On The Modeling of I-V Characteristics of InAs based Tunneling Diode including band nonparabolicity

Falguni Sinhababu
Department of Computer science & Engineering
Government College of Engineering & Leather Technology
Kolkata-700106, India

Anup Dey
Department of Electronics and Communication Engineering
Jalpaiguri Government Engineering College
Jalpaiguri-735102, India

***Abstract*—The tunneling characteristics in narrow band gap nonparabolic semiconductor differs greatly relative to that of parabolic highband gap materials. In this paper, we developed a simple analytical model for tunneling characteristics in narrow band gap nonparabolic semiconductor based diode. The model is applied to the calculation of the I-V characteristics of an InAs tunneling diode. The model is compared with the characteristics of a conventional simple parabolic band based model. With proper consideration of band nonparabolicity the results of the analysis of tunneling characteristics of the narrow-gap materials show significant deviations from the results when simple parabolic band approximation is considered. The model is also validated with the atomistics simulations and the results reveal high consistency besides dictating the necessity to include the band nonparabolicity in current modeling in tunnel diodes.**

Keywords—Kane model; Band-to-Band tunneling; I-V characteristics; band nonparabolicity.

I. INTRODUCTION (*Heading 1*)

Since the first theoretical study of interband tunneling mechanism by Zener [1] to explain the breakdown mechanism in solid dielectric under the influence of strong electric field, the tunneling in semiconductor diode gained fresh impetus after the successful experimental demonstration of tunnel diode by L. Esaki [2]. Interband tunneling is also currently considered as the principal mechanism for modeling the drive current in tunneling field effect transistors or tunnel FETs (TFETs) [3] as well as accurately evaluating the gate leakage current in conventional simple MOSFETs. Thus, modeling interband tunneling has still been of much research interest both theoretically [4] and experimentally [5, 6] even today, for gaining insight of the electronic behavior of modern nano-dimensional devices. However, most of these models rely on modeling tunneling phenomena with simplistic two band model of energy band structure, specifically parabolic band structure based model. Though these simple two band models are adequate for modeling and characterizing the tunneling phenomena in wide gap semiconducting materials (for example Si) and their device applications, a more accurate analysis is often necessary for modeling tunneling characteristics in diode made of narrow gap semiconductors [7]. Recently narrow and direct band gap semiconductors, such as InAs and InSb, are widely been considered for application in Tunnel field-effect transistors (TFETs) due to their interesting on current features at low operating voltages [8], primarily for low effective mass(m^*) arising from nonparabolic band structure. In low band gap materials the energy dispersion relation is often modeled in terms of three band energy model of Kane [9,10] in which the $k.p$ and spin-orbit interactions between the lowest singlet conduction band and the highest triplet valence band are only considered. The energy dispersion becomes nonparabolic for all the three bands except for the heavy-hole band which retains its parabolic nature. The band-to-band-tunneling (BTBT) current, being directly dependent on energy dispersion through the effective mass, energy gap and density of states, the interband tunneling current variation as a function of applied voltage is quite different in case of the materials with significant band nonparabolicity relative to the materials with parabolic energy band structure. Taking into account all these factors, the paper provides an accurate approach for modeling I-V characteristics of tunneling diodes made up of narrow gap semiconductors.

The article has the following organization. Our formulation of tunneling current of direct band gap semiconductors considering the nonparabolicity of energy band structure in the three band energy model of Kane has been summarized in section II of Theoretical Formalism. Subsequently for the sake of verification of this generalized formulation, certain limiting conditions specific to wide band gap semiconductors are employed to reduce these results to the well known results of tunneling current for materials having parabolic energy band in the same section. In Section III the band coupling effect and nonparabolicity on tunneling current have been investigated with due consideration to treating the exact valence band structure and its relevant energy band parameters. Finally, the article is concluded in section IV.

