

## Interface trap density metrology from sub-threshold transport in highly scaled undoped Si n-FinFETs

Abhijeet Paul,<sup>1,a)</sup> Giuseppe C. Tettamanzi,<sup>2,b)</sup> Sunhee Lee,<sup>1</sup> Saumitra R. Mehrotra,<sup>1</sup> Nadine Collaert,<sup>3</sup> Serge Biesemans,<sup>3</sup> Sven Rogge,<sup>2</sup> and Gerhard Klimeck<sup>1</sup>

<sup>1</sup>*School of Electrical and Computer Engineering, Network for Computational Nanotechnology, Purdue University, West Lafayette, Indiana 47907, USA*

<sup>2</sup>*Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands and Centre for Quantum Computation and Communication Technology,*

*University of New South Wales, Sydney, New South Wales 2052, Australia*

<sup>3</sup>*IMEC, 3001 Leuven, Belgium*

(Received 19 February 2011; accepted 14 October 2011; published online 20 December 2011)

Channel conductance measurements can be used as a tool to study thermally activated electron transport in the sub-threshold region of state-of-art FinFETs. Together with theoretical tight-binding (TB) calculations, this technique can be used to understand the dependence of the source-to-channel barrier height ( $E_b$ ) and the active channel area ( $S_{aa}$ ) on three important parameters: (i) the gate bias ( $V_{gs}$ ), (ii) the temperature, and (iii) the FinFET cross-section size. The quantitative difference between experimental and theoretical values that we observe can be attributed to the interface traps present in these FinFETs. Therefore, based on the difference between measured and calculated values of (i)  $S_{aa}$  and (ii)  $|\partial E_b/\partial V_{gs}|$  (channel to gate coupling), two new methods of interface trap density ( $D_{it}$ ) metrology are outlined. These two methods are shown to be very consistent and reliable, thereby opening new ways of analyzing *in situ* state-of-the-art multi-gate FETs down to the few nanometer width limit. Furthermore, theoretical investigation of the spatial current density reveals volume inversion in thinner FinFETs near the threshold voltage.

© 2011 American Institute of Physics. [doi:10.1063/1.3660697]

### I. INTRODUCTION

The non-planar tri-gated FinFET geometry (Fig. 1(a)) provides a viable solution to the channel length ( $L_{ch}$ ) scaling due to its better gate to channel electrostatic coupling and reduced short channel effects (SCEs).<sup>1–5</sup> In a recent experimental study of undoped Si n-FinFETs,<sup>6</sup> thermionic emission in the sub-threshold region was used to measure (1) the active channel cross-section area ( $S_{AA}$ ) (Fig. 1(b)), which shows the region of channel where the charge prevalently flows and (2) the source to channel barrier height ( $E_b$ ) (Fig. 1(c)), which reflects on the ease with which electrons travel from the source/drain to the channel. Understanding the evolution of the active area “ $S_{AA}$ ” and the barrier height “ $E_b$ ” with gate bias, temperature, and cross-section size, opens up new ways to investigate these FinFETs.

To shed light into the complicated transport phenomena that can arise in these undoped FinFETs, we expand our previous work<sup>6,7</sup> and theoretically investigate the evolution of  $S_{AA}$  and  $E_b$ . Since these devices are small and have finite number of atoms in the channel, modeling transport requires an atomistic representation of the device. A 20 band  $sp^3d^5s^*$  atomistic tight-binding (TB) model with spin-orbit coupling (SO) (Refs. 8–10) is well suited for modeling the band structure of these confined Si channels, since TB can easily take into account the material, geometrical, strain, and potential fluctuations at the atomic scale.<sup>10,11</sup> This model also takes

into account the coupling of the conduction (CB) and the valence bands (VB), which is neglected in simple models like the effective mass approximation (EMA).<sup>12</sup> Thermally activated transport is modeled using a semi-classical “top of the barrier” (ToB) model (Fig. 1(c)).<sup>10,13</sup> The simple ToB approach has been shown to model thermionic emission accurately.<sup>14</sup>

Qualitatively, we found similar theoretical and experimental trends for  $S_{AA}$  versus gate bias ( $V_{gs}$ ) and  $E_b$  versus  $V_{gs}$ .<sup>6</sup> However, the theoretically obtained  $S_{AA}$  and  $E_b$  values quantitatively over-estimated the experimental values. The reduced experimental values can be attributed to the presence of interface traps in these FinFETs.<sup>5,6,15,16</sup> The effect of interface traps on channel property are even more dominant in the extremely thin FinFETs.<sup>7</sup> This difference in  $S_{AA}$  and  $E_b$  has been utilized to directly estimate the interface trap density ( $D_{it}$ ) in these FinFETs, thereby eliminating the need to implement special FinFETs geometries to determine  $D_{it}$ .<sup>15</sup> These methods now enable the direct implementation of interface trap density metrology in state-of-the-art undoped Si n-FinFETs.

The trap extraction method outlined in this paper is new and different from the older trap extraction techniques such as capacitance-voltage (C-V), charge pumping, and inductance methods.<sup>15,17</sup> The older methods rely on special structures like the gated diodes<sup>15</sup> and large capacitors. However, the final FinFETs used in the circuits undergo different process steps like extra etching, deposition, higher thermal budgets, etc. These processes result in different interface quality in the final FETs compared to the test structures.

<sup>a)</sup>Electronic mail: abhijeet.rama@gmail.com.

<sup>b)</sup>Electronic mail: g.tettamanzi@unsw.edu.au.

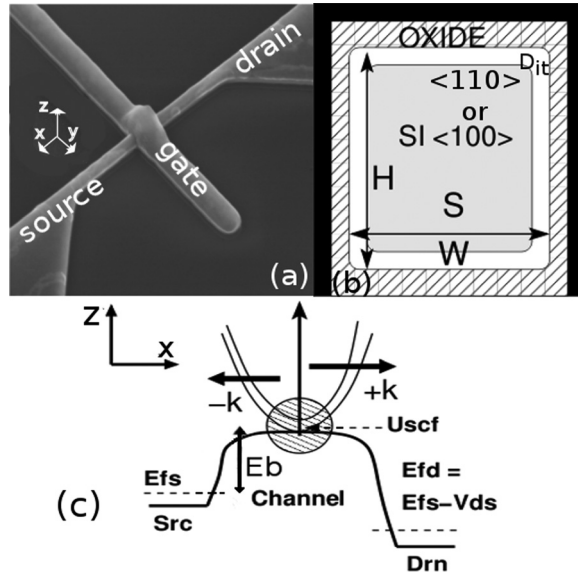


FIG. 1. (a) Scanning-electron-microscope (SEM) image of a Si n-FinFET with [100] channel orientation and single fin. (b) The schematic of the cross-sectional cut in the Y-Z plane of a typical tri-gated FinFET. The active cross-section ( $S_{aa}$ ) is in gray,  $H$  and  $W$  are the physical height and width, respectively. (c) Ballistic top of the barrier model employed for calculating the thermionic current in the FinFETs.

