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Exact analytical Model for the Evaluation of complex Einstein relation for disordered semiconductor with parabolic band

Abstract

The present manuscript exhibits a simple analytical model for the evaluation of the Einstein Relation(ER) of a disordered semiconductor having band-tail in energy spectrum as well as density-of-states (DOS) functions, through the presence of exponential and error functional behavior with respect to Normalized energy(E/η_e), demonstrates a complex functions, containing both real as well as imaginary terms of different Fermi-Integrals (FIs) and their derivatives. Their module provides an oscillatory function of $\left[\eta, \eta_e, k_B T\right]$. The total ER, over the entire energy regions ($\infty > E \geq -\infty$) of the band-tail curve is described as Cumulative Effects denoted a complex value. On the other band, the same ER for the positive and negative energy region of the band of the band-tail curves are known as the Distributive Effects in the band-zone and tail zone, respectively. The distributive effects are real and positive values. The Cumulative effect is a sum of the two distributive effects which has no mathematical justification. These contradictions are systematically explained with the proper justification in the manuscript.

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Introduction

In the context of current advanced technologies, reliable theories elucidating the electronic phenomena, such as created in devices, like homojunction, heterojunction, bipolar and field- effect decides, solar cells with degenerately doped and uniform structures are highly important in the field of solid-state electronics.[1–6] With the advent of MBE, MOCVD, PLL and other experimental techniques for the development of doped semiconductor materials;[7,8] the impact of energy spectrum and the density- of- states (DOS) functions are of paramount importance. It has been well established that the charge transport phenomenon in heavily doped disordered semiconductor are not fully characterized by the conventional current-continuity equation.[9,10] In a semiconductor, the doping concentration (Ni) that satisfies the relation for heavily doped case, $\left[\left(a_D . Ni^{1/3}\right) > 1.0\right]$, where a_D is the Bohr's radius of impurity state.[11] The calculations of the Fermi-energy (E_f) and the Fermi-Integrals (FIs) in heavily doped cases are emerging as a challenging area of research and development.[12] To the best of our knowledge, the study of the FIs in energy-spectrum and the density -of-states function with tail have not been made as yet in literatures.[10–14] It was reported recently15 that the FI of the (DOS) functions in a degenerately doped disordered semiconductor; showing band-tail in energy spectrum as well as in (DOS) functions, through the presence of exponential and error functional behavior with respect to (E/η_e); [where (E) is the electron-energy and (η_e), the impurity screening potential]; demonstrates a complex functions, containing both real as well as imaginary terms of different (FIs). Their module provides an oscillatory function and a phase angle of the functions of $\left[\eta, \eta_e, k_B T\right]$, where η is the reduced Fermi-energy, T is the absolute temperature and k_B is the Boltzmann constant.

Understanding the diffusion co-efficient (D) and the mobility (μ), one has attributed to considerable attention[3,10] due to its significance in device applications. Many attempts have been made to derive at a simple relation between (D) and (μ) ratio (i.e.DMR); also widely known as Einstein relation (ER) for the case of a disordered semiconductor. Possible simple model for (DMR) as suggested in literatures,[16–18] are thermodynamically, independent of scattering mechanisms. The diffusivity-mobility ratio was more accurate than the individual relationships for diffusivity and mobility.[19]

Among the various models, proposed for (DMR) the most important recent works that had been carried out by Roichman & Nessler,[3] Copuroglu & Mehmetoglu,[10] and Atanu Das & Arif Khan.[19] In,[3] the (ER), in the low density limit, is given by $D/\mu = k_B T/|e|$, calculated for a Gaussian density –of- States function (having not a tail),and also valid for organic semiconductors and few other amorphous semiconductors. Further, their model was valid for the energy distributions, smaller compared to the Fermi-energy (E_f), when the Fermi-Dirac distribution is approximated to a Boltzmann-distribution function. In[10] authors provided a simple analytical model for the evaluation of (ER) for disordered semiconductor with exponential distribution of the tail-states. The proposed analytical method was based on the binomial expansion of the (FD) distribution function (FD) or Fermi-functions and the square root of the energy band-states. In authors have calculated numerically the (ER), for heavily doped semiconductors exhibiting band gap narrowing.[19] The numerical calculations have shown that DMR are dependent on a host of semiconductor parameters including the temperature, carrier degeneracy etc.

