Temperature Dependent Band Gap Correction Model Using Tight-Binding Approach for UTB Device Simulations

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Abstract—In order to accurately determine the electrostatics of Ultra-Thin-Body (UTB) devices, the semi-empirical tight-binding (TB) approach is widely used for calculating the channel thickness dependent band structure of any material at those temperatures where TB parameters are available (generally defined at 0 K and 300 K). In this work, we analyze the variation of band structure for Si, Ge, and GaAs over different channel thicknesses at 0 K and 300 K, and show that the band curvature at the band minima remains unchanged with temperature, while the band gap changes significantly and affects the channel electrostatics. Based on this finding, we propose an approach to simulate the electrostatics of UTB devices, at any temperature between 0 K and 300 K, using the band structure obtained at 0 K, along with a suitable channel thickness and temperature-dependent band gap correction. From the results obtained for the channel charge density, we show good agreement with band structure based simulation results, at 300 K, over a wide range of channel thicknesses, for Si, Ge, and GaAs, while also showing good agreement with TCAD simulation results, at a typical intermediate temperature of 150 K, thus highlighting the accuracy, simplicity and wide applicability of the proposed approach.

Index Terms—Device simulation, full band simulation, sp3d5s* tight binding, Ultra-Thin-Body (UTB).

I. INTRODUCTION

N ORDER to enable the use of ultra-thin body (UTB) devices in electronic circuits, which could find applications in space, military and consumer electronics, these devices need to be simulated over a wide range of temperatures [1]. The band structure of the channel material, which is dependent on channel thickness and operating temperature, must be taken into account [2] in order to simulate the channel electrostatics of the UTB device. A widely used method for calculation of band structure is the tight-binding (TB) model. It is a semi-empirical scheme, which therefore requires a set of TB parameters that can replicate the band structure of the channel material at a particular temperature. In literature, TB parameters are generally defined at room temperature [3], [4], [5] or low temperature (0 K) [6] for elemental and compound semiconductors. Therefore, applying the TB model at any temperature other than 0 K and 300 K is not possible and this limits the applicability of the TB approach for temperature dependent electrostatics simulations of UTB devices.

Recently, Zacharias et al. [7] have presented a Density Functional Theory (DFT) based approach to perform electronic band structure calculation at finite temperatures. However, DFT is a computationally cumbersome approach and is not suitable for the purpose of device simulations. Similarly, Takai et al. [8] have employed the TB molecular dynamics simulations to investigate the effect of temperature dependence on the band gap in quantum dots, which also adds an extra computational load to the TB method. On the other hand, Sawamura et al. [9] have determined the sp3d5s* TB parameters for various compound semiconductors at 0 K, 77 K and 300 K, which again limits the applicability to only those specific temperatures. Some recent works [10] have also discussed a possible approach to get the ab initio band structure matching experiments under room temperature through the application of artificial hydrostatic strain to individual channel materials in order to mimic the effect of room temperature and also to compensate for the error from ab initio calculations. This approach involves including the effect of artificial hydrostatic strain through modification of the material’s lattice constant.

In this work, we propose an approach to enable the applicability of the TB method to the simulation of electrostatics of UTB devices at any temperature between 0 K and 300 K, without increasing any computational complexity. In order to do that, we firstly analyze the effects of temperature on the band structure, considering Si, which is a widely used semiconductor, along with Ge and GaAs, having lesser and wider band gap than Si, respectively. By observing from the band structures at 0 K and 300 K that the band curvatures around the band minima remain unchanged with variation in temperature, we are able to show that by suitably correcting the band gap, for a particular channel thickness, the band structure can be obtained for any temperature between 0 K and 300 K. Besides temperature dependence, another important aspect to be considered in UTB devices is the effect of structural confinement of the channel...
material resulting in an increase in the band gap compared to its bulk value. This quantum confinement based correction along with the temperature dependent band gap correction term is used to suitably modify the temperature dependent band gap model defined for bulk semiconductors [11], thus incorporating the effect of channel thickness and temperature on the band gap. By incorporating the temperature dependent band gap variation for a particular channel thickness into the band structure calculation, using the significant k-point selection scheme [12], a computationally efficient approach to simulate the electrostatics of UTB devices over a wide range of channel thicknesses and temperature variations, is proposed in this work.

