Optics Communications 334 (2015) 85–89

Contents lists available at ScienceDirect

Optics Communications

journal homepage: www.elsevier.com/locate/optcom

Absorption threshold frequency of silicon nanowires: Effect of cross section shape

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ARTICLE INFO

Article history:
Received 11 November 2013
Received in revised form
10 August 2014
Accepted 11 August 2014
Available online 23 August 2014

Keywords:
Quantum wire
Absorption threshold frequency
Cross section

ABSTRACT

In the present work, the influence of cross sectional shape on threshold frequency of absorption in Silicon nanowires is investigated. For this purpose, we have considered Silicon nanowires with three different cross-sectional shapes like square, circular and triangular. We have used the effective mass approximation to obtain energy levels and wave functions of the structures. We have obtained absorption threshold frequency for two different cases, constant and variable effective mass. In the latter case, we have calculated the mass of electron and hole as a function of cross section. Also, we have used the tight binding approximation to obtain energy levels and thereby absorption threshold frequency. The results show that: (i) the threshold energy frequency for triangular quantum wire is higher than the square and circular cases, (ii) the electron effective mass increases by increasing the cross section area and approach to bulk value for large cross section area.

1. Introduction

Physical properties of low-dimensional semiconductor structures such as quantum dots, quantum wires, quantum wells, quantum anti-dots, quantum well-wires, and quantum anti-wells has gained considerable attention in the last decade [1–7]. These structures have been fabricated by several methods like chemical lithography, molecular beam epitaxy, and etching. The structures display rather interesting size-dependent optical properties and appear to have promising perspectives in the streaming progress of nanostructured device technology. In the past few years, many studies have been made on electronic, optical and thermodynamic properties of the structures [8–12].

The low dimensional semiconductor structures confine charge carriers in one, two, and three dimensions and their size, shape, and other properties can be controlled in experiments. It has been made possible to fabricate a wide variety of quantum wires with well-controlled shape and composition. Semiconductor structures can be fabricated with practically unlimited flexibility, and the formation of quantum wires have been demonstrated in several different materials. These low-dimensional structures, where the electron motion is confined in two dimensions, are expected to play a pivotal role in many micro- and nano-optoelectronic applications.

Among low dimensional semiconductor structures, quantum wires with various cross sectional shapes such as rectangular, square, T-shaped, V-groove, triangular, parallelogram and other cross sections have received lots of attention by researchers during the last decade [13–17]. For example, Tsukamoto et al. [18] have fabricated GaAs triangular-shaped quantum wires with the lateral width of ~10 nm by metal–organic chemical vapor selective deposition growth technique. The lateral dimension is determined by both photoluminescence (PL) measurement and a high-resolution scanning electron micrograph observation. Also, Arakawa et al. [19] discussed fabrication of triangular-shaped GaAs quantum wires with a lateral width of 15 nm using an in situ MOCVD selective growth technique on SiO_2 patterned substrates. Araki et al. [20] investigated systematic growth experiments for the successful formation of InGaAs/InAlAs quantum wires on patterned InP substrates by selective molecular beam epitaxy (MBE). Multilayer test structures consisting of InGaAs and InAlAs alternate layers were formed on 7 different types of mesa patterns including stripe- and square-shaped mesas oriented along the [110], [110] and [100] directions.

To show fabrication complexity of quantum wires, here, we briefly present (for example) fabrication method of triangular quantum wire. Kim et al. [13] used the metal–organic chemical vapor deposition (MOCVD) to fabricate triangular-shaped AlGaAs/GaAs and InGaAs/GaAs quantum wire. In chemical vapor deposition a similar substrate is placed into a reactor chamber. Gaseous sources containing the elements to be incorporated are made to flow past the substrate, which is heated enough to allow the gas to

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http://dx.doi.org/10.1016/j.optcom.2014.08.025
0030-4018/

decompose on or near the surface, but not too high so that incorporation of the source elements is thermodynamically favored. Typically, pressures of a fraction of atmospheric are required to ensure a high enough growth rate. The MOCVD growth was carried out in a horizontal, IR-heated reactor at a pressure of 76 Torr. As source materials, trimethylgallium, trimethylaluminium, trimethylindium, 100% arsine, and 500 ppm of SiH4 diluted in H2 were used. The growth temperatures was varied from 550 C to 750 C, and the V/III ratio was 100. We have carried out a rapid thermal annealing (RTA) process to enhance the optical emission and transport properties of the quantum wires. The RTA process was carried out under an Ar ambient at several temperatures from 700 C to 950 C. In addition to fabrication method, the study of the optical properties of low-dimensional semiconductor structures is important, not only to know, but also in the fabrication and subsequent working of electronic and optical devices based on such systems. In the past few years, optical properties of low-dimensional semiconductor structures have attracted much attention in theoretical and applied physics [12–16].

The study of the electronic and hole subband structure is of particular interest for optical and electronic device applications. The calculation of the band structure of quantum wires (QWRs) is complicated due to the existence of the two-dimensional confinement. In general, this cannot be done analytically except for special geometries such as isotropic cylindrical QWRs with infinite potential barrier height, spherical etc. [21,22]. As the quantum wires dimension is in the nanometer regime, effects like tunneling and quantum confinement play dominant role. There have been numerous simulation works on Silicon (Si) nanowires in recent times. The electronic properties of Si nanowires have been studied using atomic orbital basis with empirical tight-binding parameters [23–25] and also using first principle calculations [26–28]. Nanowire of different orientations and shapes has been studied by several experimental groups [29,30]. Nanowires with square and circular cross-section [24,31,32] are the most frequently used shapes for simulations. Other cross sectional shapes such as pentagonal and hexagonal nanowires has been studied in references [33,34].