In our earlier work,[20] we showed for the first time, the (DOS) functions, having tails through the presence of the exponential and error functions along with the tails in the energy spectrum. Their module provides an oscillatory function and phase angle of a function of $\eta = E_f / K_B T$, the reduced Fermi energy. Further, we made no alteration of the FD distribution as in[3] as well as binomial expansion of the FD.[10] Therefore, we might conclude that the above calculations of the DMR were not exact enough. An exact equation of the ER should be made without considering any approximation to the (DOS) tail calculations as well as the FD distribution functions. Taking the aforesaid issues into account, present study aims to provide an useful general analytical model, based on the complex Fermi-Integrals FIs derived in for the evaluations of the ER is a heavily doped semiconductor.[15]

Theory and basic formulae

In the limit of non-degeneracy, satisfying the relation $\left[0.02 \leq \left(a_D Ni^{1/3}\right) < 1.0\right]$,[11] the Einstein relation ER can be written as:[12]

$$D/\mu = K_B T/|e| \quad (1)$$

where, D denotes diffusivity of the semiconductor

T is the temperature in absolute degree, K_B is the Boltzmann constant and the electron mobility (μ), $|e|$ is the electron charge. Mukherjee[21,22] and Co-workers proposed a new generalized form of ER for the disordered semiconductor. This is also known as the Diffusivity-Mobility Ratio (DMR). This relation of DMR is valid for all scattering mechanisms and all the conditions of in homogeneity at uniform temperature. The ER/ DMR as defined for a non-degenerately doped semiconductor is given as the ratio:[12]

$$\frac{D_n}{\mu_n} = \frac{k_B T}{|e|}\left[F_{1/2}(\eta)/F_{-1/2}(\eta)\right] \quad (2)$$

where, $\eta = \frac{F_f}{k_B T}$, is the reduced Fermi-energy (E_f) and $F_j(\eta)$ is the Fermi-integrals (FIs) of order (j) with j=1/2 and j= -1/2. It might be noted that Eq. (1) can be obtained from Eq.(2) in the limit, when $\eta \to 0$.

Analytical evaluation of the general (er) of a degenerately doped dis-ordered semiconductor with band-tail

It has been seen earlier[15] that the (FIs) are complex in nature of degenerately doped disordered semiconductors. More over the derived energy-spectrum as well as the (DOS) functions possesses tails; containing error functions and the exponential function of (E/η_e). The parameter η_e reflected the width of the conduction band –tail. The tail generally extended within forbidden band.

Therefore, the new generalized form of DMR of a degenerately doped semiconductor with band-tail are given for: $\overline{N_D}$

$$(D/\mu)_{DT} = \frac{k_B T}{|e|}\left\{\overline{N}_D.\left(\frac{\partial \overline{N}D}{\partial \eta}\right)^{-1}\right\} \quad (3)$$

Where, $\overline{N}D$ has two parts: real ($\overline{ND_1}$) and imaginary ($\overline{ND_2}$) represent to

$$\overline{N}D = \overline{ND_1} + \overline{ND_2} \quad (4)$$

$$\left(\frac{\partial \overline{N_D}}{\partial \eta}\right)^{-1} = \left[\left(\frac{\partial \overline{N_{D_1}}}{\partial \eta}\right)^{-1} + \left(\frac{\partial \overline{N_{D_2}}}{\partial \eta}\right)^{-1}\right] \quad (5)$$

Following[15] we have:

$$\overline{\left[\frac{N_{D1}}{(k_B T)^{3/2}}\right]} = D_{\frac{1}{2}R}(\eta, \eta_e, k_B T) \quad (6)$$

= Real function of the degenerately doped (FI).