Thus, older methods cannot provide correct  $D_{it}$  information in the final FETs. The methods presented in this work overcome this limitation by carefully analyzing the experimental measurements and comparing the data with simulation, thus, enabling the extraction of the trap density in the final FET structures.

This paper has been divided into the following sections. Section II provides the details about the FinFETs for which interface trap density metrology has been implemented and the fundamentals of our experimental procedures. The details about the self-consistent calculations are provided in Sec. III A and the theoretical extraction of  $E_b$  and  $S_{AA}$  is outlined in Sec. III B. Section IV provides the details of the two procedures for obtaining the interface trap density. The theoretical and experimental results and the discussion on them are given in Sec. V. The conclusions are summarized in Sec. VI.

## II. DEVICE AND EXPERIMENTAL DETAILS

**Device details:** In this work, seven different FinFETs (labeled A-G) with two different channel orientations of [100] ((FinFETs A-C and G)) and [110] ((FinFETs D-F)) have been used<sup>4</sup> (see Table I). All the FinFETs have the same channel length ( $L = 40$  nm). The channel height ( $H$ ) is either 40 nm or 65 nm (Table I). The channel width ( $W$ ) varies between 3 and 25 nm. All the FinFETs consist of one or more Si channel(s) (fins) running between the same source and drain contacts. These fins are etched on an intrinsic Si film with wraparound gates covering the three faces of each of the channel fins (Fig. 1(a)).<sup>4</sup> An HfSiO (high- $\kappa$ ) layer isolates a TiN layer from the intrinsic Si channel.<sup>4</sup> In particular the FETs used in this study, have either one fin (FinFETs A-C and G) or ten fins (FinFETs D-F) between a given source

TABLE I. Si n-FinFETs used in this study along with their labels. The surface hydrogen annealing detail is also shown. The channel is intrinsic Si, while the source and the drain are n-type doped for all the FinFETs.

Label	H [nm]	W [nm]	L [nm]	Channel Orientation	$H_2$ anneal
A	65	25	40	[100]	Yes
B	65	25	40	[100]	No
C	65	~5	40	[100]	No
D	40	18	40	[110]	Yes
E	40	18	40	[110]	Yes
F	40	~3-5	40	[110]	Yes
G	65	~7	40	[100]	Yes

and drain. The measured drain current is normalized by the number of fins in the channel to obtain the current per fin, which allows a fair comparison between different types of FinFETs. These devices have two different surface treatments (with or without  $H_2$  annealing) as shown in Table I.

**Measurement procedure:** The experimental value of  $E_b$  and  $S_{AA}$  are obtained using a differential conductance ( $G = \partial I_D / \partial V_{ds}$ ) method. The conductance data are taken at  $V_{ds} = 0$  V using a lock-in technique. The full experimental method and the required ambient conditions have been outlined in detail in Ref. 6.

In the next section details of the theoretical approach to calculate the experimental values of  $E_b$  and  $S_{AA}$  in tri-gated n-FinFETs are outlined.

## III. MODELING APPROACH

### A. Self-consistent calculation

The band structure for the Si channel is calculated using TB.<sup>10,11,13</sup> The TB calculation is coupled self-consistently to a 2D Poisson solver to obtain the charge and the potential.<sup>10,13</sup> Once the convergence between the charge and the potential is achieved the thermionic current in the FinFETs is obtained using a semi-classical ballistic ToB model as shown in Fig. 1(c).<sup>10,13,18</sup> Due to the extensively large cross-section of the devices that combines up to 44 192 atoms (for  $H = 65$  nm,  $W = 25$  nm FET) in the simulation domain, a new NEMO-3 D code has been integrated in the top of the barrier analysis.<sup>19</sup> Since the FinFETs studied here show (i) negligible source-to-drain tunneling current and (ii) reduced SCEs,<sup>6</sup> the ToB model is applicable to such devices.<sup>13</sup> All the FinFETs are n-type doped in the source and drain to a value of  $5 \times 10^{19}$  cm<sup>-3</sup>. A 1.5 nm SiO<sub>2</sub> cover is assumed.

The ballistic ToB model has been chosen for simulations due to the following reasons. The FinFETs used in the study have undoped channels,<sup>6</sup> which reduce impurity scattering. Also a small channel length of 40 nm along with a small signal drain bias ( $V_{ds}^{dc} = 0$  V,  $V_{ds}^{ac} \sim 1$  mV coming from the lock in technique)<sup>6</sup> further suppresses back-scattering in the sub-threshold operation regime.

The simulation methodology in the present study has been validated against experimental data from ultra-scaled Si nanowires as outlined in Ref. 20. The benchmarking with

electro-static results<sup>20</sup> along with the feasibility of using ballistic transport (due to the reasons mentioned above) paved the way for extracting the trap density information using the experimental I-V data in these devices. Moreover, the C-V of ultra-scaled FinFETs is very noisy when measured using the common split CV technique, which calls for special C-V measurement methods as outlined in Ref. 20. Hence, due to the lack of experimental C-V data benchmarking using simulations was not performed for these FinFETs.

As it is difficult to extract the gate work function (WF) from the experimental results, a midgap gate WF value of 4.5 eV is utilized in the simulations for all the FinFETs. The simulated  $I_{ds} - V_{gs}$  curves are then shifted such that the simulated and the experimental  $V_T$  overlap. Then the  $V_{gs}$  range is chosen from the matched  $V_T$  point ( $V_2$  in Eq. (13)) down to a constant gate under-drive,  $(V_{gs} - V_T) \sim 1/3V_{dd}$  ( $V_1$  in Eq. (13)), where  $V_{dd} = 0.9$  V (according to Ref. 1). This analysis method is outlined in detail in Ref. 21. In this way the  $V_{gs}$  range is selected for the trap calculation using  $E_b$ .

Next we outline the procedure to calculate  $E_b$  and  $S_{AA}$ .

## B. Calculation of $E_b$ and $S_{aa}$

For pure thermionic emission any carrier energetic enough to surmount the barrier from the source (Src) to the channel (C) (Fig. 1(c)) will reach the drain (Drn) provided the transport in the channel is close to ballistic.<sup>18</sup> Typically Src/Drn in FETs are close to thermal and electrical equilibrium (since heavy scattering in the contacts is assumed, which leads to instantaneous carrier relaxation). This allows us to make the assumption that most of the carriers in the Src/Drn are thermalized at their respective Fermi-levels ( $E_{fs}$ ,  $E_{fd}$  in Fig. 1(c)). Also the channel potential ( $U_{scf}$ ) can be determined under the application of  $V_{gs}$  using the self-consistent scheme (discussed in Sec. III A). Hence, for the source-to-channel homo-junction inside a FET, the barrier height ( $E_b$ ) can be determined as a function of  $V_{gs}$ ,

$$E_b(V_{gs}) = U_{scf}(V_{gs}) - E_{fs}. \quad (1)$$

This definition of  $E_b$  implicitly contains the temperature dependence since the simulations are performed at different temperatures ( $T$ ), which enters through the Fermi-Dirac distribution of the Src/Drn. We show in a later section that the temperature dependence of  $E_b$  in the sub-threshold region is very weak. Therefore, all the theoretical  $E_b$  results shown in this work are at  $T = 300$  K.