In the past few years, many works have been done on optical properties of nanostructures under various circumstances. Among the optical properties of nanostructures, the interest in the light interband absorption coefficient and the absorption threshold frequency has grown significantly [35–39]. Previous studies have been focused on spherical, parabolic, and cylindrical quantum dots. For example, Atoyan et al. [38] have investigated interband light absorption in parabolic and cylindrical quantum dot in presence of magnetic field. According to our knowledge, the influence of cross sectional shape on absorption threshold frequency of quantum wires has not been studied so far. For this goal, we have intended to study this problem for a Si nanowire. We know that this work requires numerical computation.

The development of nanotechnological and microelectronics applications has provided some of the most challenging problems in computational science. Moving to nanosize devices opens new opportunities for computational scientists, and many important problems in nanoscience have already been solved with computational tools. More recently, the light scattering and the optical absorption of Si nanowires have been found to vary with the diameter of Si nanowires [40]. Such size effects affect the photoconductive gain and stress the need for additional investigations of the nanowire length and diameter dependence on their optoelectronic properties in order to better control the photosensitivity of future devices. Also, knowing the dependence of the optical properties such as absorption threshold frequency, with the size and shape of the quantum wires can be used in the design and fabrication of photodetectors.

In this paper, we have intended to study the effect of cross sectional shape on the absorption threshold frequency (ATF) of Si quantum wires. We have obtained ATF in square, circular and triangular nanowires. We have considered the variation of effective mass and energy band gap with respect to confinement.

2. Energy spectrum and wave functions

The Hamiltonian of an electron (hole) in a quantum wire in the effective mass approximation is given by

$$H=-\frac{\hbar^2}{2m^*}\nabla^2+V(x,y), \tag{1}$$

where m^* is effective mass of electron (hole) and $V(x,y)$ is confining potential as:

$$V(x,y)=\begin{cases}0, & inside\\ \infty, & outside\end{cases}. \tag{2}$$

The wave functions and energy levels for a quantum wire with square cross section can be written as:

$$\Psi_{mnn_z}(x,y,z)=C\ \sin\left(\frac{n\pi x}{a}\right)\sin\left(\frac{m\pi y}{a}\right)\sin\left(\frac{n_z\pi z}{L}\right) \tag{3}$$

$$E_{nmk_z}=\frac{\hbar^2}{2m^*a^2}(n^2+m^2)+\frac{\hbar^2n_z^2\pi^2}{2m^*L^2} \tag{4}$$

where C, a and L are normalization constant, side length of square, and wire length respectively.

The wave functions and energy levels for a quantum wire with circular cross section can be written as:

$$\Psi_{mnn_z}(\rho,\varphi,z)=CJ_n\left(\frac{\chi_{nm}\rho}{a}\right)e^{im\varphi}\ \sin\left(\frac{n_z\pi z}{L}\right) \tag{5}$$

$$E_{nmk_z}=\frac{\hbar^2{\chi_{nm}}^2}{2m^*a^2}+\frac{\hbar^2n_z^2\pi^2}{2m^*L^2} \tag{6}$$

where C, a and L are normalization constant, radius of the circle, and wire length. J_n is nth Bessel function and χ_{nm} is mth zero of nth Bessel function.

The wave functions and energy levels for a quantum wire with triangular cross section can be written as:

$$\begin{aligned}\Psi_{pqn_z}(x,y,z)=C\Bigg[&\cos\left(\frac{2\pi qx}{a}\right)\sin\left(\frac{2\pi(2p+q)y}{\sqrt{3}a}\right)\\ &-\cos\left(\frac{2\pi px}{a}\right)\sin\left(\frac{2\pi(2q+p)y}{\sqrt{3}a}\right)\\ &-\cos\left(\frac{2\pi(p+q)x}{a}\right)\sin\left(\frac{2\pi(p-q)y}{\sqrt{3}a}\right)\Bigg]\sin\left(\frac{n_z\pi z}{L}\right)\end{aligned} \tag{7}$$

$$E_{pqk_z}=\frac{3h^2}{4m^*a^2}(p^2+q^2+pq)+\frac{\hbar^2n_z^2\pi^2}{2m^*L^2} \tag{8}$$

where $q=0,1,2,3,\ldots$, $p=q+1$, $q+2$, $q+3,\ldots\ldots$, $n_z=0,1,2\ldots$. Also, C, a, and L are normalization constant and side length of the triangle, and wire length, respectively.

3. Absorption threshold frequency

Expressions (3)–(8) show the charge carriers energy spectrum and wave functions of quantum wires with different cross sectional shapes. These relations allow calculating the direct interband light absorption coefficient and the threshold frequency of absorption in such systems. The light absorption coefficient can be expressed by [13–15]

$$\alpha=N\sum_{\eta}\sum_{\eta'}\left|\int\Psi_{\eta}^{e}\Psi_{\eta}^{h}d\mathbf{r}\right|^2\delta(\Delta-E_{\eta}^{e}-E_{\eta'}^{h}) \tag{9}$$