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New accurate approximation of the Einstein Relation for heavily-doped semiconductor devices

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ABSTRACT

The modern electronic devices have been scaled down significantly. The scaling rules would dictate higher doping concentrations which lead us to consider the degeneracy in the calculations. One of the semiconductor device quantities that would be impacted by considering the degeneracy is the Einstein Relation. The commonly used formula of Einstein Relation assumes that it is constant and independent of doping. The doping-independent Einstein Relation would cause serious inaccuracy in the calculations. This paper offers a *closed-form* solution for*doping-dependent* Einstein Relation. The proposed expression employs approximations of Fermi-Dirac Integrals (FDI) needed in the Einstein Relation. The quality and accuracy of the proposed approximations have been determined.

1. Introduction

Due to the lateral scaling of the electronic devices, the vertical dimensions need to be reduced as well. Consequently, the doping level will have to be increased. Thus the degeneracy comes into play in semiconductor device calculations. One of the significant quantities is the Einstein Relation which is the ratio of the diffusivity to the mobility. The form of the Einstein Relation that has been extensively used in textbooks and software is a *doping-independent* expression as follows:

$$\frac{D}{\mu} = \frac{kT}{q} \tag{1}$$

where D is the diffusion coefficient, μ is the mobility, k is the Boltzmann's constant, T is the Temperature, and q is the magnitude of electron charge. Landsberg noticed that the diffusivity-mobility ratio (DMR) for semiconductors that have degenerate electron concentration is determined by their band structure [1]. As a result of the variations in the band structure due to the variations in the electron concentration, the DMR increases as the electron concentration increases [2]. Furthermore, the degeneracy becomes a significant factor in determining the performance of the semiconductor devices at the device terminal and their switching speed [2]. Therefore, the form of Einstein Relation in Eq. (1) cannot be valid because it is independent of the electron concentration. Thus the Einstein Relation should be expressed in a form that is *doping-dependent*. Lindholm and Ayers evaluated the Einstein Relation shown in Eq. (1) and found that it could not be employed in Silicon semiconductor devices when the carrier density reached approximately 10^{18} cm^{-3} [3]. The principle of detailed balance, which states that the current density for electrons or holes in thermal equilibrium equals to zero, has been used to develop a generalised formula of Einstein Relation that turns to be *doping-dependent* as illustrated in Eq. (2) [3].

$$\frac{D_{n,p}}{\mu_{n,p}} = \frac{1}{q}\frac{n,p}{\frac{dn,p}{dE_f}} \tag{2}$$

where n the electron density, p is the hole density, and E_f is the Fermi-Level.

Fick's law states that the diffusive flux of particles at a local spatial point is proportional to the spatial gradient of the particle concentration. Because the electron concentration is given by the Fermi–Dirac integrals as shown in Eq. (3), Li and Lindholm developed a generalised expression of Einstein Relation as illustrated in Eq. (4) [4].

$$n = N_C F_{\frac{1}{2}}(\eta) \tag{3}$$

$$\frac{D}{\mu} = \frac{kT}{q}\frac{F_{\frac{1}{2}}(\eta)}{F_{-\frac{1}{2}}(\eta)} \tag{4}$$

where $N_C = 2\left(\frac{2\pi m_n^* kT}{h^2}\right)^{3/2}$ is the effective density of states in the