The study of thermionic emission model is applicable when the barrier height is much larger than the thermal broadening ( $E_b \gg k_B T$ ,<sup>22</sup> where  $k_B$  is the Boltzmann constant). For this reason, Eq. (1) works only in the sub-threshold region where  $E_b$  is well defined.<sup>13</sup> Once the FinFET is above the threshold,  $E_b (\leq k_B T)$  is not a well defined quantity.<sup>13</sup> Using the  $E_b$  value,  $S_{AA}$  can be extracted using the conductance ( $G$ ) in the thermionic emission regime for a 3 D system<sup>6,22</sup> as

$$G_{3D} = S_{AA} A^* T \frac{e}{k_B} \exp\left(-\frac{E_b(V_{gs})}{k_B T}\right) \quad (2)$$

where  $A^*$  is the effective 3D Richardson constant ( $A_{Si,3D}^* = 2.1 \times 120 \text{ Acm}^{-2} \text{ K}^{-2}$ ),<sup>22</sup> and  $e$  is the electronic charge. This will hold only when the cross-section size of the FinFET is large enough (i.e.,  $W, H > 20$  nm) to be considered a 3D bulk system. For a very narrow width FinFET,  $S_{AA}$  cannot be extracted using Eq. (2) since the system is close to 1D. For a 1D system the  $G$ , under a small drain bias ( $V_{ds}$ ) at a temperature  $T$ , is given by the following relation (for a single energy band<sup>23</sup>):

$$G_{1D} = \frac{2e^2}{h} \cdot \left[1 + \exp\left(\frac{E_b(V_{gs})}{k_B T}\right)\right]^{-1}, \quad (3)$$

where  $h$  is the Planck's constant. Since Eq. (3) lacks any area description,  $G$  for 1D systems is no more than a good method to extract  $S_{AA}$ .

The conductance measurements are performed at low temperature ( $T \sim 40$  K-220 K) (Ref. 7) where phonon scattering is negligible. The undoped FinFET channel also results in negligible impurity scattering. Due to these experimental conditions and the devices, scattering has been neglected in the simulations. However, in a future refinement to the present work the effects of scattering could be investigated.

## IV. TRAP EXTRACTION METHODS

In Ref. 6 it was observed that the active cross-section area ( $S_{AA,sim}$ ) obtained theoretically was an over-estimation of the experimental value ( $S_{AA,expt}$ ). In the results section, it will be further shown that also the theoretical  $E_b$  value can over estimate the experimental  $E_b$  value. These mismatches can be attributed to the presence of traps at the oxide-channel interface of multi-gate FETs where these traps can enhance the electrostatic screening and suppress the action of the gate on the channel.<sup>6,7,15,16</sup> This simple idea is a powerful tool used for the estimation of interface trap density ( $D_{it}$ ) in these undoped Si n-FinFETs.

### A. Method I: $D_{it}$ from active area

Based on the difference between the simulated and the experimental active area ( $S_{AA}$ ) values, a method to calculate the density of interface trap charges,  $\sigma_{it}$ , in the FinFETs is outlined. The method is based on the assumption that the total charge in the channel at a given  $V_{gs}$  must be the same in the experiments and in the simulations. This requirement leads to the following:

$$S_{AA,sim} \cdot L_{ch} \cdot \rho_{sim} = S_{AA,expt} \cdot L_{ch} \cdot \rho_{expt} + e \cdot \sigma_{it} \cdot L_{ch} \cdot P, \quad (4)$$

where  $S_{AA,sim}$  ( $S_{AA,expt}$ ) is the simulated (experimental) active area,  $P$  is the perimeter of the channel under the gate ( $P = W + 2H$ ) and  $\rho_{sim}$  ( $\rho_{expt}$ ) is the simulated (experimental) charge density. By applying Gauss's law at the oxide channel interface,  $\rho_{expt}$  is obtained from  $\rho_{sim}$  and  $\sigma_{it}$  as,

$$\rho_{expt} = \rho_{sim} - \rho_{it} = \rho_{sim} - (e \cdot \sigma_{it} \cdot P)/(W \cdot H). \quad (5)$$

Using Eqs. (4) and (5) the final expression for  $\sigma_{it}$  is obtained as

$$\sigma_{it}(V_{gs}) = \frac{\rho_{sim}(V_{gs})S_{AA,sim}(V_{gs})}{e \cdot P} \times \left[ \frac{\left[ 1 - \frac{S_{AA,expt}(V_{gs})}{S_{AA,sim}(V_{gs})} \right]}{\left[ 1 - \frac{S_{AA,expt}(V_{gs})}{W \cdot H} \right]} \right] \left[ \#/\text{cm}^2 \right]. \quad (6)$$

This method is useful for wider devices for which Eq. (2) is valid. For very thin FinFETs (close to a 1D system) this method cannot be utilized. All the comparisons for the interface trap charges is made at the same gate under-drive,  $V_{gt} = V_{gs} - V_T$ .

**Assumptions in Method I:** The extra charge contribution completely stems from the interface trap density ( $D_{it}$ ) and any contribution from the bulk trap states has been neglected. All the interface traps are assumed to be completely filled, which implies  $\sigma_{it} \cong D_{it}$ . The interface trap charges are assumed to be situated very close to the oxide-channel interface for Eq. (5) to be true. Also the interface trap density is assumed to be constant and identical for the top and the side walls of the FinFET, which is generally not the case.<sup>15,16</sup> This method of extraction works best for undoped channel since any filling of the impurity/dopant states is neglected in the calculation. Orientation dependent  $D_{it}$  for different surfaces could be included as a further refinement.

## B. Method II: $D_{it}$ from barrier control

The second method does not utilize the  $E_b$  value directly but its derivative w.r.t  $V_{gs}$ . The term  $\alpha = |\partial E_b / \partial V_{gs}|$  represents the channel to gate coupling.<sup>6</sup> The presence of interface traps weakens this coupling due to the electrostatic screening. This method of trap extraction is based on the difference in the experimental and the simulated  $\alpha$  value. The  $\alpha$  value can be represented in terms of the channel and the oxide capacitance. The equivalent capacitance model for a MOSFET with and without interface traps ( $D_{it}$ ) is shown in Fig. 2.

