Theoretical evaluation of maximum electric field approximation of direct band-to-band tunneling Kane model for low bandgap semiconductors

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Abstract. The two-band Kane model has been popularly used to calculate the band-to-band tunneling (BTBT) current in tunnel field-effect transistor (TFET) which is currently considered as a promising candidate for low power applications. This study theoretically clarifies the maximum electric field approximation (MEFA) of direct BTBT Kane model and evaluates its appropriateness for low bandgap semiconductors. By analysing the physical origin of each electric field term in the Kane model, it has been elucidated in the MEFA that the local electric field term must be remained while the nonlocal electric field terms are assigned by the maximum value of electric field at the tunnel junction. Mathematical investigations have showed that the MEFA is more appropriate for low bandgap semiconductors compared to high bandgap materials because of enhanced tunneling probability in low field regions. The appropriateness of the MEFA is very useful for practical uses in quickly estimating the direct BTBT current in low bandgap TFET devices.

1. Introduction
The band-to-band tunneling (BTBT) has been proposed as the main mechanism to generate the conduction current in three-terminal tunnel devices which were initially named “surface tunnel transistors” [1] or tunnel field-effect transistors (TFETs) as widely known today. The most important innovation of employing the BTBT mechanism is to produce a sub-60 mV/decade subthreshold swing at room-temperature [2]-[4] which is a key requirement for scaling the threshold voltage and associated dynamic power consumption of transistors [5]. Furthermore, the off-state power dissipation of BTBT-based transistors is also relatively low since they are always operated in the highly reverse-biased condition of p-n junctions [6], [7]. With the breakthrough of the 60 mV/decade swing limit of conventional metal-oxide-semiconductor field-effect transistors (MOSFETs), TFETs have drawn much attention to serve as a promising candidate for energy-efficient applications [8], [9].

Properly calculating the BTBT generation rate in TFET devices is an important issue to study their physical operation, electrical characteristics and device design. Several full-quantum models based on

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the k·p or tight-binding methods have been developed to accurately simulate the tunneling current in TFETs with different structures and materials [10], [11]. However, there are significant disadvantages of using full-quantum models due to their sophisticated mathematical formalisms such as huge memory space, long simulation time, big difficulties in extracting physics and design. Therefore, the two-band Kane model [12] has been popularly employed for TFET devices because of its simple formalism, applicability for both direct and indirect semiconductors, favorable integration in numerical simulation tools [13] and acceptable validity [4], [14], [15]. However, the Kane model was only derived for tunnel junctions with a uniform electric field. In cases of nonuniform electric field, an appropriate approach must be applied in the Kane model to calculate the tunneling generation rate. An intuitive approach by using nonlocal electric field in the Kane formula has demonstrated a good agreement with experiment data [14], [16], [17]. The electric field is nonlocally determined along the tunneling path of electrons. However, the nonlocal BTBT models may be relatively complicated for engineers who wish to quickly estimate the tunneling current in TFETs for design purposes. In this case, one can use another approximation in which the maximum electric field at the tunnel junction is used in the Kane model. The appropriateness of the maximum electric field approximation (MEFA) has been experimentally verified for reverse-biased p-n junctions with high bandgap semiconductor of silicon [18]. Regrettably, applying the MEFA of Kane model for TFET devices has not been clarified because previous researches have not realized local and nonlocal field terms in the Kane formula. In addition, it has been shown that low and direct bandgap semiconductors must be used in TFETs to achieve sufficient on-current for practical applications. The modeling and properties of the tunneling in low bandgap materials are quite different from those in high bandgap semiconductors [19], [20]. Therefore, the appropriateness of the MEFA of direct BTBT Kane model for low bandgap semiconductors remains questionable.