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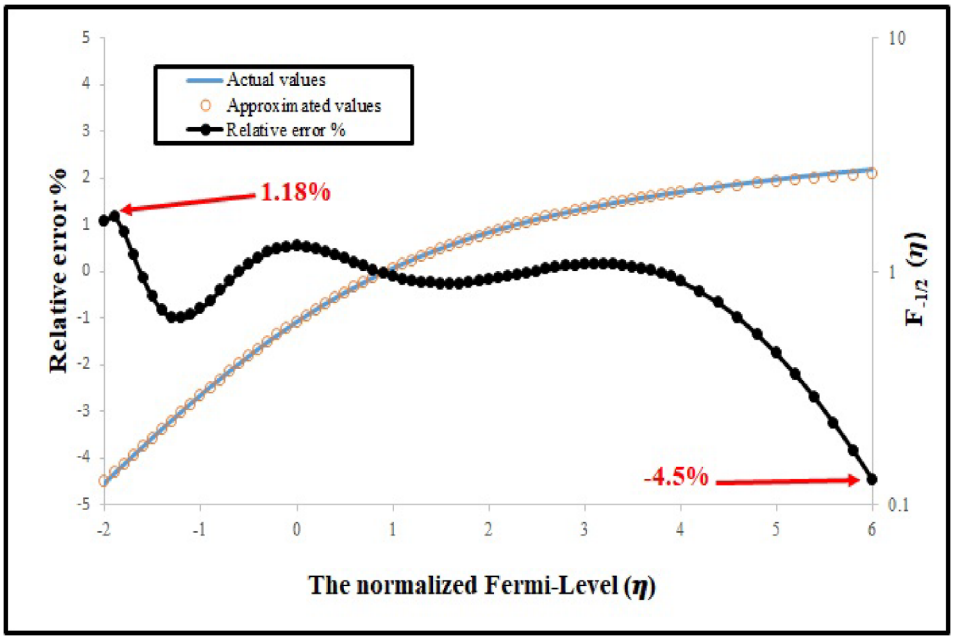

Fig. 1. Approximated and actual values of Fermi-Dirac negative half-integral.

conduction band, $\eta = \frac{-(E_C - E_f)}{kT}$ is the normalized Fermi-Level, and $F_{\frac{1}{2}}(\eta)$ and $F_{-\frac{1}{2}}(\eta)$ are the Fermi-Dirac Integrals of positive and negative half orders, respectively.

There is a physical reason behind the appearance of $\left(F_{\frac{1}{2}}(\eta)/F_{-\frac{1}{2}}(\eta)\right)$ factor in Eq. (4) other than the mathematical reason, which is the appearance of $\left(F_{\frac{1}{2}}(\eta)\right)$ in the calculation of the electron concentration as expressed in Eq. (3). The form of DMR in Eq. (1) is restricted to the Maxwell–Boltzmann statistics, which allow the electrons to occupy the same quantum state [5].If this restriction is removed, a large number of electrons with the same quantum state and high occupation probability at a low energy level will jump to higher energy empty state in order to accommodate Pauli's exclusion principle, which is the fundamental law in the Fermi- Dirac statistics [6]. As a result, the average kinetic energy of electron will be higher than the average value that resulted from the Maxwell–Boltzmann statistics, and the diffusivity of several electrons at given mobility will be more significant.

The actual values of Einstein Relation in Eq. (4) can be calculated using the tabulated functions of $F_{\frac{1}{2}}(\eta)$ and $F_{-\frac{1}{2}}(\eta)$ [7]. The method used to determine the accuracy when applying Eq. (1) compared to applying Eq. (4) is the Mean Absolute Error (MAE) which can be expressed as follows [8]:

$$MAE = \frac{1}{m}\sum_{i=1}^{m}\left|\frac{(Actual)_i - (Approximated)_i}{(Actual)_i}\right| \tag{5}$$

The Mean Absolute Error of using Eq. (1) compared to using Eq. (4) over the range of η values from -2 to $+4$ is 34.7%. In this paper, we propose a closed-form solution of *doping-dependent* Einstein Relation. The new expression takes into account the Fermi–Dirac Integrals (FDI) by approximating the negative half order of FDI $F_{-\frac{1}{2}}(\eta)$ and its integration $F_{\frac{1}{2}}(\eta)$. Approximation of the $F_{-\frac{1}{2}}(\eta)$ is being achieved by the Prony's method which is the same method we used in a previous work [9].

2. Prony's method

Prony published a method in 1795 which is a systematic way to approximate a function with a sum of a series of exponential functions [10]. The Prony's method has been used to approximate specific functions in the field of semiconductors such as the Two-Step Diffusion Profile [11].