The  $\alpha$  value can be associated to the oxide, interface, and semiconductor capacitance that is given in Eq. (38) on page 383 in Ref. 22 This leads to the following relation:

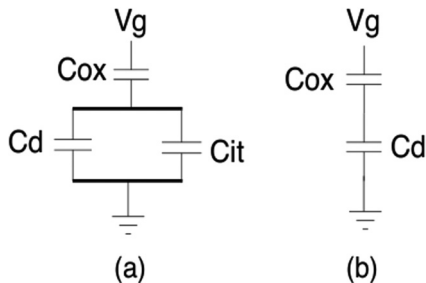


FIG. 2. Equivalent circuits (a) with interface-trap capacitance ( $C_{it}$ ) and (b) without interface capacitance.  $C_d$  and  $C_{ox}$  are the depletion and the oxide capacitance, respectively. The idea for this equivalent circuit is obtained from page 381 in Ref. 22.

$$\left| \frac{\partial E_b}{\partial V_{gs}} \right| = 1 - \frac{C_{tot}}{C_{ox}}, \quad (7)$$

where  $C_{tot}$  is the total capacitance. For the two cases, as shown in Fig. 2, the total capacitance is given by

$$C_{tot}^{exp} = \frac{C_{ox} \cdot (C_d + C_{it})}{C_d + C_{ox} + C_{it}}, \quad (8)$$

$$C_{tot}^{sim} = \frac{C_d \cdot C_{ox}}{C_d + C_{ox}}, \quad (9)$$

where  $C_{it}$ ,  $C_{ox}$ , and  $C_d$  are the interface trap capacitance, the oxide capacitance and the semi-conductor capacitance, respectively. Equation (8) represents the capacitance in the experimental device, and Eq. (9) represents the capacitance in the simulated device under ideal conditions without any interface traps. Combining Eqs. (7), (8), and (9) and after some mathematical manipulations, we obtain

$$\frac{1}{\alpha_{exp}} = \frac{1}{\alpha_{sim}} + \frac{C_{it}}{C_{ox}}. \quad (10)$$

Manipulating Eq. (10) gives the following relation for  $C_{it}$ :

$$C_{it} = C_{ox} \cdot \left( \frac{1}{\alpha_{sim}} \right) \cdot \left[ \frac{\alpha_{sim}}{\alpha_{exp}} - 1 \right]. \quad (11)$$

Also  $C_{it}$  can be related to the interface charge density ( $\sigma_{it}$ ) as<sup>22</sup>

$$C_{it} = e \cdot \frac{\partial \sigma_{it}}{\partial V_{gs}}. \quad (12)$$

In Eq. (11) all the values are dependent on  $V_{gs}$  except  $C_{ox}$ . Combining Eqs. (11) and (12) and integrating w.r.t  $V_{gs}$  yields the final expression for the integrated interface charge density in these FinFETs as

$$\sigma_{it} = \frac{C_{ox}}{e} \cdot \int_{V_1}^{V_2=V_T} \left( \frac{1}{\alpha_{sim}(V_{gs})} \right) \times \left[ \frac{\alpha_{sim}(V_{gs})}{\alpha_{exp}(V_{gs})} - 1 \right] dV_{gs} \left[ \#/\text{cm}^2 \right], \quad (13)$$

where  $V_T$  is the threshold voltage of the FinFET and  $V_1$  is the gate under-drive. Thus,  $V_1$  and  $V_2$  is the integration range for Eq. (13) in the sub-threshold region. The second method derived from barrier control has the advantage that it is independent of the dimensionality of the FinFET. Hence, Eq. (13) can be used for wide as well as thin FinFETs.

**Assumptions in Method II:** The most important assumption is that the rate of change of the surface potential ( $\Psi(V_{gs})$ ) is the same as  $E_b$  w.r.t  $V_{gs}$ . The extra charge contribution completely originates from the density of interface trap charges ( $\sigma_{it}$ ) and any contribution from the bulk trap states have been neglected. Also all the interface traps are assumed to be completely filled, which implies  $\sigma_{it} = D_{it}$ . This method works best when the change in the dc and the

ac signal is low enough, such that the interface traps can follow the change in the bias sweep.<sup>22</sup>

### C. Limitations of the methods

It is important to understand the limitations of the new trap metrology methods to apply them properly. One of the main limitations is how closely the simulated FinFET structure resembles the experimental device structure. This depends both on the SEM/TEM imaging as well the sophistication of the model. In the present case, we create the FinFET cross-section structure using the TEM image making the simulated structure as close to the experimental device as possible. With the development of better TCAD tools, the proximity of the simulated structure to experimental structure has increased. The physical device model needs to comprehend the crystal directions, atomistic details, strain, and gating realistically to realize the working of the nano-scale FETs. Effective mass models fail to properly represent the band structure in these types of ultra-scaled nanowires/FinFETs.<sup>12</sup> Our model enables the calculation of theoretical conductance value with good confidence to be used in the trap calculation. Furthermore, the calculated  $G$  is calculated as close to ideal as possible and all the difference between the ideal and experimental  $G$  is attributed to the traps, which may not be true always. An important difference between the two methods is that they are calculated over different  $V_{gs}$  ranges. This is important since the trap filling and their behavior changes with  $V_{gs}$  range, which should be taken into account accurately. One must also be aware of the embedded assumption of complete interface trap filling and the neglect of the bulk traps in the gate dielectric.

## V. RESULTS AND DISCUSSION

In this section the theoretical results as well as their comparison with the experimental data are provided.

### A. 3D versus 1D system

The conduction band structure (E-K) can be utilized to distinguish a 1D system from a 3D system. The bulk silicon conduction band (CB) has 6 degenerate valleys ( $\Delta_6$ ) (see inset of Figs. 3 and 4), which split into 2 sets of degenerate valleys called the “4-2 configuration” ( $\Delta_4 - \Delta_2$ ) for [100] and [110] 1D nanowires (NWs) due to the geometrical confinement.<sup>10</sup> In Si bulk the  $\Delta_2$  valleys are along the [100] direction. For a [100] Si nanowire channel the bulk  $\Delta_2$  valleys are projected along the channel axis away from the  $\Gamma$  point due to the folding of the Brillouin Zone (Figs. 3(a) and 3(b)).<sup>10</sup> The bulk  $\Delta_4$  valleys are projected at the  $\Gamma$  point.<sup>10</sup> The band structure of conduction band for silicon channel with  $W=3$  nm and  $H=15$  nm, and  $W=H=15$  nm is shown in Figs. 3(a) and 3(b), respectively. For [110] oriented Si channel the valley projection is different compared to the [100] channel. The CB minima is at the Off- $\Gamma$  position as shown in Fig. 4. This happens due to the different atomic positions and geometrical confinement in [100] and [110] channels.<sup>10</sup>

The energy separation between the  $\Gamma$  and Off- $\Gamma$  valleys is given by

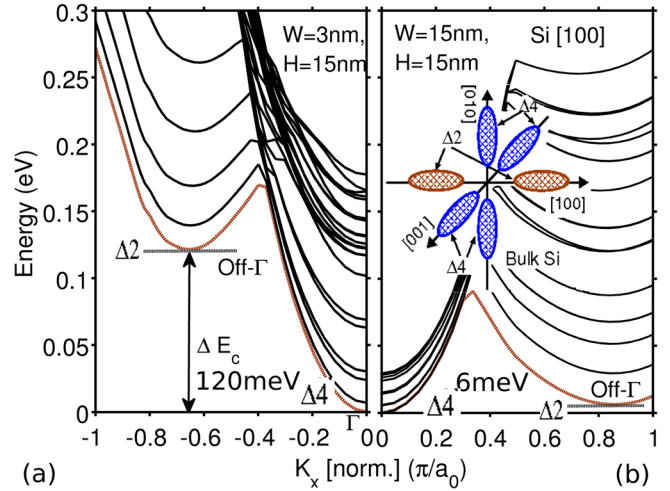


FIG. 3. (Color online) Simulated conduction band E-K, using TB, for [100] Si channel with  $H=15$  nm for (a)  $W=3$  nm and (b)  $W=15$  nm. The inset shows 6 equivalent bulk Si conduction band ellipsoids. The  $\Delta_2$  valleys are along the transport direction [100] whereas the  $\Delta_4$  valleys are in the quantized plane.