And

$$\overline{\left[\frac{N_{D2}}{(k_B T)^{3/2}}\right]} = i D_{\frac{1}{2}\text{Im}}(\eta, \eta_e, k_B T) \quad (7)$$

$$` = S_1 - \exp(-\eta).S_{2....} \quad (8)$$

Where

$D_{\frac{1}{2}\text{Im}}$ = Imaginary part of the degenerately doped (FI) with $i = \sqrt{-1}$.

From Eqn.4, we find: the following[15]

Total carrier concentration, $\overline{N}_D(\infty > E \geq -\infty)$,over the entire zone of energy (E) = [Partial carrier concentration, $\overline{\overline{N_{D_1}}}(\infty > E \geq 0_+)$ over the positive energy region or zone] + [partial carrier concentration, $\overline{\overline{N_{D_2}}}(0\_ > E \geq -\infty)$ over the negative energy region or zone] (9)

Now, $\overline{N}_D$ is the total FI over the entire energy (E) i.e $(\infty > E \geq -\infty) = [\overline{N_{D_1}}$ is the total FI over the positive energy(E) region i.e $(\infty > E \geq 0_+) + [\overline{N_{D_2}}$ is the total FI over the negative energy region i.e $(0\_ > E \geq -\infty)$] (10)

Differentiating Eqn. (10) with respect to η, on both side,

we find

$$\frac{\partial \overline{N}_D}{\partial \eta} = \frac{\partial \overline{N_{D_1}}}{\partial \eta} + \frac{\partial \overline{N_{D_2}}}{\partial \eta} \quad (11)$$

Therefore, from Eqns. (3)-(5), we have

$(D/\mu)_{DT}$ = Total (DMR)

$$= \frac{k_B T}{|e|}\left\{\overline{N}D.\left(\frac{\partial \overline{N}D}{\partial \eta}\right)^{-1}\right\}$$

$$= \frac{k_B T}{|e|}\left[\frac{\overline{N_{D_1}} + \overline{N_{D_2}}}{\frac{\partial \overline{N_{D_1}}}{\partial_\eta} + \frac{\partial \overline{N_{D_2}}}{\partial_\eta}}\right] \quad (12)$$

From Eqns (6), (7) and (12), we have

$$= \frac{k_B T}{|e|}.\left[\frac{\left(D_{\frac{1}{2}}R + iD_{\frac{1}{2}}\,\text{Im}\right)}{\frac{\partial D\frac{1}{2}R}{\partial \eta} + i\frac{\partial D\frac{1}{2}/\text{Im}}{\partial \eta}}\right] \quad (13)$$

Therefore, we find from Eqn.(13) that

$(D/\mu)_{DT}$ = Total (DMR) or total Einstein Relation (ER) of a degenerately doped with band-tailing conditions of a parabolic band semiconductor is a complex value.

$$= \frac{k_B T}{|e|}\left[A(\eta, \eta e, k_B T)\right] \quad (14)$$

Taking the module of $(D/\mu)_{DT}$, from Eqn(14), we may write:

$$\left|\left(\frac{D}{\mu}\right)DT\right| == \frac{k_B T}{|e|}\left\{\left[\sqrt{A^2(\eta, \eta e, k_B T) + B^2(\eta, \eta e, k_B T)}\right] * \text{Cos}\left[\alpha(\eta, \eta e, k_B T)\right]\right\} \quad (15)$$

with

$\alpha = \text{Tan}^{-1}\left[B(\eta, \eta e, k_B T)/A(\eta, \eta e, k_B T)\right]$ in radian It might be noticed that the unit of $\left|\left(\frac{D}{\mu}\right)DT\right|$ is volt and the angle α is determined in Radian.

From Eqns.(6), we find

$$[B]=\frac{k_BT}{|e|}\left[\overline{N_{D_1}}\cdot\left(\frac{\partial\overline{N_{D_1}}}{\partial\eta}\right)^{-1}\right]\quad \text{(valid for}(\infty > E \geq 0_+))\quad (16)$$

$$=\frac{k_BT}{|e|}\left[D\frac{1}{2}R.\left(\frac{\partial D\frac{1}{2}R}{\partial\eta}\right)^{-1}\right]$$

= a real and positive value.