This study theoretically evaluates the maximum electric field approximation of direct BTBT Kane model for low bandgap semiconductors. Since important low bandgap semiconductors have a direct energy bandgap, the Kane model for direct semiconductors was considered. To compare the validity of the MEFA in low bandgap semiconductors with that in high bandgap materials, two fitting factors for the electric field terms in the pre-exponential and exponential terms were separately introduced. InSb with a direct bandgap of 0.17 eV was typified as a low bandgap semiconductor while Ge with a direct bandgap of 0.8 eV was considered as a high bandgap material. The paper consists of four sections, including the Introduction and the Conclusion. Section 2 first summaries the direct BTBT Kane model with decoupled the local and nonlocal electric field terms and then describes the device structure used for investigations. The analyses of the MEFA of direct BTBT Kane model for different bandgap semiconductors are subsequently presented in section 3.

2. Tunneling model and device structure

The nonlocal BTBT Kane model of which all electric field terms are identically specified by the nonlocal value of electric field along the tunneling path have been widely used to calculate the tunneling generation in the nonuniform field junctions of TFET devices. However, it is noted that this approach is an approximation because the Kane model was initially derived for a uniform electric field. For more accurate calculations, the physical origin and associated roles of each electric field term in the Kane model must be clarified to answer the question which value of electric field, the local or nonlocal field, should be used when considering nonuniform field tunnel junctions. This section first summaries the direct tunneling model to explicitly show the reason why the local and nonlocal electric field terms have to be decoupled appropriately. The device structure used in this study is then described and explained.

2.1. Direct tunneling model

To illustrate and calculate the direct BTBT in semiconductors, Figure 1 shows the schematic energy-band diagram of a p-n junction under reverse-biased condition. The electric field is assumed to be uniform in the region of tunnel junction. In the quantum picture, it is physically allowable for electrons
to tunnel through the forbidden bandgap from the left-side valence band to the right-side conduction band. Generally, the tunneling generation rate per unit volume ($G_{BTBT}$) is obviously equal to the product of flux of electrons reaching to the high field junction for possible tunneling transitions, tunneling probability and transmission factor:

$$G_{BTBT} = \int dN_F \times P \times F_T$$

where $dN_F$ is the incident electron flux in a ring of perpendicular momentum between $k_{\perp}$ and $k_{\perp} + dk_{\perp}$ ($k_{\perp}$ is perpendicular component of wave vector), $P$ is the tunneling probability and $F_T$ is the transmission factor defined as the number of available conduction band states into which transmission of a valence electron can be performed. It is clearly that the transmission factor of direct BTBT is equal to one because both electron energy and momentum are strictly conserved.

The direct BTBT probability can be calculated by using the two-band Kane model [12]. In the Kane model, the tunnel electric field is treated as a constant perturbation field which causes the transition from the initial valence band state to the final conduction band state of tunneling electrons. The time-dependent perturbation theory limited to the first-order is employed to estimate the transition probability. Using the Fermi golden rule, the direct tunneling probability can be approximated as:

$$P = \frac{\pi^2}{9} \exp\left(-\frac{\pi m_{\perp}^{1/2} E_{\perp}^{3/2}}{2 \hbar q \xi}\right) \exp\left(-\frac{2E_{\perp}}{E_{\perp}}\right)$$

where

$$E_{\perp} = \frac{\hbar^2 (k_x^2 + k_y^2)}{4m_{\perp}}, \quad E_{\perp} = \frac{\hbar q \xi}{\pi m_{\perp}^{1/2} E_{\perp}^{3/2}}.$$  

$m_{\perp}$ is the reduced mass, $\xi$ is the electric field, $\hbar$ is reduced Plank’s constant, $E_g$ is the semiconductor bandgap, $q$ is the elementary charge, $k_x$ and $k_y$ are perpendicular components of wave vector.

Logically, the tunneling probability depends on the electric field at anywhere along the tunneling path. Therefore, the electric field terms in equations (2) and (3) must be nonlocally determined along this tunneling path. In other words, the electric field terms related to the tunneling probability should be specified to be the nonlocal electric field.