$$\Delta E_c = E(\Gamma) - E(\text{Off} - \Gamma), \quad (14)$$

which gives a measure of how close (or far) a 1D NW system is from a 3D bulk system. The observation of a large  $\Delta E_c$  value strongly points toward a 1D system, whereas a value close to zero points to a bulk system. Tight-binding simulations predict a  $\Delta E_c$  value of around 120 meV for a [100] Si nanowire channel with  $W=3$  nm and  $H=15$  nm (Fig. 3(a)) while this value reduces to 6 meV for a Si nanowires channel with  $W=H=15$  nm (Fig. 3(b)). For a [110] Si channel the  $\Delta E_c$  value is around 34 meV for  $W=3$  nm and  $H=15$  nm (Fig. 4(a)), which reduces to 3.4 meV for  $W=15$  nm and  $H=15$  nm (Fig. 4(b)). This indicates that larger cross-section silicon channels are closer to the 3D bulk system for both [100] and [110] oriented channels.

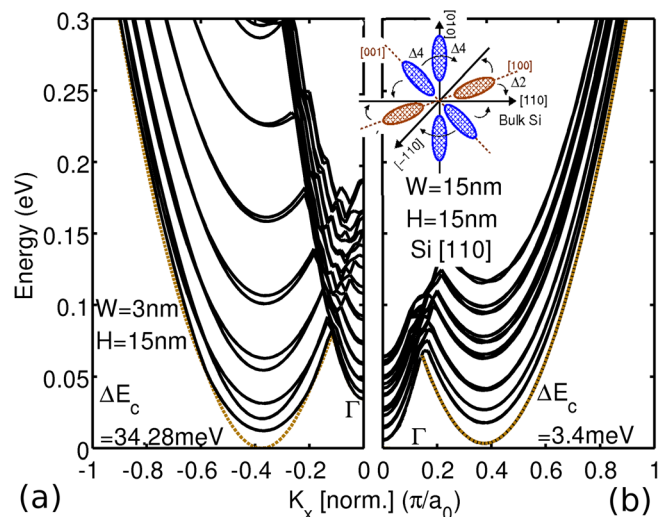


FIG. 4. (Color online) Simulated conduction band E-K, using TB, for [110] Si channel with  $H=15$  nm for (a)  $W=3$  nm and (b)  $W=15$  nm. The CB minima is at Off- $\Gamma$  position for the thinner [110] Si channel. Inset shows the bulk Si 6 equivalent conduction valleys.

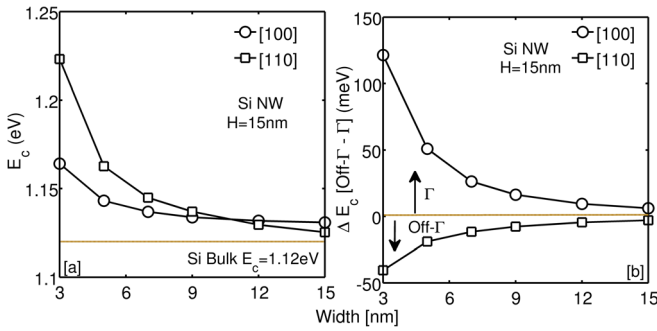


FIG. 5. (Color online) (a) Variation of the conduction band minimum ( $E_c$ ) for [100] and [110] oriented Si channels with width for a fixed height of 15 nm. (b) The separation of the  $\Delta_2$ - $\Delta_4$  valleys with width ( $W$ ) for rectangular [100] and [110] Si channel for a fixed height of 15 nm.

The conduction band minimum (CBM) decreases with increasing channel width for both [100] and [110] SiNWs (Fig. 5(a)). Also the  $\Delta E_c$  value decreases with silicon channel width for a fixed height of 15 nm (Fig. 5(b)). The  $\Delta E_c$  value is negative for [110] channel since the Off- $\Gamma$  valley is lower in energy compared to  $\Gamma$  valley. For  $W > 15$  nm the  $\Delta E_c$  is less than 5 meV ( $\leq k_B T_{300K}$ ) for both [100] and [110] Si channels. *This suggests that silicon channels with  $W \geq 15$  nm, and  $H = 15$  nm behave electrically close to the bulk Si system at room temperature.*

**B. Temperature dependence of  $E_b$**

The source-to-channel barrier height has been assumed to be temperature independent in the sub-threshold region. Figure 6 shows the results of a temperature dependent ToB calculations and proves that the barrier height ( $E_b$ ) is only weakly temperature dependent. In the sub-threshold region, the  $E_b$  value for a device identical to FinFET C is the same at four different temperatures ( $T = 140$  K, 200 K, 240 K, and 300 K). The variation with temperature becomes more prominent when the FinFET transitions into the on-state. Thus,  $E_b$  has a weak temperature dependence in the sub-threshold

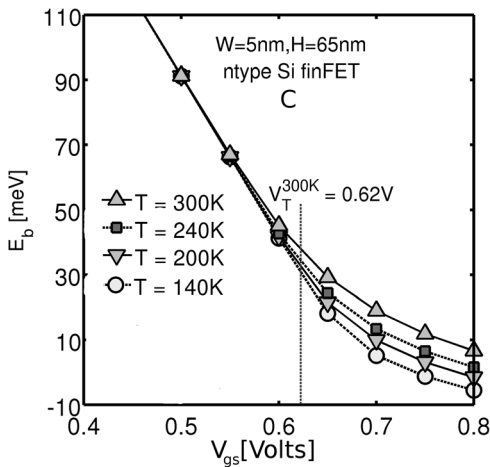


FIG. 6. Temperature dependence of the simulated barrier height ( $E_b$ ) in n-FinFET C. At  $T = 300$  K,  $V_T$  of the FinFET is 0.62 V. The overlap of the curves at different temperatures with  $V_{gs}$ , below  $V_T$  at 300 K, shows a weak temperature dependence of  $E_b$  in the sub-threshold region. The impact of temperature becomes prominent after  $V_{gs}$  goes above  $V_T$ .