The detailed steps of Prony's method are described [12]. The general form of Prony's function is expressed as shown in Eq. (6).

$$F(x_k) = \sum_{i=1}^{n} C_i \exp(a_i * x_k) = \sum_{i=1}^{n} C_i \mu_i^{x_k} \tag{6}$$

where $k = 1, 2, \ldots, N$ (number of equally spaced chosen points), C is the coefficient multiplying the exponential term in the function, a is an exponent, and $i = 1, 2, \ldots, n$ (number of terms in Prony's approximation).

One of the advantages of Prony's approach is the easiness with which the approximation function can be differentiated and integrated. This can be efficient in calculating the Einstein Relation.

3. Results and discussion

In this section, we present the approximation of $F_{-\frac{1}{2}}(\eta)$ and examine its quality by differentiating and integrating it. Then we employ the approximation and its first integrated function into the Einstein Relation equation.

3.1. Approximation of $F_{-\frac{1}{2}}(\eta)$

We developed an analytical expression of $F_{-\frac{1}{2}}(\eta)$ by using the Prony's method that we used in our previous work [9]. The expression of $F_{-\frac{1}{2}}(\eta)$ in the previous work showed inaccuracy (i.e., MAE = 2.15%) which leads to a significant error in the Einstein Relation (i.e., MAE = 1.94%). The proposed approximation is required to be accurate enough and simple enough to be employed in Einstein Relation. The proposed approximation is expressed as follows:

$$F_{-\frac{1}{2}}(\eta) = \sum_{i=1}^{4} A_i \exp(a_i * \eta) \tag{7}$$

where $A_1 = 4.6554, \quad a_1 = -0.03903.$
$A_2 = -6.5272, \quad a_2 = -0.28836$
$A_3 = 3.5205, \quad a_3 = -0.61818$
$A_4 = -1.0405, \quad a_4 = -0.82426$

As depicted in Fig. 1, the approximated values are quite close to the

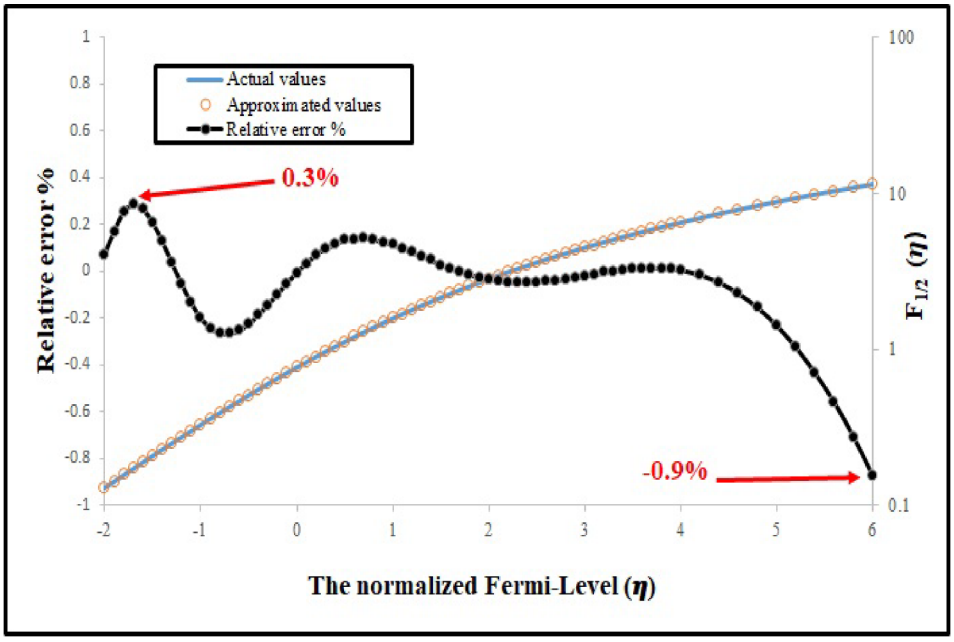

Fig. 2. Relative error of the approximation as a function of Fermi-level position.

actual values, tabulated by Blakemore [7]. The Mean Absolute Error denoted as MAE has been calculated to be MAE = 0.0031. Fig. 2 shows the relative error of the proposed approximation as a function of the normalized Fermi-Level.

