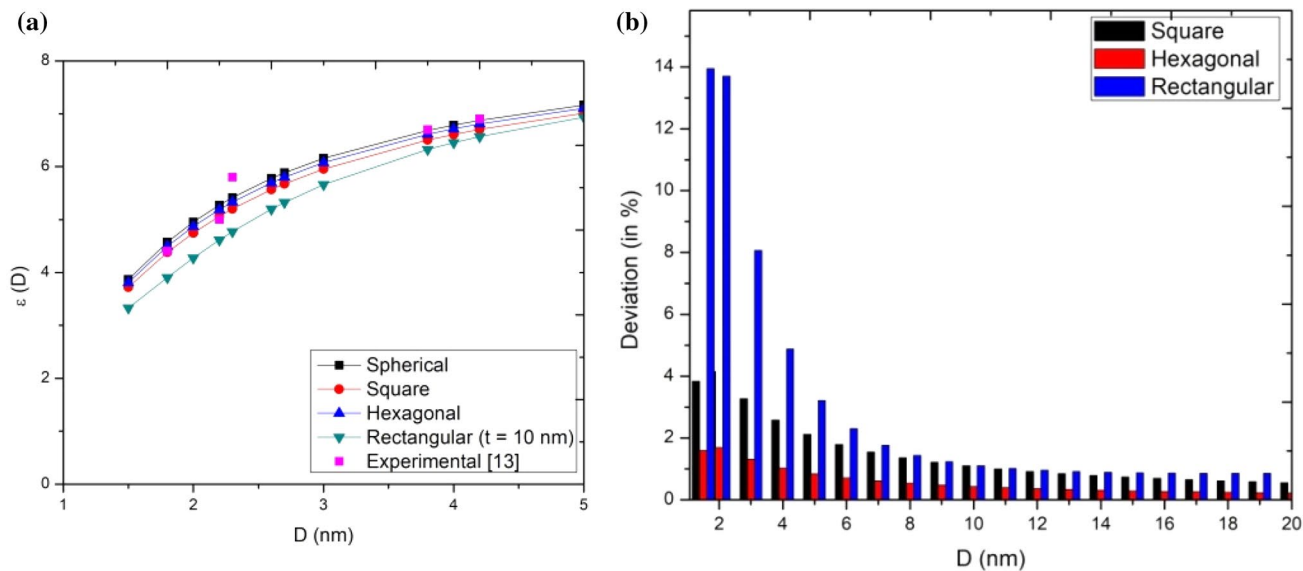


Fig. 10 **a** Variation of dielectric constant with size for different cross-sectional shapes of CdS semiconductor nanowires. **b** % deviation in dielectric constant of different cross-sectional shapes from spherical CdS semiconductor nanowires