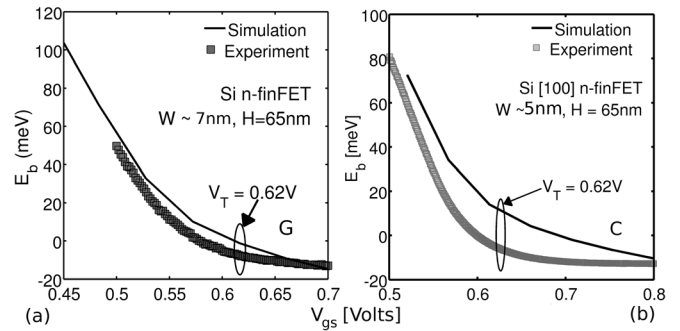


FIG. 7. Experimental and simulated barrier height ( $E_b$ ) in n-FinFET (a) G and (b) C. Both the devices have same  $V_T$ . Both experiment and simulation show a decreasing value of  $E_b$  with  $V_{gs}$ , but the absolute values are different.

region allowing us to evaluate  $E_b$  from the 300 K simulations only.

**C. Evolution of  $E_b$  and  $S_{aa}$  with  $V_{gs}$**

Experimentally, it has been shown that, for undoped silicon n-FinFETs,<sup>6</sup>  $E_b$  reduces as  $V_{gs}$  increases. Theoretically, the  $E_b$  value is determined using Eq. (1), which depends on the self-consistent channel potential ( $U_{scf}$ ). As the gate bias increases, the channel can support more charge. This is obtained by pushing the channel CB lower in energy to be populated more by the source and drain Fermi level.<sup>10</sup> Figures 7 and 8 show the experimental and theoretical evolution of  $E_b$  in FinFETs G, C and D, E, respectively. Theory provides correct qualitative trend for  $E_b$  with  $V_{gs}$ . Few important observations here are (i) *the theoretical  $E_b$  value is always higher than the experimental value and* (ii) *[110]. Si devices (D and E) show a larger mismatch to the experimental values.* The reason for the first point is suggested to be the presence of interface traps in the FinFETs, which screen the gate from the channel.<sup>6,7</sup> The second observation can be understood by the fact that [110] channels with (110) sidewalls have higher interface trap density due to the higher surface bond density<sup>22</sup> and poor anisotropic etching of the (110) sidewalls.<sup>15,16</sup>

The active channel area ( $S_{AA}$ ) represents the part of the channel where the charge flows.<sup>6</sup> Experimentally  $S_{AA}$  is shown to be decreasing with gate bias since the inversion charge moves closer to the interface, which electro-statically

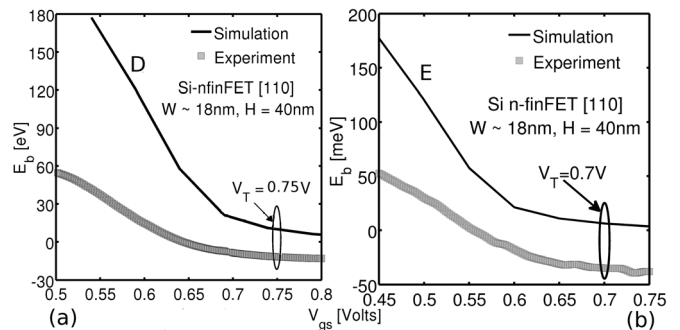


FIG. 8. Experimental and simulated barrier height ( $E_b$ ) in n-FinFETs (a) D and (b) E. The devices have different  $V_T$ , which is attributed to process induced variations. Both experiment and simulation shows a decreasing value of  $E_b$  with  $V_{gs}$ , but the absolute values are different.

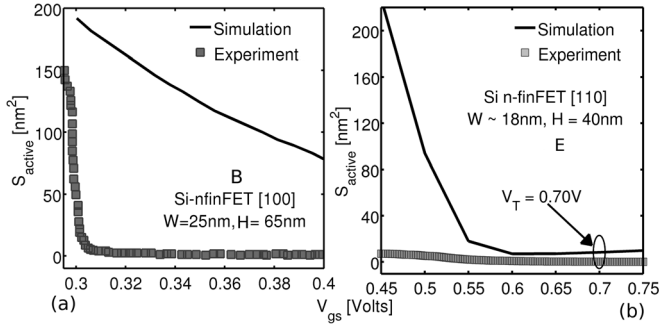


FIG. 9. Experimental and simulated channel active cross-section ( $S$ ) in n-FinFETs (a) B and (b) E. Both experiment and simulation show a decreasing value of  $S_{aa}$  with  $V_{gs}$ , but the absolute values are different. The simulated graph is for the same FinFET in both the cases, however, the  $V_{gs}$  ranges are different due to the different  $V_T$  of the experimental devices.

screens the inner part of the channel from the gate.<sup>6</sup> This gives a good indication of how much channel area is used for the charge transport. Figures 9(a) and 9(b) show the experimental evolution of  $S_{AA}$  in FinFET B and E, respectively. The theoretical value of  $S_{AA}$  decreases with  $V_{gs}$ , which is in qualitative agreement to the experimental observation.<sup>6,7</sup> However, the absolute values do not match. In fact theory over-estimates the experimental  $S_{AA}$  value (Fig. 9), which is attributed to the interface traps.

#### D. Trap density evaluation

In this section we present the results on the interface trap density ( $D_{it}$ ) in the undoped Si n-FinFETs.

##### 1. $D_{it}$ using $S_{AA}$ : Method I

The calculated  $D_{it}$  values for FinFET B and E are  $1.02 \times 10^{12} \text{ cm}^{-2}$  and  $1.81 \times 10^{12} \text{ cm}^{-2}$  (Figs. 10(a) and 10(b), respectively). The  $D_{it}$  values compare quite well with the experimental  $D_{it}$  values presented in Ref. 15 and also shown in Table II. As expected the  $D_{it}$  value for FinFET E (with [110] channel and (110) sidewalls) is higher than FinFET B ([100] channel with (100) sidewalls). This is attributed to the higher  $D_{it}$  ( $\sim 2\times$ ) on the (110) surfaces.<sup>15,16</sup> Our results show  $\sim 1.8\times$  more  $D_{it}$  for (110) sidewalls, in close agreement to the experiments. This method allows one to obtain the  $D_{it}$  in the actual FinFETs rather than custom made FETs.

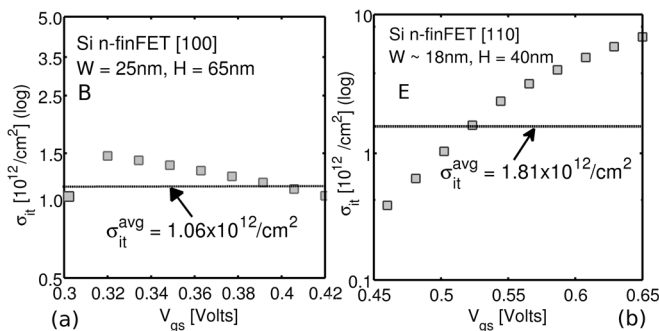


FIG. 10. Extracted trap density using the difference in active device area (method I) for n-FinFETs (a) B and (b) E.

TABLE II. Values of  $D_{it}$  obtained from all the n-FinFETs as well as from Ref. 15.

