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J–V characteristics of GaN containing traps at several discrete energy levels

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A B S T R A C T

Mathematical modeling is presented to calculate the space charge limited current (SCLC) in a semiconductor containing traps at several discrete single energy levels. The effect of trap depths and trap densities is investigated in detail. If the difference in the trap energies is large, the J–V curves show humps as many as the number of trap levels. Each hump can be used to calculate a value of trap concentration. This trap concentration is the sum of all the traps at this and deeper energy levels. Accurate trap densities can only be obtained by fitting theoretical curve to the experimental J–V characteristics. The theory is compared with the experimental data taken from the literature. A very good agreement between theory and experiment is found.

1. Introduction

In disorder materials like polymers and amorphous semiconductors the traps are generally distributed exponentially in the energy space [1–5]. In crystalline materials such as Si, GaAs and GaN the traps are located at discrete energy levels and the separation of trap levels in energy space varies from semiconductor to semiconductor [6–8]. The traps affect the current flow in these materials. As the current determines the device performance it is very important to investigate the trap densities and their distribution for designing the devices. The study of space charge limited currents (SCLC) in these materials provides a powerful method to determine both the trap depths and trap concentrations [6–8] and their effect on current flow. The investigations of traps by SCLC studies have been made by several authors [6–8]. In general GaN has been observed to contain traps, distributed in two single energy levels [7]. Analytical expressions for the J–V curves of a sample containing traps, confined only in a single level are given in Refs. [2,3]. These analytical expressions use approximations, which hold only at very low voltages [9]. In the past regional approximations were used to analyze the SCL J–V curves and to obtain the information about trap energies and trap concentrations [6,8]. The importance and limitations of the regional approximation method are discussed later in Section 4. In Section 4 it is shown that the regional approximations have very limited value and cannot be used to reproduce experimental curves with realistic values of material parameters. Shen et al. [7] studied the J–V characteristics of GaN Schottky diodes that show two humps [7]. They assumed that the first hump occurs due to the filling of the traps which exist at the deepest energy level and the voltage at which hump starts was considered to be the trap filled limit. Similarly the second hump was attributed to the trap filled limit of the traps existing at the second shallow energy level. The relation between trap filled limit voltage (V_{TFL}) and trap concentration is given by the following equation [9]:

$$V_{TFL} = 0.5\frac{qHd^2}{\varepsilon\varepsilon_0}, \tag{1}$$

where ε and ε_0 are respectively the dielectric constant and permittivity of free space, d is the sample thickness and H is the density of traps. Shen et al. [7] used Eq. (1) and determined the trap concentrations $H_1 = 10^{15}\ \mathrm{cm}^{-3}$ and $H_2 = 3.6 \times 10^{15}\ \mathrm{cm}^{-3}$ corresponding to first and second humps respectively. The value of trap concentrations corresponding to each hump is an approximate value and to get the correct values of trap densities at each level new mathematical modeling is required to analyze the J–V characteristics. We now present a mathematical modeling for J–V characteristics of a semiconductor diode containing traps, existing at discrete energy levels. Our modeling leads to the accurate determination of trap concentrations at the respective energy levels.

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Nomenclature

ε	dielectric constant of the material	V	voltage (V)
ε_0	permittivity of the free space	p	free charge carrier density (cm^{-3})
q	electronic charge (C)	p_t	trapped charge carrier density (cm^{-3})
μ	mobility of charge carriers ($cm^2\,V^{-1}\,s^{-1}$)	N_v	effective density of traps (cm^{-3})
k	Boltzmann's constant ($eV\,K^{-1}$)	F	electric field (V/cm)
T	absolute temperature (K)	E_t	trap energy (eV)
H	density of traps (cm^{-3})	E_f	difference of Fermi level from the conduction band (eV)
J	current density (A/cm^2)	δ	Dirac-Delta function