3.2. Applicability of the approximation

The type of approximation we have obtained can be differentiated and integrated to examine the quality of the approximation. This can demonstrate its applicability in the calculations of Einstein Relation. In this section, the expression used for the approximation is being differentiated and integrated and their accuracies evaluated.

3.2.1. The differentiation

The differentiation of Fermi-Dirac Integrals follows the rule in (8).

$$F_{j-1}(x_k) = \frac{dF_j}{dx_k} \tag{8}$$

When differentiating $F_{-\frac{1}{2}}(\eta)$, one can get $F_{-\frac{3}{2}}(\eta)$ which is expressed as follows:

$$F_{-\frac{3}{2}}(\eta) = \sum_{i=1}^{4} B_i \exp(b_i{*}\eta) \tag{9}$$

where $B_1 = -0.1817$, $b_1 = -0.03903$.
$B_2 = 1.8822$, $b_2 = -0.28836$

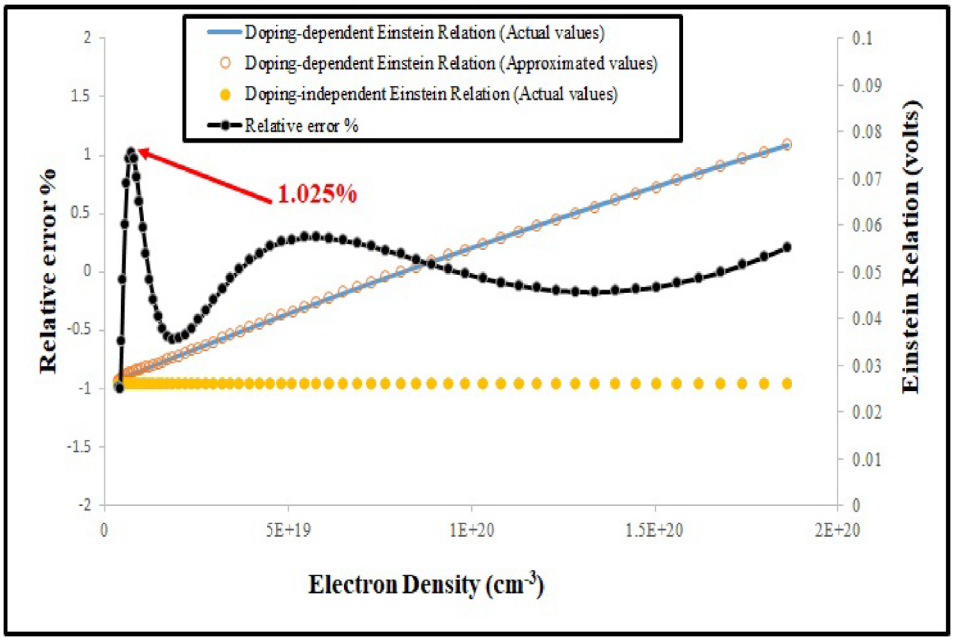

Fig. 3. The differentiated function $F_{-\frac{3}{2}}(\eta)$ compared to the Tabulated Blakemore's values.