In order to validate this approach, the integrated charge density obtained using the proposed model is compared against the integrated charge density obtained using the TB parameters given by Boykin et al. (Ge) and [3] Tan et al. (Si and GaAs) [4] at 300 K, for various channel thicknesses and is found to be in good agreement. Also good agreement of the integrated charge density obtained from the proposed model, at a typical intermediate temperature of \( T = 150 \text{ K} \), with TCAD simulation [13] results, further validates this model.

The rest of the article is organized as follows: In Section II, firstly, the full band structure approach followed by the details of the band gap correction model is discussed. Further in this section a computationally efficient algorithm for simulating the electrostatics of UTB devices over a wide range of temperatures is proposed by incorporating a temperature dependent band gap correction model into the band structure calculation. The validation of the proposed approach with the band structure simulations at room temperature and with TCAD simulation results, at \( T = 150 \text{ K} \), is shown in Section III, followed by the conclusion in Section IV.

II. APPROACH

In this section, we discuss an approach to use the Tight-Binding model for simulating the electrostatics of UTB DG-MOS devices over a wide range of temperatures. In Section II-A, a procedure is discussed to obtain the full band structure of UTB DG-MOS devices with an intrinsic (100) surface for diamond (Si, Ge) or zinc-blend (GaAs) structures, which is shown in Fig. 1. Then, the formulation based on using TB parameters at 0 K to obtain the band structure while incorporating a temperature and channel thickness dependent band gap correction is discussed subsequently in Section II-B which will enable us to simulate the electrostatics of UTB devices efficiently through selecting significant k-points from the band structure, discussed in Section II-C, over a wide range of channel thicknesses and temperatures.

A. Full Band Structure Approach

The sp\(^3\)d\(^5\)s\(^*\) tight-binding (TB) model has been used to obtain the full band structure of the thin semiconductor channel [14], [15]. In this model, the two centre overlap integrals considering four nearest neighbours per atom are taken into account. Infinite crystal periodicity and thus Bloch’s theorem is assumed to hold good along the channel length and width directions. However, given the ultra thin nature of the channel, the crystal cannot be assumed to be periodic along the thickness direction, \( z \). The TB Hamiltonian has been constructed using the well known procedure outlined in literature [14], [15], [16] which is also shown in Supplementary material S1. The TB fitting parameters for Si and GaAs given by Tan et al. [4] and Ge given by Boykin et al. [3] are used at 300 K, while those from Jancu et al. (Si, Ge and GaAs) are used at 0 K [6]. The top and bottom surfaces are assumed to be hydrogen passivated [17].

B. Band Gap Correction Model

In order to calculate the band structure for different channel materials, at 0 K, it is first important to establish the correctness of using the TB model parameters proposed by Jancu et al. [6], which have been defined at low temperatures. In Table I, we compare the band gap values obtained using Jancu’s TB model parameters at a channel thickness of 50 nm (where quantum confinement effects are no longer seen) with the experimentally obtained bulk band gap values [18], for different channel materials, at 0 K, showing excellent agreement.

Through very good agreement, shown in Table I, it may be seen that the TB model parameters proposed by Jancu et al. are indeed valid at 0 K.

Therefore, by using the TB parameters given by Jancu et al., at 0 K, and Boykin et al., Tan et al., at 300 K, the band structure is obtained for \( T_{ch} = 2 \text{ nm} \) and 10 nm, for different channel materials and is plotted in Fig. 2. In order to match the band minima at 0 K and 300 K, an offset of \( \Delta E_{min} \) is subtracted from the band structure obtained at 0 K. This offset corresponds to a change in band gap due to temperature.

From Fig. 2, it can be noted that for both \( T_{ch} = 2 \text{ nm} \) and 10 nm, the band gap corrected band structure, at \( T = 0 \text{ K} \), in case of Si, Ge and GaAs (anion terminated), shows very good

![Fig. 1. Typical schematic of Ultra-thin body (UTB) double gate (DG) MOS device with Si (100) surface having 7 atomic layers (ALs).](image-url)
agreement with the band structure at $T = 300$ K, particularly around the band minima. It may also be noted that even for GaAs (cation terminated), the band minima at $T = 0$ K, will align with the band minima at $T = 300$ K with a band gap correction of $\Delta E_{\text{min}} = 0.0841$ eV and $0.1047$ eV for $T_{ch}=2$ nm and $T_{ch}=10$ nm, respectively. Given the demonstration of the applicability of the temperature dependent band gap correction approach to enable the alignment of the band minima between $T = 0$ K and $T = 300$ K, for both GaAs (anion terminated) and GaAs (cation terminated), in this article, we consider the case of anion termination.