Intuitively, the incident electron flux in a ring of perpendicular momentum is the product of the velocity in $k$-space, the density of states in $k$-space, the area of ring, and the occupancy of states. Using the expressions of the electron velocity and the density of state in $k$-space:
(4) the incident electron flux can be formulated as:

\[ dN_F = v_k \times \rho(k) \times 2\pi k_x dk_x \times (F_v - F_c) = \frac{q}{2\pi h} (F_v - F_c) v_k \xi dk_x \text{,} \]

(6) where \( F_v \) and \( F_c \) are Fermi-Dirac distribution functions in valence and conduction bands, respectively. The presence of the conduction band Fermi-Dirac function in equation (6) is to exclude occupied conduction band states. From equation (6), we see that there is one term of electric field related to the electron velocity in \( k \)-space at the tunnel junction. This electric field term determines the number of electrons reaching to the tunnel junction for possible tunneling transitions. Therefore, the electric field term in equation (6) must be locally specified at the initial point of the tunneling. In other words, the electric field term related to the tunneling electron number has to be the local electric field.

Inserting equations (2) and (6) into equation (1) with denoting \( \xi \) for local electric field and \( \bar{\xi} \) for nonlocal electric field, we can express a full form of BTBT generation rate as:

\[ G_{BTBT} = q^2 m_{tr}^{1/2} \frac{\xi \bar{\xi}}{\sqrt{2}} \exp \left( -\frac{\pi m_{tr}^{1/2} E_0^{3/2}}{2h\bar{\xi}} \right) \left[ 1 - \exp \left( -\frac{2E_0}{E_x} \right) \right] \text{.} \]

(7) By ignoring the negligible term of the exponential in square bracket in equation (7), the direct BTBT Kane model is simply formulated in a compact form [21]:

\[ G_{BTBT} = A \frac{\xi \bar{\xi}}{E_0^{3/2}} \exp \left( -\frac{B E_0^{3/2}}{\bar{\xi}} \right) \text{,} \]

(8) where material dependent parameters \( A \) and \( B \) are given by:

\[ A = \frac{q^2 m_{tr}^{1/2}}{18\pi h} \text{,} \quad B = \frac{\pi m_{tr}^{1/2}}{2h\bar{\xi}} \text{.} \]

(9) It is emphasized that only one electric field term in the prefactor of the Kane formula associated with the tunneling electron number is the local field whereas the remaining terms related to the tunneling probability are the nonlocal field.

2.2. Device structure
The direct BTBT Kane model presented in previous subsection is for tunnel junctions with a uniform electric field. In practical terms, the electric field profile of tunnel junctions in TFET devices are usually nonuniform. In this study, one-sided p-n junctions were chosen to represent nonuniform field tunnel junctions in TFETs, as schematically shown in figure 2(a). An important reason for this choice is that tunnel junctions in TFETs are all one-sided p-n junctions regardless of point- or line-tunneling TFET structure. Furthermore, the structure of one-sided p-n junction provides a simple calculation of nonuniform electric field profile [22]. Figure 2(b) shows the energy-band diagram in reverse-biased condition of one-sided p-n junction with lightly-doped p-type left side and heavily-doped n-type right side. The depletion region and associated nonzero electric field region almost penetrate into the lightly-doped p-side. The electric field is maximum at the most right of the depletion region and it nonlinearly decreases when going to the left.

3. Maximum electric field approximation (MEFA)

Clearly, the question arises of which value of electric field should be used in the Kane formula when the model is applied for a nonuniform electric field. There is no definite standard for choosing the value of electric field in the Kane model since we cannot know the exact and explicit expression of potential barrier in the classically forbidden region II in figure 1 [21]. Some authors have suggested the average field [12], [21], [23] but also another suggestion of using the maximum field has been made [24], [25]. Based on the investigation of the reverse-biased p-n junctions of silicon with a relatively high bandgap, Hurkx has experimentally shown that the maximum field is appropriate for use in the Kane model. In this section, the maximum electric field approximation of direct BTBT Kane model applied for nonuniform field junctions is discussed to theoretically evaluate its validity for low bandgap semiconductors.

3.1. MEFA of direct BTBT Kane model

Starting from the Kane model of equation (8) with noting the local electric field $\xi = -(qN_A/e)x$, the tunneling current in the one-sided p-n junction in reverse-biased voltages can be calculated by:

$$I = A \frac{qV_a}{E_g^{3/2}} \exp \left(-B \frac{E_g^{3/2}}{\xi} \right), \quad (10)$$

where $V_a$ is the reverse-biased voltage.