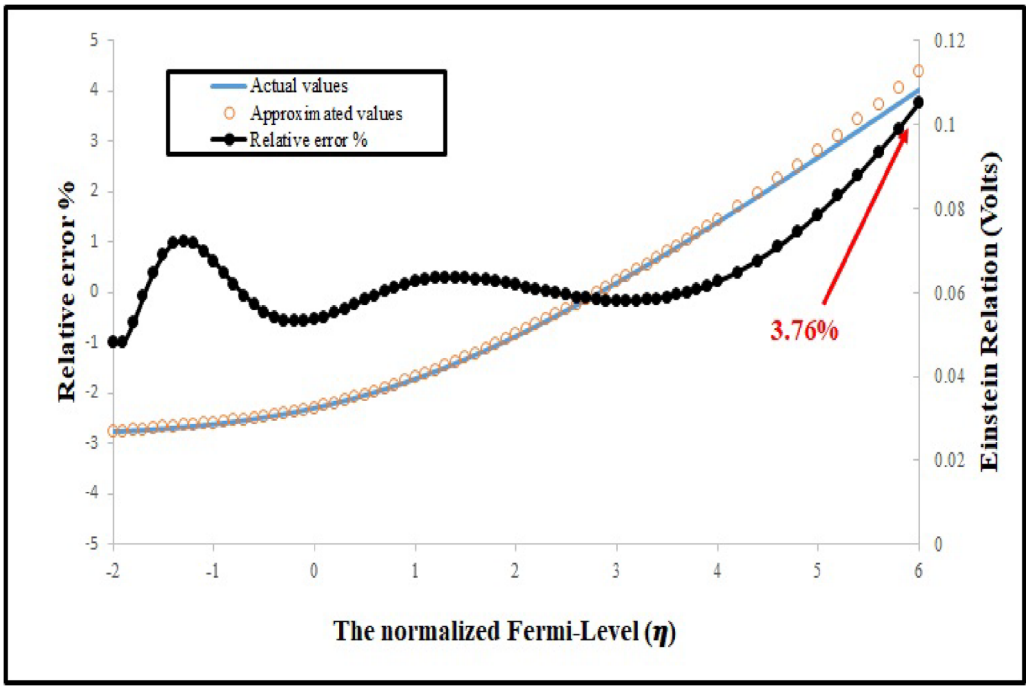

Fig. 4. The integrated and actual values of Fermi-Dirac positive half-integral $\left(+\frac{1}{2}\right)$.

$B_3 = -2.1763, \quad b_3 = -0.61818$
$B_4 = 0.8576, \quad b_4 = -0.82426$

Fig. 3 shows the differentiated function $F_{-\frac{3}{2}}(\eta)$ compared to the tabulated function of $F_{-\frac{3}{2}}(\eta)$ [7]. The Mean Absolute Error of the differentiated function is 1.82% which is smaller compared to the MAE of $F_{-\frac{3}{2}}(\eta)$ in our previous work [9].

3.2.2. The integration

The integration of Fermi-Dirac Integrals follows a rule similar to the differentiation's rule shown in Eq. (8) with a few modifications. Integrating the negative half-order of FDI will result in a function as follows:

$$\int F_{-\frac{1}{2}}(\eta)d\eta = F_{\frac{1}{2}}(\eta) \tag{10}$$

The integrated function is expressed as shown in Eq. (11) where the constant of the integration appears.

$$F_{\frac{1}{2}}(\eta) = \sum_{i=1}^{4} D_i \exp(d_i{}^*\eta) + K_1 \tag{11}$$

where $D_1 = -119.29, \quad d_1 = -0.03903.$
$D_2 = 22.636, \quad d_2 = -0.28836$
$D_3 = -5.6949, \quad d_3 = -0.61818$
$D_4 = 1.2623, \quad d_4 = -0.82426$