Similarly, from Eqn.(7), we can show

$$[C]=\frac{k_BT}{|e|}\left[\overline{N_{D_2}}\cdot\left(\frac{\partial\overline{N_{D_1}}}{\partial\eta}\right)^{-1}\right]\quad \text{(valid over }(0_- > E \geq -\infty))$$

$$=\frac{k_BT}{|e|}\left[i\,D_{\frac{1}{2}}\mathrm{Im}.\left(\frac{\partial i\,D_{\frac{1}{2}}\mathrm{Im}}{\partial\eta}\right)^{-1}\right]$$

$$=\frac{k_BT}{|e|}\left[D_{\frac{1}{2}}\mathrm{Im}\left(\frac{\partial D_{\frac{1}{2}}\mathrm{Im}}{\partial\eta}\right)^{-1}\right]\quad (17)$$

= a real and positive value

Therefore, we designate $[B]=\frac{k_BT}{|e|}\left[\overline{N_{D_1}}\cdot\cdot\frac{\partial}{\partial\eta}(\overline{N_{D_2}})^{-1}\right]$ as the "Distributive effect" over the energy region $(\infty > E \geq 0_+)$ (i.e, the Band-zone (BZ))

Similarly, we may write:

$[C]=\frac{k_BT}{|e|}\left[\overline{N_{D_2}}\cdot\cdot\frac{\partial}{\partial\eta}(\overline{N_{D_2}})^{-1}\right]$ as the "Distributive effect" over the energy region (0_->E≥-∞) (i.e, the Tail-zone (TZ).

From Eqn.(14), we get the Total (DMR) as the "Cumulative Effect" over the entire energy region i.e, (∞>E≥ -∞), we may designate it as [A] and in general "A" is complex value.

Therefore, we can observe from Eqns, (13), (14), (16) and (17) that

[A] is a complex value [Cumulative Effect]

[B] is a Real and positive value [Distributive effect]

[C] is a Real and positive value [Distributive effect] (18)

Therefore, we can write Eqn(18) as

[A] ≠ [B] + [C] (19)

(i.e, Total "Cumulative Effect" ≠ the sum of the two "Distributive effect"

From Eqn.(19), we find that it might be a contradictory statement of a physical system, of degenerately Doped with band-tailing semiconductor.

The physics of the contradiction could be given as under

The Fermi-Dirac (FD) distribution for $\overline{ND_1}$, the energy(E) is valid from i.e ($\infty > E \geq 0_+$) (BZ)

The Fermi-Dirac (FD) distribution for $\overline{ND_2}$, the energy(E) is valid from i.e , ($0_- > E \geq -\infty$),(TZ)

In order to demonstrate the above (i.e Eqn (19)) phenomena, we have drawn a Figure 1 with different colors to distinguish the various effects.

(A) Total (DMR) covers the entire energy region i.e, (∞>E≥ -∞), covered by the solid band-tail curve: carriers are distributed as Yellow and Violet color region [Cumulative Effect].

(B)Total (DMR) over the positive energy region i.e, ($\infty > E \geq 0_+$) indicated by dotted curve: carriers are distributed in Yellow and Green color region, this zone is named as Band-zone (BZ) and the effect is [Distributive effect].

(C) Total (DMR) cover the negative energy region i.e, ($0_- > E \geq -\infty$),indicated by solid curve: that is extended in the band-tail region: here, carriers are distributed as violet color region, This zone is named as Tail-zone (TZ) and the effect is [Distributive effect].

Now, Eqn.(19) can also be proved from Figure 1 in the following way:

Figure 1 shows that the "Green color carriers lie outside the solid Band-Tail curve and within the dotted curve regions. Here, This carriers the physically do not exist. So, we designate Green color zone as the (FmZ) (i.e, forbidden mobility carrier zone) where the carrier mobility is imaginary.