Device	Method	$D_{it}$ ( $10^{11} \text{ cm}^{-2}$ )	FET type	Observations
L = 140 nm (Ref. 15)	Charge	1.725	Special body	–
L = 240 nm (Ref. 15)	Pumping	2.072	tied FET	–
A	I	5.560	Std. FET	$H_2$
B	I	10.60	Std. FET	anneal,
	II	8.860	Std. FET	reduces $D_{it}$
C	II	9.26	Std. FET	Thin fin, more $D_{it}$
D	II	18.31	Std. FET	(110) side-wall,
E	I	18.1	Std. FET	thin fin,
	II	15.3	Std. FET	more etching,
F	II	36.3	Std. FET	more $D_{it}$
G	II	4.33	Std. FET	$H_2$ anneal, less $D_{it}$

##### 2. $D_{it}$ using $|\partial E_b/\partial V_{gs}|$ : Method II

The  $C_{ox}$  value needed in this method is taken as  $\sim 0.0173 \text{ F/m}^2$  which is assumed to be the same for all the devices since these FinFETs have similar oxide thickness. The calculated  $D_{it}$  values for FinFET C and D are  $9.26 \times 10^{11} \text{ cm}^{-2}$  and  $1.563 \times 10^{12} \text{ cm}^{-2}$  (Figs. 11(a) and 11(b), respectively). These calculations also show that the [110] channel device (FinFET E) shows a higher  $D_{it}$  compared to the [100] channel device (FinFET C), again consistent to the observations made in Ref. 15. The advantage of this method is that it can be used to obtain  $D_{it}$  in extremely thin FinFETs (close to 1D system) unlike method I, which is applicable only to wider FinFETs (due to the reasons discussed in Sec. III B).

##### 3. Discussion on the two methods and $D_{it}$ trends

The  $D_{it}$  values for all the FinFETs used in this study are shown in Table II. The important outcomes about the two methods are outlined below:

- The  $D_{it}$  values obtained by the two methods compare very well with the experimental measurement in Ref. 15 for similar sized FinFETs (A and B), demonstrating the validity of these new methods.
- The  $D_{it}$  values calculated using methods I and II (for B and E) compare very well with each other, which shows

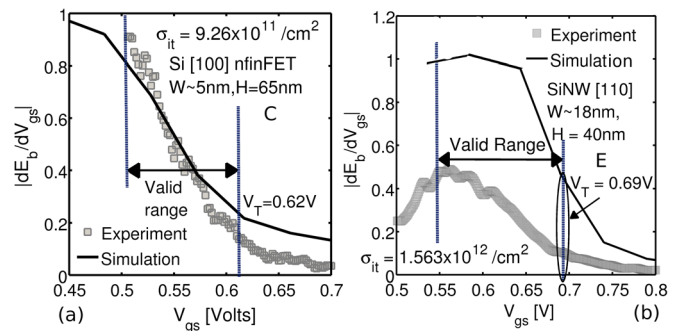


FIG. 11. (Color online) Experimental and simulated value of  $\alpha$  in n-FinFETs (a) C and (b) E.

that the two methods are complimentary<sup>7</sup> for large cross-section devices.

- The Dit values calculated for the two similar FinFETs (D and E) compare very well showing the reproducibility of the methods.<sup>7</sup>

The calculated  $D_{it}$  values also reflect some important trends about the FinFET width scaling and surfaces (Table II). The central points are as follows:

- Hydrogen passivation considerably reduces Dit.<sup>5</sup> This is observed for FinFETs A and B where H<sub>2</sub> passivation results in  $\sim 2\times$  less Dit in FinFET A.<sup>7</sup>
- Width scaling requires more etching, which also increases Dit.<sup>15,16</sup> The same trend is observed in devices A to C and D to F (decreasing W).
- (110) sidewalls show higher Dit compared to (100) sidewalls.<sup>15</sup> The same trend is also observed for FinFETs A, B, C, G ((100) sidewall) compared to FinFETs D, E and F ((110) sidewall).

### E. Current distribution

The spatial current distribution in FinFETs can provide a better insight for optimizing the channel cross-section area utilization. Theoretical calculations show that the charge flow in n-FinFETs depends strongly on the geometrical confinement. For very small width FinFET ( $W \sim 5$ ) the entire body gets inverted (Fig. 12(a)) and shows little change in  $S_{AA}$  with  $V_{gs}$ .<sup>6</sup> For wider FinFETs ( $W \sim 25$ ) the current flow starts from a weak volume inversion and moves toward surface inversion as  $V_{gs}$  increases (Fig. 12(b)).<sup>6</sup> For extremely thin n-FinFETs ( $W = 5$  nm,  $H = 65$  nm) the charge flows through the entire body (volume inversion) compared to the wider n-FinFETs ( $W = 25$  nm,  $H = 65$  nm) where the charge flows at the edges. Thus thin FinFETs can show better channel area utilization for the charge flow compared to the wider devices. However thin FinFETs show an increase in  $D_{it}$  due to more side-wall etching (Table II), which can severely limit the action of the thin FinFETs. The advancement of fabrication methods and strain technology may improve the performance of thin FinFETs as reported by some experimental works.<sup>24–26</sup>

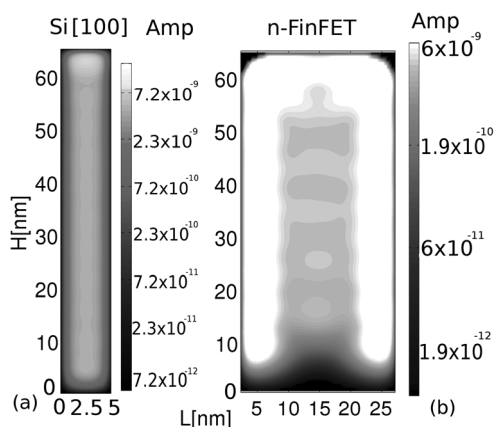


FIG. 12. Spatial current distribution in the  $\langle 100 \rangle$  undoped Si n-FinFET intrinsic with  $H = 65$  nm and (a)  $W = 5$  nm and (b)  $W = 25$  nm.  $V_{gs} = 0.4$  V and  $V_{DS} = 30$  mV at 300 K. 5 nm device shows a complete volume inversion. In the 25 nm device the current mainly flows at the edges.

## VI. CONCLUSIONS

Two new trap charge density metrology methods in ultra-scaled Si n-FinFETs are presented. The top-of-the-barrier model, combined with tight-binding calculations, explains very well the thermally activated sub-threshold transport in state-of-the-art Si FinFETs. The qualitative evolution of  $E_b$  and  $S_{AA}$  with  $V_{gs}$  are well explained by the theory. The systematic mismatch in the experimental and theoretical values of  $E_b$  and  $S_{AA}$  led to the development of two new interface trap density metrology schemes. The advantage of these schemes is that they do not require any special MOSFET structure as needed by the present experimental methods allowing one to probe the interface quality of the ultimate channel. These methods are shown to provide consistent and reproducible results, which compare very well with the independent experimental trap measurement results. The calculated trends of interface trap density with channel width scaling, channel orientation, and hydrogen passivation of the surfaces show a good correlation with the experimental observations. Thin width FinFETs could lead to a better channel utilization due to strong volume inversion only if surface roughness and the density of interface traps created during the extreme etching of these ultra-scaled devices can be reduced.