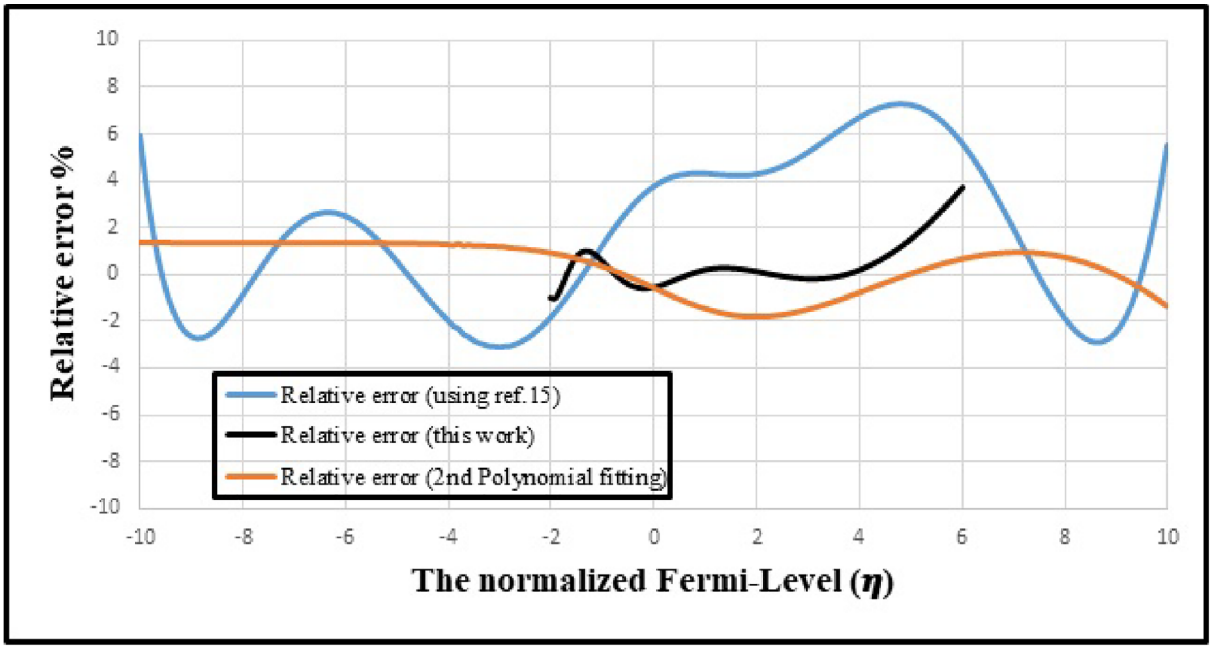

Fig. 5. The approximated values of *Doping-Dependent* Einstein Relation for different electron concentrations in Silicon where $N_C = 2.8 * 10^{19}$ cm^{-3} [13].

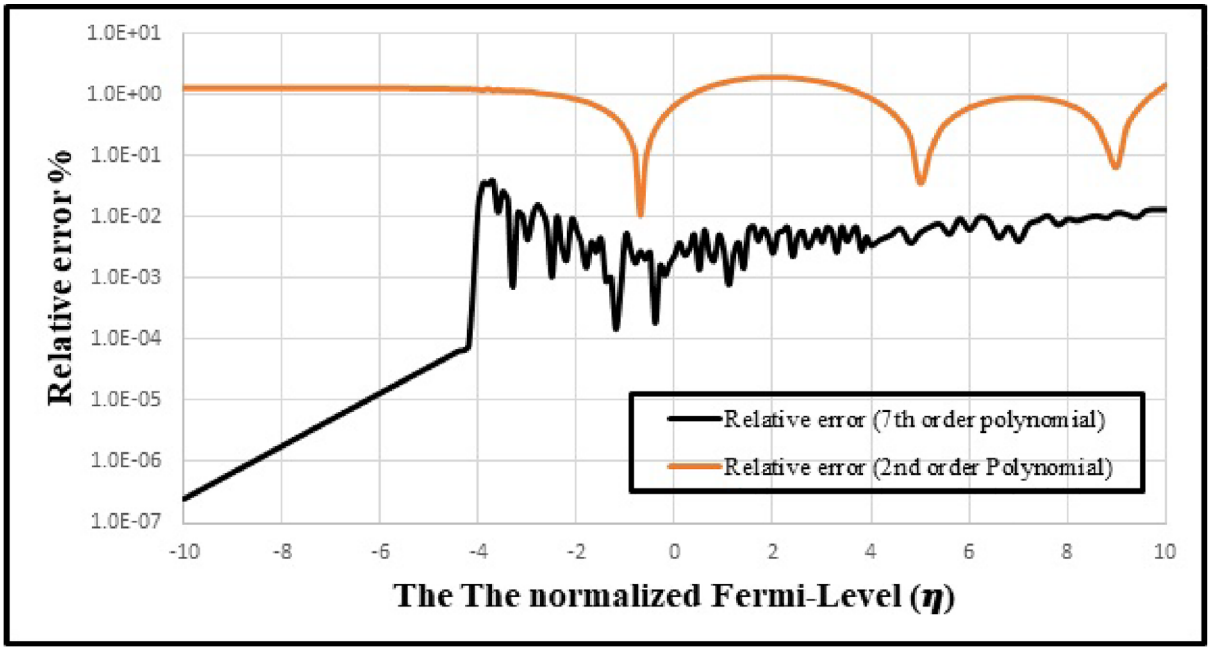

Fig. 6. Relative error of Einstein Relation calculated by Eqs. (4), (7) and (11) as a function of electron concentrations in Silicon where $N_C = 2.8 * 10^{19}$ cm^{-3} [13].