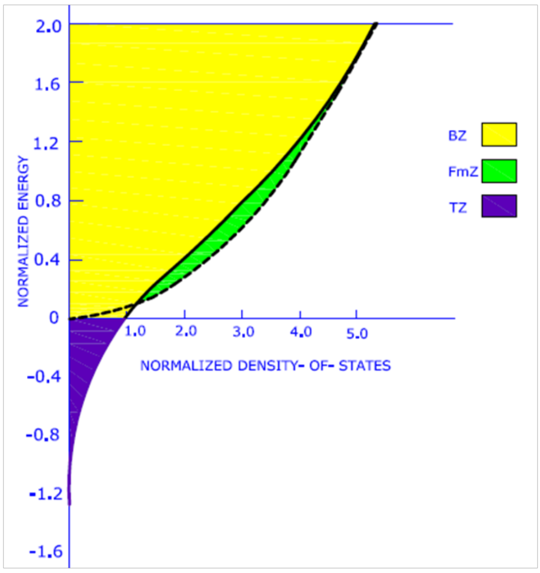

Figure 1 Color graphs are plotted for (a) Normalized Density –of- states (DOS) function against the normalized energy (E/ ηe); when the semiconductor is not heavily doped (Dotted line) [Yellow + Green].
(b) Normalized Density –of- states (DOS) function curve with Band-Tail, denoted by solid thick curve, against normalized energy(E/ ηe); [Yellow + Violet] color for the case, semiconductor is headily doped.

We have seen from above discussion that Eqn(19) is a contradiction, mathematically.

Also, in Figure 1, the Green color zone i.e (Fmz) is a contradiction of a physical system. Similarly, from physics point view, we have discussed above the existence of the contradiction based on the Fermi-Dirac distribution functions for $\overline{ND_1}$ valid for (∞>E≥0_+) and $\overline{ND_2}$ valid for (0_->E≥-∞).

Results and discussion

From Fig.1, we can draw the following points:-

1. Color graphs are plotted for normalized Density-of-States (DOS) function, (indicated by the dotted line), against normalized energy, when the semiconductor is not heavily doped. In this case, the mobile carriers are shown by [yellow+Green] colors region and the mobility of the carrier are [Real and positive value]. In this case, no-tail is present, as shown. This is called as the Band-zone (BZ).
2. When the semiconductor is degenerately doped, the normalized (DOS) function curve is denoted by the solid-thick curve, including the tail curve. In this case, Tail is present along with the (DOS) one. The mobile carriers are shown by [violet] color region. Here, the mobility is real and positive and the zone is named as Tail-zone (TZ).
3. But because of tailing, the [Green] color zone does not enclosed within the solid curve, rather enclosed within solid and dotted curves. So, in this region, carrier mobility do not exist physically, i.e., the carrier mobility is an imaginary value. Hence, we might denote it as the (FmZ) ≡ Forbidden mobility zone; i.e, the zone where the mobility could be imaginary

In Figure 2a, we have plotted the module of complex (DMR), $\left\|\left[(D/\mu)_{DT}(\eta,\ \eta_e,\ k_B T)\right]\right\|$ against (η), for (η_e) =0.01 eV and T=4.2K, using Eqns (13) and (14).

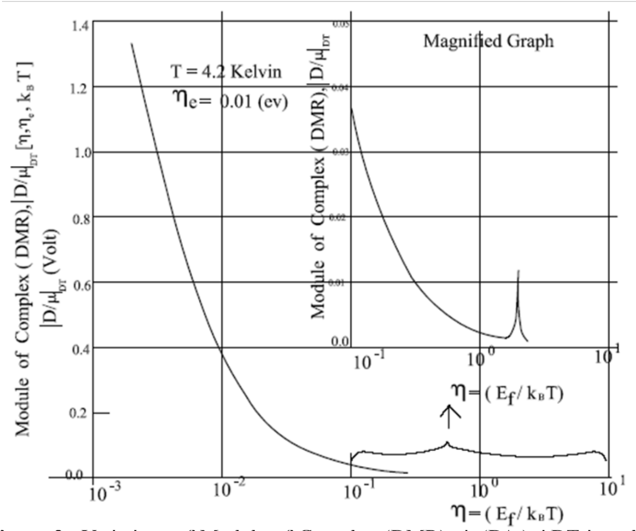

Figure 2a Variations of Module of Complex (DMR), ∣ (D/μ) ∣DT in volts against η with heavily doped case at T=4.2K and ηe= 0.01 eV; when η varies from 10-3 to 100.