From Fig. 2, it is seen that the band gap of the UTB device depends on temperature ($T$) and channel thickness ($T_{ch}$), which can be formulated as,

$$E_g(T_{ch}, T) = E_g(\text{bulk}, 0) + \Delta E_g^C(T_{ch}, 0) - \Delta E_g^T(T_{ch}, T).$$

(1)

where, $E_g(\text{bulk}, 0)$ is the bulk band gap of the semiconductor at 0 K [11], while $\Delta E_g^C(T_{ch}, 0)$ is the increase in band gap due to confinement in UTB devices and $\Delta E_g^T(T_{ch}, T)$ is the temperature dependent reduction in the band gap. $\Delta E_g^C(T_{ch}, 0)$

can be defined as,

$$\Delta E_g^C(T_{ch}, 0) = E_g(T_{ch}, 0) - E_g(\text{bulk}, 0).$$

(2)

where, $E_g(T_{ch}, 0)$ can be obtained using the TB model with parameters defined at 0 K [6]. Similarly, $E_g(\text{bulk}, 0)$ is obtained as the band gap value at $T_{ch} \gg a_B$ (excitonic Bohr radius), where Quantum confinement effects can be neglected.

$\Delta E_g^T(T_{ch}, T)$ can be defined using the well-known model of temperature dependent band gap for bulk semiconductors [11], while making one of its parameter as $T_{ch}$ dependent so as to apply it to UTB devices, as shown in (3).

$$\Delta E_g^T(T_{ch}, T) = \frac{\alpha T^2}{\beta(T_{ch}) + T}. $$

(3)

where, $\alpha$ is taken as a material constant defined by Varshni et al. [11] and $\beta$ is a parameter which is material as well as channel thickness dependent. In order to apply equation (3), the value of $\beta$, which is a function of $T_{ch}$, needs to be determined for Si, Ge and GaAs. By rearranging (1)–(3), for $T = 300$ K, $\beta$ is obtained, as shown in (4)

$$\beta(T_{ch}) = \frac{9 \times 10^4 \alpha}{E_g(T_{ch}, 0) - E_g(T_{ch}, 300)} - 300. $$

(4)

From (4), it may be seen that in order to obtain the parameter $\beta$, the values of the band gap at $T = 0$ K and $300$ K need to be determined. The required values of $E_g$ at various $T_{ch}$ are obtained by determining the full band structure, while using parameters given by Jancu et al. [6] for 0 K and Boykin et al. [3], Tan et al. [4] for 300 K.

The obtained $E_g$ and thus obtained $\beta$ are plotted in Figs. 3 and 4, respectively, for Si, Ge and GaAs. By substituting the Band gap ($E_g$) and $\beta$ into the algorithm, shown in Fig. 5, the temperature and channel thickness dependent Band gap correction term, $\Delta E_g^T(T_{ch}, T)$, can be obtained.

C. Simulation of the Channel Electrostatics

Through the incorporation of a temperature dependent band gap correction term ($\Delta E_g^T(T_{ch}, T)$) into the band structure
Fig. 4. The required value of the parameter $\beta$ for getting the band gap model to fit the band gap obtained from the TB model, for various channel thicknesses, at 0 K and 300 K.

Using TB parameters from Jancu et al. [6], calculate Band Structure at $T = 0$ K for particular channel thickness and channel material (See Supplementary S1)

Determine $E_g(T_{ch}, 0)$

Using TB parameters from Boykin et al. (Ge) and Tan et al. (Si and GaAs) [3][4] respectively, calculate Band Structure at $T = 300$ K

Determine $E_g(T_{ch}, 300)$

Determine $\beta$, given $\alpha$ from Equation 4

Substitute Equation 4 into Equation 3, for determining $\Delta E_g^T(T_{ch})$ for 0 $\leq T < 300$ K

Fig. 5. Algorithm for determination of $\Delta E_g^T$ for temperature between $T = 0$ K and 300 K.

