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k.p based closed form energy band gap and transport electron effective mass model for [100] and [110] relaxed and strained Silicon nanowire

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ABSTRACT

In this paper, we address a physics based closed form model for the energy band gap (E_g) and the transport electron effective mass in relaxed and strained [100] and [110] oriented rectangular Silicon Nanowire (SiNW). Our proposed analytical model along [100] and [110] directions are based on the **k.p** formalism of the conduction band energy dispersion relation through an appropriate rotation of the Hamiltonian of the electrons in the bulk crystal along [001] direction followed by the inclusion of a 4×4 Lüttinger Hamiltonian for the description of the valance band structure. Using this, we demonstrate the variation in E_g and the transport electron effective mass as function of the cross-sectional dimensions in a relaxed [100] and [110] oriented SiNW. The behaviour of these two parameters in [100] oriented SiNW has further been studied with the inclusion of a uniaxial strain along the transport direction and a biaxial strain, which is assumed to be decomposed from a hydrostatic deformation along [001] with the former one. In addition, the energy band gap and the effective mass of a strained [110] oriented SiNW has also been formulated. Using this, we compare our analytical model with that of the extracted data using the nearest neighbour empirical tight binding $sp^3d^5s^*$ method based simulations and has been found to agree well over a wide range of device dimensions and applied strain.

1. Introduction

Emergence of Silicon Nanowires (SiNWs) as one-dimensional transistors has generated a challenging task to investig ate two of its fundamental band structure dependent electronic properties, one being the energy band gap (E_g) and the other being the electron effective mass along the carrier transport direction which drastically affects the carrier transport mechanism. However as the experimental study of these parameters at the nanoscale regime is extremely challenging, usually one relies on the atomic level simulations, the results of which are at par with the experimental observations.

In recent years, there has been an extensive study on the behaviour of E_g and the electron effective mass along different transport orientations in both relaxed and strained SiNWs by using ab initio and different empirical methods [1–5]. Albeit of these existing simulation results, there still lies a provocative challenge in developing an analytical solution of these electronic parameters due to the following reasons.

- enhanced electron mobility in relaxed and strained [100] and [110] channel Si [6],
- crossing of primed and unprimed subbands in SiNW when **k.p** formalism is used [3,4,7].
- closed form relation of E_g and electron effective mass in the presence of strain, and
- standardizing energy parameters in TCAD software for applications in nanodevices [8].

In this work we use a degenerate **k.p** theory in a relaxed bulk Si crystal to obtain the conduction band dispersion relation and quantized subband energies at the Γ and off-Γ axes in a [100] oriented SiNW together with 4×4 Lüttinger Hamiltonian dispersion relation of heavy holes (HHs) and light holes (LHs) subbands. This is followed by an appropriate rotation of the conduction band and valence band Hamiltonian to explain the corresponding dispersion relation and subband energies at both the axes of a [110] oriented SiNW. By including the quantum confinement effects, we next formulate the direct and indirect energy band gap and the transport electron effective masses considering both the channel orientations. In case of [100] SiNW, we have studied the effect of a uniaxial and a biaxial strain on the E_g and the transport electron effective mass. The uniaxial strain has been applied along the [100] direction while the biaxial strain consists of a hydrostatic deformation strain along [001] together with the same uniaxial one. The effect

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of these strains together with a shear strain on the variation of transport electron effective mass in a [1 1 0] oriented SiNW has further been investigated. In this case, the uniaxial strain is along [1 1 0] direction while the biaxial part contains the same hydrostatic one together with the [1 1 0] uniaxial. Both the tensile and compressive strain is being associated with this uniaxial and biaxial strain to investigate the variation of these two parameters. We have formulated the energy band gap and effective electron mass in a (0 0 1) wafer along [1 0 0] and [1 1 0] channel directions, which can also be extended for (0 0 1)/[1 1 1] case, as this is preferable to control the carrier mobility both in the absence and presence of strain. The analytical results of the band gap and the electron transport effective masses in both relaxed and strained rectangular SiNW along the former two channel orientations are further being compared with the data extracted from the Atomistix ToolKit (ATK) [9] which uses a nearest neighbour empirical tight binding $sp^3d^5s^*$ method. Our analytical model stands valid for the cases where the strain is within 1% and the spin–orbit coupling does not influence the conduction energy band.

2. Model and discussions

2.1. Importance of **k.p** approach over EMA

The importance of **k.p** method over EMA in the proper description of the energy band structure of Si lies in the fact that the non-degenerate EMA equation used for [0 0 1] valleys fails to describe the conduction band wrapping and the subband structure correctly in (1 1 0) oriented Si films [6,10]. In particular, to correlate a complete analytical conduction band dispersion relation with the advanced empirical tight binding model like $sp^3d^5s^*$, a two band degenerate **k.p** model should be used where a second conduction band close to the first conduction band must be taken into account, the two of which becomes degenerate just at the X point [10]. These are generally called as primed and unprimed bands respectively. This phenomenon is however not arrested in the simple non-parabolic EMA analyses [4]. Further the EMA also neglects any change in the nature of the energy band gap with the application of strain properly [7].