Since the tunneling probability is strongly dependent on the length of tunneling path, the tunneling probability is only significant at the highest field region where the tunneling path is minimized. For
simplicity, therefore, the nonlocal field terms in the Kane model are set with a maximum value of electric field at the tunnel junction. An important point in the MEFA has not been previously clarified because we usually use the Kane model in the form of equation (8), and thus it allows us to apply the MEFA for TFET devices. Using the MEFA, the tunneling current is written as:

\[ I = A \frac{q V}{\varepsilon_{\text{max}}} \exp \left( -B \frac{E_{g}^{3/2}}{\varepsilon_{\text{max}}} \right), \]  

(11)

where \( \varepsilon_{\text{max}} \) is the maximum electric field at the tunnel junction. In this study, we use the Hurkx’s results to assume that the MEFA of direct BTBT Kane model is appropriate for high bandgap semiconductors.

3.2. Theoretical evaluation of MEFA for low bandgap semiconductors

To evaluate the MEFA for low bandgap semiconductors, we introduce two separate fitting parameters \( a \) and \( b \) for the nonlocal field terms in the prefactor and the exponential of equation (11), respectively:

\[ I_{\text{fit}} = A \frac{q V}{\varepsilon_{\text{max}}} \exp \left( -B \frac{E_{g}^{3/2}}{\varepsilon_{\text{max}}} \right), \]  

(12)

The fitting parameters are determined so that the tunneling current \( I_{\text{fit}} \) is best fitted to the accurate solution of the Kane model. By comparing the values of fitting parameters for low bandgap semiconductors with those for high bandgap materials, the MEFA of direct BTBT Kane model for low bandgap semiconductors can be evaluated properly.

Although the full form of Kane model in equation (7) provides the more accurate solution of the tunneling generation rate, its compact form in equation (8) is much simpler for calculations. To decide which form of the Kane model should be used for the fitting procedure, figure 3 shows the calculated current-voltage characteristics of one-sided p-n tunnel diodes with different bandgap semiconductors. For high bandgap Ge in figure 3(a), the compact form of equation (8) is excellently fitted to the full model of equation (7). For low bandgap InSb in figure 3(b), the compact form presents a remarkable deviation from the full model because of very small applied voltages [19]. For exactly evaluating the MEFA, therefore, the tunneling current \( I_{\text{fit}} \) is fitted to the full Kane model of equation (7) using the least-square method.

Figure 4 shows the current-voltage curves of one-sided p-n tunnel diodes using high bandgap Ge

\[ \text{Figure 4. Calculated current-voltage curves of reverse-biased one-sided p-n tunnel diodes with (a) high bandgap Ge and (b) low-bandgap InSb using different forms of the Kane model.} \]
and low bandgap InSb calculated by using the full Kane model, the MEFA without and with fitting parameters. Firstly, the deviation between the MEFA curve and the full model curve of low bandgap InSb tunnel diode is almost comparable to that of high bandgap Ge counterpart. It means that if the MEFA is considered as a good approximation for high bandgap materials, it is also a good approximation for low bandgap semiconductors. Basically in both high and low bandgap devices, the results of fitted MEFA are fitted well to those of the full model that confirms the appropriateness of the fitting procedure. The fitting parameter $a$ in the case of low bandgap InSb is significantly larger than that in the case of high bandgap Ge, whereas the values of parameter $b$ are slightly different between the two cases.

To further investigate the dependences of fitting parameters on semiconductor bandgap and doping concentration of tunnel junction, figure 5 shows the values of fitting parameters as a function of the energy bandgap with different doping concentrations. It is seen from figure 5(b) that parameter $b$ does not depend on the bandgap except the region of very low bandgaps. The exponential change of parameter $b$ when decreasing the bandgap in extremely low bandgap region is solely attributed to the contribution of the exponential in the square bracket in equation (7). The change of parameter $b$ is more rapid in the tunnel junction with higher doping concentration because of the larger curvature of energy-band diagram. As shown in figure 5(a), in general, parameter $a$ always increases with decreasing energy bandgap irrespective of doping concentration. The increase of parameter $a$ approaching to one when decreasing energy bandgap implies that the role of maximum field in determining the tunneling probability approaches to that of the nonlocal field. This is because the tunneling is extended far from the maximum field region due to high tunneling probability in low bandgap semiconductors [19]. Moreover, for a high doping concentration, a large curvature of energy-band diagram results in a narrow tunneling path, a high tunneling probability and thus a large value of parameter $a$. In the mathematical point of view, therefore, the MEFA of direct BTBT Kane model is more appropriate for low bandgap semiconductors and high doping concentrations.