K_1 = Constant of the integration = 101.85.

The integrated function values are very close to the Blakemore's tabulated values as shown in Fig. 4 The Mean Absolute Error of the integrated function is $9.0893 * 10^{-4}$.

3.3. A new approximation of Einstein Relation

The DMR in Eq. (4) depends on the values of Fermi–Dirac Integrals for negative and positive half orders which leads the Einstein Relation that depends on the Fermi-Level position. Developing an expression of Einstein Relation that considers the degeneracy in the field of the semiconductor is required. Thus the degree of the accuracy that the approximations of FDI we have achieved is high enough to be employed in the expression for Einstein Relation.

The new approximation is employing Eqs. (7) and (11) in Eq. (4) to obtain approximated values of the Einstein Relation as illustrated in Fig. 5. The Mean Absolute Error of the approximated values is 0.31%. The relative error of the approximated values for different electron concentrations in Silicon, where $N_C = 2.8 * 10^{19}$ cm^{-3} [13], is shown in Fig. 6. The proposed expression of Einstein Relation can be employed in the textbooks and software modules instead of the Boltzmann's approximation since it is more accurate and simple enough to be implemented.

4. Conclusion

Einstein Relation is one of the important relationships in the analysis of semiconductor devices. The conventional Einstein Relation cannot be used in the modern semiconductor devices because it leads to considerable errors in the calculation of many device quantities. This paper proposed a new approximation of Einstein Relation, taking into consideration the degeneracy of the regions.

The new expression includes an approximation of the negative order of FDI and its integrated function. The Mean Absolute Error of the new Einstein Relation is 0.31%. The new approximation can be readily employed in the textbooks and software instead of the inadequate Boltzmann's approximation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, athttps://doi.org/10.1016/j.sse.2020.107869.

References

[1] Landsberg P. On the diffusion theory of rectification. Proc R Soc London Ser A Math Phys Sci 1952;213(1113):226–37.
[2] Ghatak KP, Bhattacharya S, De D. Einstein Relation in Compound Semiconductors and Their Nanostructures vol. 116. Springer Science & Business Media; 2008.
[3] Lindholm F, Ayers R. Generalized einstein relation for degenerate semiconductors. Proc IEEE 1968;56(3):371–2.
[4] San Li S, Lindholm F. Alternative formulation of generalized einstein relation for degenerate semiconductors. Proc IEEE 1968;56(7):1256–7.
[5] McKelvey JP. Solid state and semiconductor physics. Harper and Row.
[6] Jyegal J. Thermal energy diffusion incorporating generalized einstein relation for degenerate semiconductors. Appl Sci 2017;7(8):773.
[7] Blakemore JS. Semiconductor statistics. Courier Corporation; 2002.
[8] Chai T, Draxler RR. Root mean square error (rmse) or mean absolute error (mae)?–arguments against avoiding rmse in the literature. Geosci Model Develop 2014;7(3):1247–50.
[9] AlQurashi A, Selvakumar CR. A new approximation of fermi-dirac integrals of order

1/2 for degenerate semiconductor devices. Superlatt Microstruct 2018;118:308–18.
[10] De Prony BGR.Essai éxperimental et analytique: sur les lois de la dilatabilité de fluides élastique et sur celles de la force expansive de la vapeur de l'alkool, a différentes températures, Journal de l'école polytechnique 1795;1(22):24–76.
[11] Selvakumar CR. Approximations to two-step diffusion process by prony's method. Proc IEEE 1982;70(5):514–6.
[12] Hildebrand FB. Introduction to numerical analysis. Courier Corporation; 1987.
[13] Sze SM. Semiconductor devices: physics and technology. John wiley & sons; 2008.

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