For complex (DMR), the “Data” that required in Eqn.13, are provided from Table 1 for various values of η. Finally, in Table 2, , the module of [$\left|(D/\mu)\right|_{DT}(\eta,\ \eta_e,\ k_B T)\right|$ in volts] are calculated against η, as well as the phase angle, in $\left[\alpha(\eta,\ \eta_e,\ k_B T)\right]$ (radian). Thus “Data” obtained from Table 2, were plotted in Figure 2a for various values of η with η_e =0.01 eV and T=4.2K. Similar plots are made in Figure 2b, against η, with η_e =0.05 eV and T=4.2K in order to observe the effect of η_e on $|DMR|$.

Table 1 Comparative result of Fermi-Integral functions obtained by computer calculations

$\eta = E_f/K_B T$, $\eta_e = 0.01eV$, $T = 4.2K$	Real Functions		Imaginary Functions	
	$D_{\frac{1}{2}R}(\eta,\eta e,K_B T)$	$\frac{\partial}{\partial n}\left[D_{\frac{1}{2}R}(\eta,\eta e,K_B T)\right]$	$i\ D_{\frac{1}{2}Im}\left[(\eta,\eta e,K_B T)\right]$	$\frac{\partial}{\partial n}\left[D_{\frac{1}{2}Im}(\eta,\eta e,K_B T)\right]$
1.0×10⁻³	0.036397	0.0008227	14.505143	0.0030341
5.0×10⁻³	0.032393	-0.003395	14.501133	0.00672
1.0×10⁻²	0.027335	-0.0087601	14.496171	0.0112797
5.0×10⁻²	-0.013054	-0.0537988	14.458448	0.0458812
1.0×10⁻¹	-0.0742894	-0.1159625	14.416017	0.0846497
5.0×10⁻¹	-0.8165663	-0.8913279	14.224525	0.2549007
1.0×10⁰	-2.4426024	-2.5690713	14.198433	0.2681601

Our results, $\left|(D/\mu)\right|$ against η are of decreasing trend unlike [3, 7, and 16] in magnitude. Also, our report which was a complex value, having phase angle $\alpha(\eta,\ \eta_e,\ k_B T)$ and module values $\left|(D/\mu)\right|_{DT}$ against η; their results were only and positive values [3,10, 19].

In Figure 3, we plotted the phase angle, $\alpha(\eta,\ \eta_e,\ k_B T)$ against η; when η_e =0.01 eV and T=4.2K. The Eqn.(15) was used for calculating $\alpha(\eta,\ \eta_e,\ k_B T)$ in Table 2. It could be inferred from Figure 3, that at η≈ 1.0×10^{-3}, the value of $\alpha(\eta,\eta_e,k_B T)$ reached to minimum value of ≈ -0.05 radian. Eqn.(15) concluded that (i) when $\left|\alpha(\eta,\ \eta_e,\ k_B T)\right| \to 0$, the imaginary component, $\left|B(\eta,\ \eta_e,\ k_B T)\right| \to 0$ | i.e vanishes.

(ii) When $\left|\alpha(\eta,\ \eta_e,\ k_B T)\right| \to$ maximum, the real component of DMR vanished. This corresponds to the value of η→1.0. In the intermediate values of η between 1.0×10^{-3} to 1.0, the angle $\alpha(\eta,\ \eta_e,\ k_B T)$ has definite value, as indicated in Figure 3.