4. Conclusions
The maximum electric field approximation of direct BTBT Kane model has been theoretically elucidated to show that the local field term must be remained while the nonlocal field terms are replaced by the maximum electric field. It has been mathematically demonstrated that the MEFA can be applied more appropriately for low bandgap semiconductors and associated physical explanations have also been made adequately. The meaning of these conclusions is that the BTBT current in low bandgap TFET devices can be calculated easily and quickly for practical uses in device modeling and design.
Acknowledgment: This work was funded by the Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.02-2015.58.

References

[1] Baba T 1992 *Jpn. J. Appl. Phys.* **31**, L455
[2] Appenzeller J, Lin Y-M, Knoch J and Avouris Ph 2004 *Phys. Rev. Lett.* **93** 196905
[3] Zhang Q, Zhao W and Seabaugh S A 2006 *IEEE Electron Device Lett.* **27** 297
[4] Krishnamohan T, Donghyun K, Raghunathan S and Saraswat K 2008 *Tech. Dig. IEEE Int. Electron Devices Meeting* (15-17 December 2008, San Francisco) p 1
[5] 2013 *International Technology Roadmap for Semiconductor*
[6] Reddick W M and Amaratunga G A J 1995 *Appl. Phys. Lett.* **67** 494
[7] Wang P-F, Hilsenbeck K, Nirschl Th, Oswald M, Stepper Ch, Weis M, Schmitt-Landsiedel D and Hansch W 2004 *Solid-State Electron.* **48** 2281
[8] Ionescu A M and Riel H 2011 *Nature* **479** 329
[9] Zhao Q T et al. 2015 *IEEE Journal of Electron Devices Society* **3** 103
[10] Shin M 2009 *J. Appl. Phys.* **106** 054505
[11] Luisier M and Klimeck G 2009 *IEEE Electron Device Lett.* **30** 602
[12] Kane E O 1961 *J. Appl. Phys.* **31** 83
[13] 2010 *Synopsys MEDICI User’s Manual* (California: Synopsys Inc.)
[14] Nayfeh O M, Hoyt J L and Antoniadis D A 2009 *IEEE Trans. Electron Devices* **56** 2264
[15] Shih C-H and Chien N D 2013 *J. Appl. Phys.* **113** 134507
[16] Peng J Z, Haddad S, Hsu J, Chen J, Longcor S and Chang C 1995 *Proc. Int. Conf. Solid-State and Integrated Circuit Technology* (24-28 Oct 1995, Beijing) p 141
[17] Kao K-H, Verhulst A S, Vandenberghhe W G, Sorée B, Groeseneken G and Meyer K D 2012 *IEEE Trans. Electron Devices* **59** 292
[18] Hurkx G A M 1989 *Solid-State Electron.* **32** 665
[19] Shih C-H and Chien N D 2014 *J. Appl. Phys.* **115** 014507
[20] Shih C-H and Chien N D 2014 *IEEE Trans. Electron Devices* **61** 1907
[21] Moll J L 1970 *Physics of Semiconductors* (New York: McGraw-Hill) pp 252-255
[22] Pierret R F 1970 *Semiconductor Device Fundamentals* (USA: Addison-Wesley Publishing Company) pp 209-225
[23] Logan R A and Chynoweth A G 1963 *Phys. Rev.* **131** 89
[24] Singh Tyagi M 1968 *Solid-State Electron.* **11** 99
[25] Fair R B and Wivell H W 1976 *IEEE Trans. Electron Devices* **23** 512