2. Theory

For the purpose of illustration we consider the case of a sample where traps are distributed in three single energy levels only. The case can be extended to any number of trap levels quite easily. Let H_a, H_b and H_c be the concentrations of traps existing at the single levels of energies E_{t1}, E_{t2} and E_{t3} respectively. The continuity and Poisson's equations for such a sample are given below [1–3]

$$J = q\mu p(x)F(x), \tag{2}$$

and

$$\frac{dF(x)}{dx} = \frac{q}{\varepsilon\varepsilon_0}(p(x) + p_t(x)). \tag{3}$$

Here μ is the carrier mobility, $p(x)$ is free carrier density, $p_t(x)$ is trapped carrier density and $F(x)$ is the electric field. The trap distribution will now be given by,

$$h(E) = H_a\delta(E - E_{t1}) + H_b\delta(E - E_{t2}) + H_c\delta(E - E_{t3}), \tag{4}$$

where δ is Dirac-delta function. The number of filled traps at any voltage can be obtained by the integration of Eq. (4)

$$p_t(x) = \int_{-\infty}^{\infty} \frac{(H_a\delta(E - E_{t1}) + H_b\delta(E - E_{t2}) + H_c\delta(E - E_{t3}))}{1 + \exp\left(\frac{E_f(x) - E}{kT}\right)} dE. \tag{5}$$

The $E_f(x)$ is the difference between conduction band and Fermi level. $E_f(x)$ is a function of x because of conduction band bending. Eq. (5) can be simplified to

$$p_t(x) \approx \frac{H_a}{1 + \exp\left(\frac{E_f(x) - E_{t1}}{kT}\right)} + \frac{H_b}{1 + \exp\left(\frac{E_f(x) - E_{t2}}{kT}\right)} + \frac{H_c}{1 + \exp\left(\frac{E_f(x) - E_{t3}}{kT}\right)}, \tag{6}$$

or

$$p_t(x) \approx \frac{H_a}{1 + \frac{H_a\theta_1}{p(x)}} + \frac{H_b}{1 + \frac{H_b\theta_2}{p(x)}} + \frac{H_c}{1 + \frac{H_c\theta_3}{p(x)}}, \tag{7}$$

where

$$\theta_1 = \frac{N_v}{H_a}\exp\left(\frac{-E_{t1}}{kT}\right), \tag{8a}$$

$$\theta_2 = \frac{N_v}{H_b}\exp\left(\frac{-E_{t2}}{kT}\right), \tag{8b}$$

$$\theta_3 = \frac{N_v}{H_c}\exp\left(\frac{-E_{t3}}{kT}\right), \tag{8c}$$

and

$$p(x) = N_v\exp\left(\frac{-E_f}{kT}\right). \tag{8d}$$

Now the integration of Eq. (3) would give

$$\int_0^d dx = \frac{\varepsilon\varepsilon_0}{q}\int_{F(0)}^{F(d)} \frac{dF}{p(x) + \frac{H_a}{1+\frac{H_a\theta_1}{p(x)}} + \frac{H_b}{1+\frac{H_b\theta_2}{p(x)}} + \frac{H_c}{1+\frac{H_c\theta_3}{p(x)}}}, \tag{9}$$

where $F(0)$ and $F(d)$ are the electric fields at the injecting contact ($x = 0$) and at the exit contact ($x = d$) respectively. $F(0)$ can be obtained from the following condition of continuity:

$$J = q\mu p(0)F(0). \tag{10}$$

Eq. (9) cannot be integrated analytically. Therefore we wrote a numerical program where Eq. (9) was solved numerically to obtain $F(x)$ for a given current J. The voltage V was obtained by integrating $F(x)$ over the thickness of the film. The procedure is repeated for every J and J–V characteristics are obtained [10].

3. Results and discussion

The dash double dotted curve in Fig. 1 represents the well known Mott's V^2 law [11]. Dashed curve represents the J–V curve calculated using the theory given in Section 2 for $E_{t1} = 0.9$ eV,