2.2. Relaxed [1 0 0] SiNW

Intrinsic relaxed bulk Si crystal consists of six equivalent conduction band minima located symmetrically along ⟨1 0 0⟩ at a distance of approximately $k_0 = 0.15\left(\frac{2\pi}{a_0}\right)$ from the X point along Γ direction in a three dimensional Brillioun zone, in which a_0 is the relaxed lattice constant of Si. The electron energy dispersion relation using this two band degenerate **k.p** model for relaxed bulk Si crystal along [0 0 1] transport direction can be written as [10,11]

$$E_{\pm}(k) = \frac{\hbar^2 k_x^2}{2m_{1_\pm}} + \frac{\hbar^2 k_y^2}{2m_{2_\pm}} + \frac{\hbar^2 (k_z + k_{min})^2}{2m_{3_\pm}} \pm \sqrt{\left(\frac{\hbar}{m_0} k_z p\right)^2 + \left(\frac{\hbar^2 k_x k_y}{M_\pm}\right)^2} \quad (1)$$

in which E is the electron energy as measured from the bottom of the conduction band minimum, ± represents the primed and unprimed band (± at the subscript of the effective masses represents their corresponding values at the primed and unprimed valleys), the momentum matrix element identity [10,11] is $\frac{p}{m_0} = \frac{h_0}{m_{3_\pm}}$, $\frac{1}{M_\pm} \approx \frac{1}{m_{1_\pm}} - \frac{1}{m_0}$. In case of unprimed band the effective masses are $m_{1_-} = m_t, m_{2_-} = m_t\ m_{3_-} = m_l$ and for the primed band the effective masses are $m_{1_+} = m_l, m_{2_+} = m_t, m_{3_+} = m_t$ where m_l(=0.91m_0) and m_t(=0.19m_0) are the longitudinal and transverse electron effective mass [2] in which m_0 is the free electron mass, $\hbar = \frac{h}{2\pi}$, h is the Planck's constant and k_x, k_y and k_z are the electron wave vectors along x, y and z direction respectively. Neglecting the spin–orbit interaction between the HH and LH with split-off holes, the hole dispersion relation at the Γ point can be written as [12]

$$E = Ak^2 \pm \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2\right)\right]^{1/2} \quad (2)$$

where in this case, E is the hole energy as measured from the top of the valance band maxima, ± indicates the HH and LH bands, $k^2 = k_x^2 + k_y^2 + k_z^2$ and $A = -(4.1 \pm 0.2)(\hbar^2/2m_0)$, $|B| = (1.6 \pm 0.2)(\hbar^2/2m_0)$ and $|C| = (3.3 \pm 0.5)(\hbar^2/2m_0)$ are the inverse mass band parameters [12]. It appears that due to the occurrence of the square root in Eq. (2), the HH and LH dispersion relation in general cannot be described by the effective masses [10]. Keeping this in view, we assume that the Lüttinger parameters A, B and C are independent of the cross-sectional dimensions.

The energy band structure of SiNW whose electron transport is along [1 0 0] direction is an involved task. The symmetry between the six equivalent conduction band minima is now displaced due to the difference in the effective masses as a result of the quantum confinement of the carriers along the two lateral directions as also conveyed through the earlier investigations done with the $sp^3d^5s^*$ simulation method [1,2,13]. Because of this, the six conduction band valleys are now grouped in a fourfold degenerate bands (Δ_4) at Γ-axis and twofold degenerate bands (Δ_2) at off-Γ at a distance of about $k_{x_{min}} \approx \pm 0.37\frac{\pi}{a_0}$ from the Γ-axis [13]. Due to the higher quantized electron effective mass in the Δ_4 valley along the quantized directions, the corresponding energy minimum is at a lower position than that of the Δ_2 valley, thus making the SiNW to be a direct band gap. With an increase in the SiNW cross-section, this quantized effective mass converges to its respective bulk value and the energy wave vector minimum tends to an indirect band gap [3]. Thus in [1 0 0] SiNW structure, the energy band gap depends not only on the effective masses at the band minima but also onto the subband energies along the confinement directions.

The [1 0 0] SiNW band structure diagram has been evaluated using the ATK simulator and is shown in Fig. 1. Fig. 1a exhibits the Si atomic configuration of a cleaved [1 0 0] with sp^3 passivated Hydrogen atoms. This has been done to remove the surface states in the band gap region due to dangling Si bonds on the surface of the nanowire. In this configuration we have considered the nearest Si–Si and Si–H bond lengths to be 0.235 nm and 0.152 nm respectively. The calculation of the energy band structure is done by nearest neighbour $sp^3d^5s^*$ tight binding method. In this method, each atomic lattice of the configuration is considered by a $sp^3d^5s^*$ basis and the spin–orbit interaction among them is ignored. In addition, the k-point samplings of $1 \times 1 \times 21$ grid were used with mesh cut-off energy of 10 Hartree. The energy band structure of a 1.25 nm cross-sectional dimension of a [1 0 0] oriented SiNW has been shown in Fig. 1b which clearly exhibits that the energy band gap is a direct one at the Γ axis while the off-Γ valleys exhibits an indirect energy band gap, a value higher that the former one, as already known from the existing studies [2,13]. Further, we notice that the valley splitting even at room temperature at Γ and off-Γ axis is significantly less. It should be noted that one may ignore the importance of the valley splitting for the present analyses of the determination of the band gap and transport effective electron mass. By this, we mean that it is the lowest conduction splitted valley and highest valance splitted valley which determines the gap and the transport electron effective mass for that valley. Although the valley splitting is extremely important for analysing mobility, electrical resistance, etc. which incorporates the total number of subbands and channels, however for the determination of energy