## ACKNOWLEDGMENTS

A.P., S.L., S.R.M., and G.K. would like to acknowledge the financial support from FCRP-MSD under Semiconductor Research Corporation, Nano Research Initiative (NRI) under Midwest Institute for Nanoelectronics Development (MIND) and National Science Foundation (NSF). Computational resources provided by nanoHUB.org, funded by NSF under Network for Computational Nanotechnology (NCN), is also acknowledged. G.C.T. and S.R. acknowledge FOM and the European Community Seventh Framework under the Grant Agreement No.: 214989-AFSiD for the financial support and the Australian Research Council Centre of Excellence for Quantum Computation and Communication Technology (Project No. CE110001029). G.C.T. acknowledges the kind hospitality extended by Professor A. Di Carlo at the University of Tor Vergata, Rome, during the preparation of this manuscript and D. Brousse for the help in the acquisition of the SEM images. All the authors acknowledge B. Johnson, J. McCallum, and N. Zimmerman for useful discussions. The band structure calculations for the silicon channels are done using Band structure Lab on nanoHUB.org.<sup>27</sup> The authors would like to thank the reviewer for improving this manuscript by raising important queries.

<sup>1</sup>For more details on mosFET scaling, see ITRS Report, <http://www.itrs.net/reports.html> (2010).

<sup>2</sup>H.-S. P. Wong, *IBM J. Res. Dev.* **46**, 133 (2002)

<sup>3</sup>D. Hisamo, W.-C. Lee, J. Kedzierski, H. Takeuchi, K. Asano, C. Kuo, E. Anderson, T.-J. King, J. Bokor, and C. Hu, *IEEE Trans. Elec. Dev.* **47**, 2320 (2000).

<sup>4</sup>N. Collaert, M. Demand, I. Ferain, J. Lisoni, R. Singanamalla, P. Zimmerman, Y. Yim, T. Schram, G. Mannaert, and M. Goodwin, *Symp. VLSI Tech.* 108 (2005).

<sup>5</sup>J. S. Lee, Y. K. Choi, D. Ha, S. Balasubramanian, T. J. King, and J. Bokor., *IEEE Elec. Dev. Lett.* **24**, 186 (2003).

- <sup>6</sup>G. C. Tettamanzi, A. Paul, G. P. Lansbergen, J. Verduijn, S. Lee, N. Collaert, S. Biesemans, G. Klimeck, and S. Rogge, *IEEE Elec. Dev. Lett.* **31**, 150 (2010).
- <sup>7</sup>G. C. Tettamanzi, A. Paul, S. Lee, S. R. Mehrotra, N. Collaert, S. Biesemans, G. Klimeck, and S. Rogge, *IEEE Elec. Dev. Lett.* **32**, 440 (2011).
- <sup>8</sup>G. Klimeck, F. Oyafuso, T. B. Boykin, R. C. Bowen, and P. von Allmen, *Comput. Model. Eng. Sci.* **3**, 601 (2002).
- <sup>9</sup>T. B. Boykin, G. Klimeck, and F. Oyafuso, *Phys. Rev. B* **69**, 115201 (2004).
- <sup>10</sup>N. Neophytou, A. Paul, M. Lundstrom, and G. Klimeck, *IEEE, Trans. Elec. Dev.* **55**, 1286 (2008).
- <sup>11</sup>M. Luisier, A. Schenk, W. Fichtner, and G. Klimeck, *Phys. Rev. B* **74**, 205323 (2006).
- <sup>12</sup>J. Wang, A. Rahman, A. Ghosh, G. Klimeck, and M. Lundstrom, *IEEE, Trans. Elec. Dev.* **52**, 1589 (2005).
- <sup>13</sup>A. Paul, S. Mehrotra, M. Luisier, and G. Klimeck, 13th International Workshop on Computational Electronics (IWCE), (IEEE, Pisa, Italy, 2009).
- <sup>14</sup>R. Kim, C. Jeong, and M. S. Lundstrom, *J. Appl. Phys.* **107**, 054502 (2010).
- <sup>15</sup>G. Kapila, B. Kaczer, A. Nackaerts, N. Collaert, and G. Groeseneken, *IEEE Elec. Dev. Lett.* **28**, 232 (2007).
- <sup>16</sup>J. W. Lee, D. Jang, M. Mouis, G. T. Kim, T. Chiarella, T. Hoffmann, and G. Ghibaudo, 2010 Proceedings of the European Solid-State Device Research Conference (ESSDERC), 2010, pp. 305–308.
- <sup>17</sup>E. H. Nicollian and A. Goetzberger, *Solid State Electron* **12**, 937 (1969).
- <sup>18</sup>A. Khakifirooz and D. Antoniadis, IEEE IEDM Electron Devices Meeting (IEDM, 2006), p. 1–4.
- <sup>19</sup>S. Lee, H. Ryu, Z. Jiang, and G. Klimeck, 13th International Workshop on Computational Electronics (IWCE), (IEEE, Shanghai, China, 2009).
- <sup>20</sup>H. Zhao, R. Kim, A. Paul, M. Luisier, G. Klimeck, F.-J. Ma, S. C. Rustagi, G. S. Samudra, N. Singh, G.-Q. Lo, and D. L. Kwong, *IEEE EDL* **30**, 526 (2009).
- <sup>21</sup>R. Chau, S. Datta, M. Doczy, B. Doyle, B. Jin, J. Kavalieros, A. Majumdar, M. Metz, and M. Radosavljevic, *IEEE Trans. Nanotech.* **4**, 153 (2005).
- <sup>22</sup>S. Sze and K. K. Ng, *Physics of Semiconductor Devices* (Wiley, New York, 2000).
- <sup>23</sup>For more details on ballistic conductance in 1D, see M. Lundstrom, ECE 656 Lecture 5: 1D Resistors <https://nanohub.org/resources/7361> (September 2009).
- <sup>24</sup>A. Teramoto, T. Hamada, M. Yamamoto, P. Gaubert, H. Akahori, K. Nii, M. Hirayama, K. Arima, K. Endo, S. Sugawa, and T. Ohmi, *IEEE Trans. Elec. Dev.* **54**, 1438 (2007).
- <sup>25</sup>T.-Y. Liow, K.-M. Tan, R. Lee, C.-H. Tung, G. Samudra, N. Balasubramanian, and Y.-C. Yeo, *IEEE Elec. Dev. Lett.* **28**, 1014 (2007).
- <sup>26</sup>M. Yang, E. Gusev, M. Jeong, O. Gluschenkov, D. Boyd, K. Chan, P. Kozlowski, C. D’Emic, R. Sicina, P. Jamison, and A. Chou, *IEEE Elec. Dev. Lett.* **24**, 339 (2003).
- <sup>27</sup>For more details on the bandstructure calculations, see A. Paul, M. Luisier, N. Neophytou, R. Kim, J. Geng, M. McLennan, M. Lundstrom, and G. Klimeck, <http://nanohub.org/resources/1308> (May 2006).