II. THEORETICAL FORMALISM

Adopting the theoretical formulation of tunneling probability by technique similar to the method of stationary phase for nonparabolic semiconductor was first illustrated by Kane and subsequently band –to band tunneling (BTBT) current in semiconductor diode was derived [10] for wide gap semiconductor adjusting the formulated tunneling probability for application to high band gap materials. Accordingly, the tunneling probability can in general be written as [7],

$$\Im = \frac{\pi^2}{9}\exp\left(-\frac{\pi m_r^{1/2} E_g^{3/2}}{2\sqrt{2}\hbar F}\right)\exp\left(-\frac{2E_\perp}{\overline{E}_\perp}\right) \quad (1)$$

where $$\frac{\hbar^2 k_\perp^2}{2m_r} = \frac{\hbar^2(k_x^2 + k_y^2)}{2m_r} = \gamma(E_\perp) \quad (2)$$

and $$\overline{E}_\perp = \frac{2\hbar F}{\pi(E_g m_r)^{1/2}} \quad (3)$$

in which $\gamma(E_\perp) = E_\perp(1+\alpha E_\perp)$ and $\alpha = 1/E_g$ (4)

In order to calculate the tunneling current, we shall first compute the elemental incident current per unit area in the energy range $dE_\perp dE_z$

where the total energy $E = E_\perp + E_z$ (5)

$$dJ = \frac{2e}{\hbar}\frac{2\pi dk_\perp dk_z}{8\pi^3} \quad (6)$$

Transforming the above equation in the energy space using (2) we may write

$$dJ = \frac{2e}{\hbar}\gamma'(E_\perp)dE_\perp \frac{2\pi m_\perp dE_z}{8\pi^3\hbar^2} \quad (7)$$

leading to $$dJ = \frac{em_\perp}{2\pi^2\hbar^3}\gamma'(E_\perp)dE_\perp dE_z \quad (8)$$

In (8) we have $\gamma'(E_\perp) = \alpha V'(E_\perp)$

$$V'(E_\perp) = 2E_\perp + E_g$$

Assuming m_r to be isotropic and is equal for both n and p sides, and by using (1) and (8), the tunnel current per unit area, J ,for non parabolic semiconductors can be expressed as

$$J = \Upsilon\int\left[f_1(E_n) - f_2(E_p)\right]\gamma'(E_\perp)\exp\left(-\frac{2E_\perp}{\overline{E}_\perp}\right)dE_\perp dE \quad (9)$$

where $$\Upsilon = \frac{em_r\alpha}{18\hbar^3}\exp\left(-\frac{\pi m_r^{1/2}E_g^{3/2}}{2\sqrt{2}\hbar F}\right) \quad (10)$$

Here the variables of integrations are conveniently chosen to be E and $E_\perp$ rather than E_z and $E_\perp$, and f_1, f_2 are the Fermi-Dirac occupancy probability in n and p sides of the diode. The limits of integrations for E and $E_\perp$ can be obtained from the band edges in n and p sides. Carrying out the integration over E and assuming $f_1 = 1$ and $f_2 = 0$ under degenerate electron concentrations in tunnel diode, (9) can be simplified as

$$J = \Upsilon\int_0^E (2E_\perp + E_g)\exp\left(-\frac{2E_\perp}{\overline{E}_\perp}\right)dE_\perp dE \quad (11)$$

Equation (11) can also be written as $J = \Upsilon D$ (12)

where

$$D = E_g\int_0^E\{2\alpha E_\perp + 1\}\exp\left(-\frac{2E_\perp}{\overline{E}_\perp}\right)dE_\perp dE, \quad \alpha = 1/E_g \quad (13)$$

which may be evaluated as

$$D = \frac{E_g\overline{E}_\perp}{2} \times\int\left[\left\{1-(1+2\alpha E)\exp\left(-\frac{2E}{\overline{E}_\perp}\right)\right\} + \alpha\overline{E}_\perp\left\{1-\exp\left(-\frac{2E}{\overline{E}_\perp}\right)\right\}\right]dE \quad (14)$$

This is the expression with semiconductor with band nonparabolicity. Moreover, for parabolic energy band $\alpha \to 0$ and (13) reduces to

$$J = \frac{\Upsilon E_g\overline{E}_\perp}{2}\int\left\{1-\exp\left(-\frac{2E}{\overline{E}_\perp}\right)\right\}dE \quad (15)$$

as is found extensively in the literature for mathematical modeling of tunneling devices[7].