Fig. 6. Algorithm for simulating the temperature dependent electrostatics of the UTB MOS device using significant k-points.

obtained from the TB Hamiltonian assembled at $T = 0$ K, the band structure at any temperature between $T = 0$ K and 300 K can be determined. With the selection of significant k-points [12], we self-consistently solve the band structure on those k-points with the Poisson’s equation, as shown in the algorithm in Fig. 6. This approach enables the efficient and accurate simulation of the electrostatics of a UTB DG MOS device over a wide range of channel thicknesses and temperatures (0 K to 300 K) (approach elaborated in Supplement S2).

Fig. 7. Comparison of band gap versus temperature using $\Delta E_g^T(T_{ch}, T)$ model, for $T_{ch} = 50$ nm, with the experimental band gap versus temperature data (filled symbols), for bulk Si, Ge and GaAs. The model precisely follows the data points obtained using the TB model at 0 K and 300 K (open symbols).

Fig. 8. Comparison of the integrated charge density obtained using the proposed approach for Si, Ge and GaAs at $T = 300$ K with results obtained using TB parameters by Boykin et al. (Ge) [3] and Tan et al. (Si, GaAs) [4] for (a) $T_{ch} = 2$ nm and (b) $T_{ch} = 5$ nm, where $T_{ox} = 1$ nm.
In order to demonstrate the correctness of the proposed approach, the band gap model is validated over a wide range of temperatures (0 K - 300 K). By using the correction values due to confinement and temperature (please see Supplement S3), for Si, Ge and GaAs, over different channel thicknesses, the temperature dependent band gap curve can be extracted. The obtained temperature dependent band gap behaviour is validated through comparison with the experimental data available in literature for bulk semiconductors [18]. The proposed model is found to match well with the experimental data for Si, Ge and GaAs at $T_{ch} = 50 \text{ nm}$ (equivalent to bulk) as shown in Fig. 7.

In order to validate the proposed band gap model, at $T = 300 \text{ K}$, the integrated charge density is obtained, using the algorithm, shown in Fig. 6, for two typical channel thicknesses of 2 nm and 5 nm, considering two cases:

1) Using Jancu’s TB parameters (defined at $T = 0 \text{ K}$), with a temperature dependent band gap correction term as shown in (3).

2) Using TB parameters by Boykin et al., Tan et al. (defined at 300 K) without a temperature dependent correction term.

The integrated charge densities obtained using the two cases are compared in both linear and log scale, in Fig. 8, where very good agreement may be seen. It may be noted that the efficiency of the UTB device simulation is contingent on the choice of the parameter $\eta$, which is in-turn dependent on the temperature for different channel materials (please see Supplement S4).

Furthermore, we compare the integrated charge density obtained from the proposed approach with TCAD simulation results for a typical intermediate temperature of $T = 150 \text{ K}$. We show good agreement between the proposed model and TCAD simulation results, as shown in Fig. 9.

**IV. CONCLUSION**

In this work, we present an approach to determine the band structure for different channel materials and thicknesses in UTB devices, at temperatures between 0 K and 300 K, by correcting the band structure obtained for these materials at $T = 0 \text{ K}$, with the inclusion of a channel thickness and temperature dependent band gap correction term. The temperature and channel thickness dependence of the band gap is incorporated by modifying the well known temperature dependent band gap model used in bulk semiconductors. The proposed model is shown to be applicable over a wide range of channel materials (Si, Ge and GaAs), channels thicknesses and device temperatures. From this approach, the UTB device electrostatics can be simulated at any temperature between $T = 0 \text{ K}$ and 300 K, without requiring TB parameters at those temperatures.

**SUPPLEMENTARY MATERIAL**

S1: Assembling the $sp^3d^5s^*$ Hamiltonian and obtaining the Band structure. S2: Solving the Band Structure. S3: The bulk band gap $E_g(bulk, 0)$ along with the corrections in band gap due to confinement and temperature (at $T = 300 \text{ K}$) for Si, Ge and GaAs semiconductors. S4: For efficient simulation of channel electrostatics of UTB devices, $\eta$ parameter for different channel materials is shown for various temperatures.

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