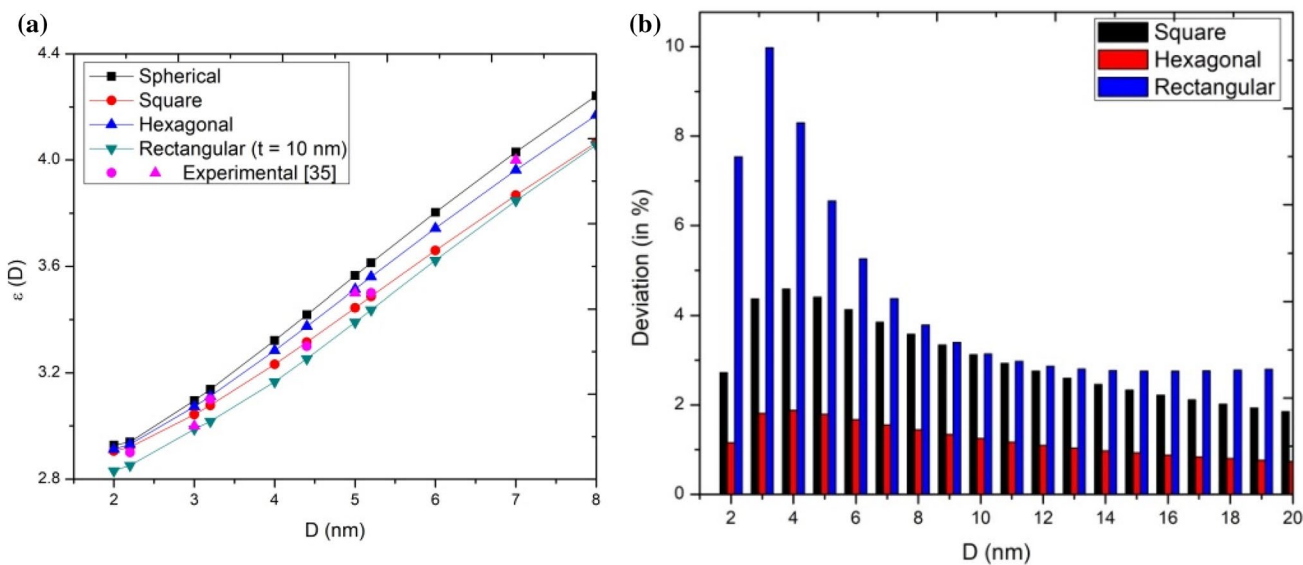


Fig. 11 **a** Variation of dielectric constant with size for different cross-sectional shapes of GaN semiconductor nanowires. **b** % deviation in dielectric constant of different cross-sectional shapes from spherical GaN semiconductor nanowires

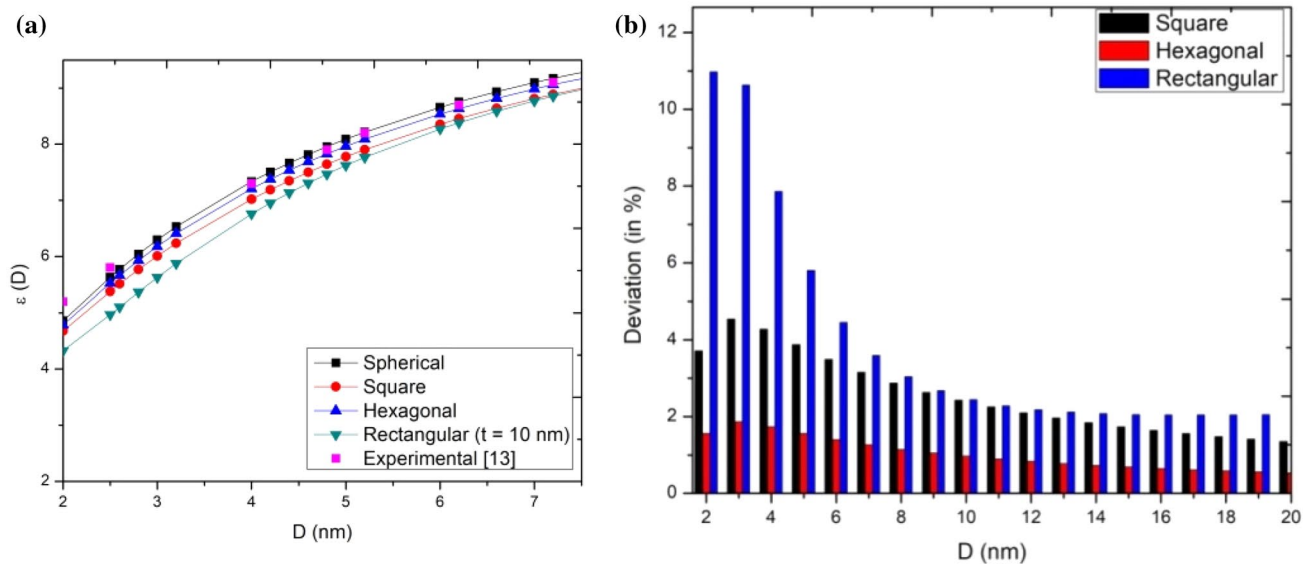


Fig. 12 **a** Variation of dielectric constant with size for different cross-sectional shapes of InP semiconductor nanowires. **b** % deviation in dielectric constant of different cross-sectional shapes from spherical InP semiconductor nanowires

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