In order to calculate the tunnel current in tunnel diode we first assume the Fermi levels of the n-side is λ_n and the p-side is λ_p. Beside, assuming the quantities D and V are positive for the forward bias and negative for the reverse bias we obtain the complete formulas as the following

$$D = \int\left[\left\{1-(1+2\alpha E)\exp\left(-\frac{2E}{\overline{E}_\perp}\right)\right\} + \alpha\overline{E}_\perp\left\{1-\exp\left(-\frac{2E}{\overline{E}_\perp}\right)\right\}\right]dE \quad (16)$$

Evaluating the above integration we get the piece-wise characteristics of D as functions of V . Towards this we define the parameters λ_s and λ_l as the smaller and larger of λ_n , λ_p , respectively. Therefore,

For $eV \le \lambda_s - \lambda_l$

$$\begin{aligned} D = {} & eVP + Q\left\{\exp(-2\lambda_p/\overline{E}_\perp) + \exp(-2\lambda_n/\overline{E}_\perp) - 2\exp(-(\lambda_p+\lambda_n-eV)/\overline{E}_\perp)\right\} \\ & + \alpha\overline{E}_\perp\left\{\lambda_p\exp(-2\lambda_p/\overline{E}_\perp) + \lambda_n\exp(-2\lambda_n/\overline{E}_\perp) - (\lambda_p+\lambda_n-eV)\exp(-(\lambda_p+\lambda_n-eV)/\overline{E}_\perp)\right\} \end{aligned} \quad (17)$$

for $\lambda_s - \lambda_l \le eV \le \lambda_s, \lambda_l - \lambda_s$

$$\begin{aligned} D = {} & eVP + Q\left\{\exp(-2\lambda_s/\overline{E}_\perp) - \exp(-2(\lambda_s - eV)/\overline{E}_\perp)\right\} \\ & + \alpha\overline{E}_\perp\left\{\lambda_s\exp(-2\lambda_s/\overline{E}_\perp) - (\lambda_s - eV)\exp(-2(\lambda_s - eV)/\overline{E}_\perp)\right\}, \end{aligned} \quad (18)$$

for $\lambda_s \le eV \le \lambda_l - \lambda_s$

$$\begin{aligned} D = {} & \lambda_s P + Q\left\{\exp(-2\lambda_s/\overline{E}_\perp) - 1\right\}, \\ & + \alpha\overline{E}_\perp\left\{\lambda_s\exp(-2\lambda_s/\overline{E}_\perp)\right\} \end{aligned} \quad (19)$$

for $\lambda_l - \lambda_s \le eV \le \lambda_s$

$$D = eVP + Q\{2\exp(-(\lambda_p + \lambda_n - eV)/\overline{E}_\perp) - \exp(-2(\lambda_p - eV)/\overline{E}_\perp) - \exp(-2(\lambda_n - eV)/\overline{E}_\perp)\} + \alpha\overline{E}_\perp\{(\lambda_p + \lambda_n - eV)\exp(-(\lambda_p + \lambda_n - eV)/\overline{E}_\perp) - (\lambda_p - eV)\exp(-2(\lambda_p - eV)/\overline{E}_\perp) - (\lambda_n - eV)\exp(-2(\lambda_n - eV)/\overline{E}_\perp)\} \quad (20)$$

for $\lambda_s, \lambda_l - \lambda_s \le eV \le \lambda_l$

$$D = \lambda_s P + Q\{2\exp(-(\lambda_p + \lambda_n - eV)/\overline{E}_\perp) - \exp(-2(\lambda_l - eV)/\overline{E}_\perp) - 1\} + \alpha\overline{E}_\perp\{(\lambda_p + \lambda_n - eV)\exp(-(\lambda_p + \lambda_n - eV)/\overline{E}_\perp) - (\lambda_l - eV)\exp(-2(\lambda_l - eV)/\overline{E}_\perp)\} \quad (21)$$