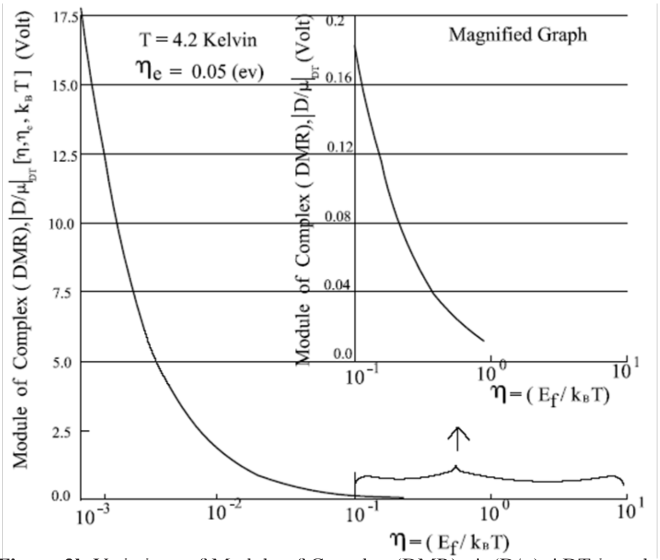

Figure 2b Variations of Module of Complex (DMR), | (D/μ) | DT in volts against η with heavily doped case at T=4.2K and ηe= 0.05 eV; when η varies from 10-3 to 100.

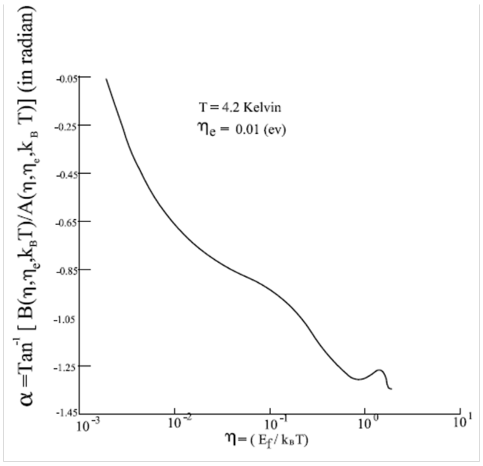

Figure 3 Variations of the phase angle, α (η, ηe, kBT) (in Rad) between real and imaginary parts of complex |[(D/μ)]_DT | (η, ηe, kBT) in volt against η for ηe= 0.01 eV and T=4.2K.

Table 2 Comparative values of complex (Einstein ratio) of a degenerately doped semiconductor with band tail

$\eta = E_f/K_BT$ $\eta_e = 0.01\text{eV}$ $T = 4.2\text{K}$	$\left\|\left(\frac{D}{\mu}\right)DT\right\|(\eta, \eta e, K_BT)$ in volt	$\alpha(\eta, \eta e, K_BT)$ in Rad.
	Computed from data	**Given in table-1**
1.0×10^{-3}	1.6737246	0.26228808
5.0×10^{-3}	0.697946447	-0.471937
1.0×10^{-2}	0.368183658	-0.662195371
5.0×10^{-2}	0.074175186	-0.863603178
1.0×10^{-1}	0.036423126	-0.935081707
5.0×10^{-1}	0.005575	-1.2349097
1.0×10^{0}	0.002023205	-1.296427157

Conclusion

We have demonstrated the effect of disordered density-of-states (DOS) functions on the complex Diffusivity-Mobility Ratio (DMR) for a semiconductor. The approach is general and relies on the energy spectrum and its corresponding (DOS) function having tails. The newly derived analytical expression for the complex (DMR) were based on both real and imaginary (FIs) and their derivatives for a disordered semiconductors. It was shown analytically via the phase angle, $\alpha(\eta, \eta_e, k_BT)$, when the real and imaginary components were vanished. In the intermediate values of η between 1.0×10^{-3} to 1.0, the phase angle α has some definite value, showing the existence of comples(DMR). Figure 2b shows that for the higher degree of heavy doping with $\eta_e = 0.05$ eV, the magnitude of $\left|(D/\mu)\right|_{DT}(\eta, \eta_e, k_BT)$ is higher than Figure 2a, where $\eta_e = 0.01$ eV.

Acknowledgments

None.

Conflicts of interest

Authors declare that there is no conflict of interests.

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