for $\lambda_l \le eV \le \lambda_p - \lambda_n$

$$D = (\lambda_p + \lambda_n - eV)P + 2Q\{\exp(-(\lambda_p + \lambda_n - eV)/\overline{E}_\perp) - 1\} + \alpha\overline{E}_\perp\{(\lambda_p + \lambda_n - eV)\exp(-(\lambda_p + \lambda_n - eV)/\overline{E}_\perp)\}, \quad (22)$$

where

$$P = 1 + \alpha\overline{E}_\perp \quad (23)$$

$$Q = \frac{\overline{E}_\perp}{2}\{1 + 2\alpha\overline{E}_\perp\} \quad (24)$$

These are in general the expressions for piece-wise effective density of states for direct tunneling in a $p^+ - n^+$ diode of nonparabolic semiconductors. These piece-wise characteristics are joined together continuously to obtain the total characteristics valid for all regions so that smooth transition occurs while going from one region to another. The expression for total tunneling current for nonparabolic materials can be obtained from combining these and using (12).

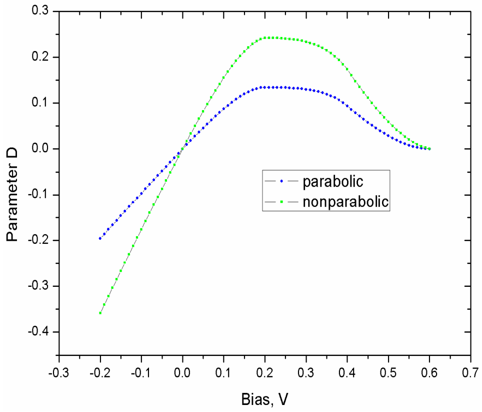

Fig. 1. Plot of Tunneling parameter D as a function of bias voltage in Volt applied along z-direction for the case of InAs ($E_g = 0.418\text{eV}$), for both the parabolic and non-parabolic energy bands to show the impact of nonparabolity on tunneling characteristics.

Substituting these values of P and Q into (17) through (22) we get the simplified expressions for D valid for wide band gap or extremely narrow band gap materials. Further, for semiconductors having parabolic energy band $\alpha \to 0$ and we have $P = 1$ and $Q = \overline{E}_\perp / 2$. Under these conditions (17) to (22) get converted into the well known expressions (17) to (22) of [7] which are extensively used in literature for tunneling device modeling.

III. Results and Discussions

The expressions of tunneling current derived in (12) together with (17) –(22) here have been used to calculate the tunneling parameter D of a degenerately doped tunneling semiconductor diode made of InAs material as a function of voltage applied across its terminals. The piece-wise characteristics are joined together continuously for obtaining the total characteristics. The following materials parameters are used [11]:

$E_g = 0.418\text{eV}, \Delta = 0.38\text{eV}, m_c = 0.026m_0, m_v = 0.45m_0,$

for the sake of numerical illustrations. We consider an abrupt junction with uniform doping in both *p* and *n*-sides. The electron concentrations in n and p sides are so chosen that $\lambda_n = 0.4$ and $\lambda_p = 0.2$. We have plotted in Fig. 1 the tunneling parameter D in case of InAs diode as a function of terminal voltage (in V) where curve labeled as 'nonparabolic' represents three-band model of Kane while the curve labeled as 'parabolic' exhibits the same dependence for isotropic parabolic energy bands. From the Fig. 1 it is clear that there is a significant modification of the tunneling characteristics in comparison with the result from conventional parabolic band model. The reason for this deviation is mainly due to the increased tunneling probability with low effective mass and increase density of states in nonparabolic band structure of InAs material. Beside the low band gap of InAs is also a factor of making the $\overline{E}_\perp$ higher thereby increased tunneling current in case of nonparabolic band model. It may also be noted that the differences of tunnel current between parabolic and nonparabolic models are more in the forward direction for small electric fields (or voltages) before the onset of usual drift current. This is due to the fact that the increased density of states on account of band nonparabolicity is more significant near high symmetry points in the Brilluin zone than that at higher energy levels. However in the reverse direction the density of band overlapping is more influential factor and hence rate of increase of current is more for nonparabolic case. Further for the sake of validation of the proposed model we made atomistic simulation evaluated by Density Functional Theory (DFT) coupled with Non-Equilibrium Green's Function (NEGF) formalism, as implemented within the Quantum Wise Atomistix Tool Kit (ATK) framework [12]. The band profile and the effective masses of electrons and holes in the InAs crystals are computed using DFT. These results, consistent with previous studies, serve as the basis for further analysis. Specifically, the 41 × 41 multiband Hamiltonian matrix and the corresponding nonorthogonal overlap matrix are taken out from ATK simulations, focusing on the conduction band minima (CBM) and valence band maxima (VBM) under relaxed conditions. These matrices are subsequently utilized to self-consistently explain the coupled Poisson and Schrödinger equations, a critical step for analyzing the InAs diode performance. We adopted the exchange and correlation interaction using the generalized gradient approximation (GGA) in the form of the Perdew-Burke-Ernzerhof (PBE) functional. The Monkhorst-Pack of 11 × 11 × 1 grid points is adopted for InAs models. Ballistic transport properties are calculated by coupling DFT with NEGF methods. The k-point meshes for the electrodes regions and central region are sampled with 16 × 1 × 216 and the double zeta polarized (DZP) basis set is used. The density mesh cut-off energy is set to 100 Hartee and the electron temperature is set at 300 K. The Fermi function of the anode and cathode are adjusted through bias and appropriate doping concentrations and the results are shown in Figure 2. We find a good agreement between the model and simulation results.

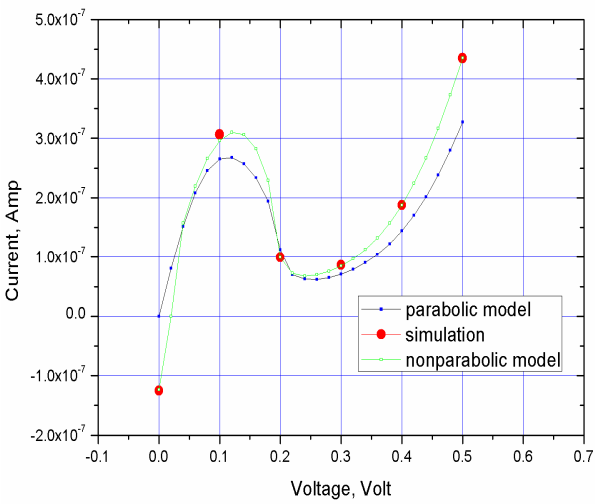

Fig. 2. Plot of Tunneling current as a function of bias applied along z-direction for InAs ($E_g = 0.418\text{eV}$), for both the parabolic and non-parabolic energy bands. Simulation results are indicated by red dots.

IV. CONCLUSIONS

In conclusion, we have presented a models incorporating realistic influence of the band nonparabolicity on the tunneling current in semiconducting tunnel diode. The calculations performed for the example of InAs show a significant modification to the I-V characteristics in comparison with the results obtained from the simple parabolic model. It should be pointed out that the generalized formulation developed here can be applicable for the determination of tunneling current of all types of *III –V* semiconducting diode based on narrow gap semiconductors. However, in order to keep the presentation short we have considered only InAs for the purpose of numerical illustrations and verifications. Further, validation of the proposed model is made with the results obtained from atomistic simulations and a strong consistency found with the model. We can conclude from the analysis that the band nonparabolicity has to be incorporated in modeling of tunneling diodes based on any narrow-gap materials. Finally, it should be stressed that the well known results of parabolic bands [10] applicable for wide gap materials diode can also be obtained from our generalized results under certain limiting conditions. This proves the accuracy and compatibility of our generalized model.

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