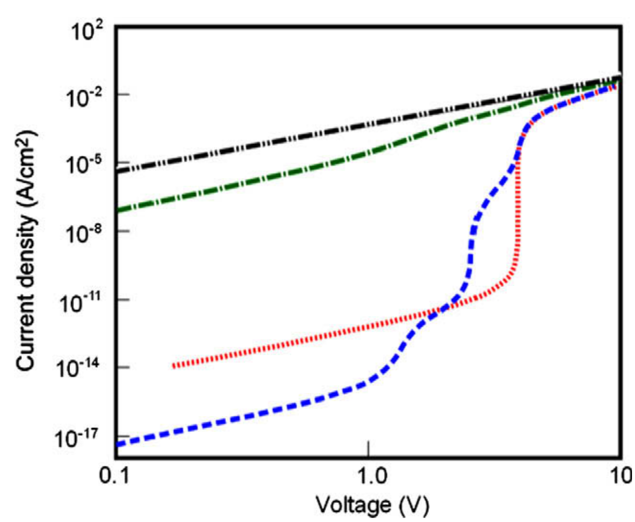

Fig. 1. Calculated J–V characteristics using theory of Section 2 for three single level traps with trap depths E_{t1}, E_{t2} and E_{t3} with the corresponding trap concentrations H_a, H_b and H_c. Dash double dotted curve represents the Mott's V^2 law. Dashed curve represents the case of $E_{t1} = 0.9$ eV, $E_{t2} = 0.7$ eV, $E_{t3} = 0.4$ eV with $H_a = H_b = H_c$ =! 4.0×10^{15} cm^{-3}. The dotted curve is for the single level trap with trap energy equal to 0.7 eV and trap density equals to $H_a + H_b + H_c = 1.2 \times 10^{16}$ cm^{-3}. Dash dotted curve is for the case of $E_{t1} = 0.3$ eV, $E_{t2} = 0.2$ eV and $E_{t3} = 0.1$ eV and the values of the trap concentrations are again the same as for the dashed curve. The values of other parameters used are $\varepsilon = 10$, $\mu = 5 \times 10^{-5}$ $cm^2\,V^{-1}\,s^{-1}$ and $N_v = 10^{19}$ cm^{-3}.

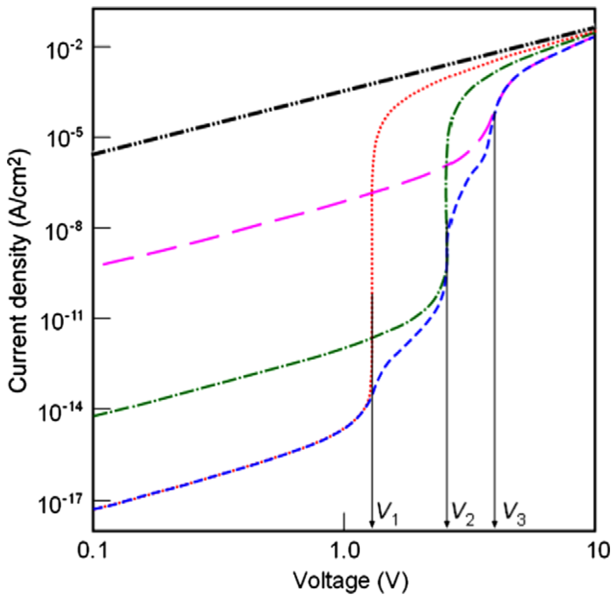

Fig. 2. Calculated J–V curves using the theory of Section 2 are plotted for three single level traps. The short dash curve in this figure is the same as the dashed curve in Fig. 1. For the dotted curve and for the first hump, trap energy (E_t) = 0.9 eV and $H_a = 4 \times 10^{15}$ cm^{-3}. For the dash dotted curve the trap concentration used is $H_a + H_b = 8 \times 10^{15}$ cm^{-3}, and E_t = 0.7 eV. For long dashed curve E_t = 0.4 eV and the trap concentration used is $H_a + H_b + H_c = 1.2 \times 10^{16}$ cm^{-3}. Dash double dotted curve is the Mott's curve as before.

E_{t2} = 0.7 eV, E_{t3} = 0.4 eV and the corresponding trap densities are same, i.e. $H_a = H_b = H_c = 4 \times 10^{15}$ cm^{-3}. The values of rest of the parameters are given in the caption of Fig. 1. The trap depths for the three levels are sufficiently different from each other. Three humps corresponding to the three trap levels can be seen clearly. The low voltage part of dashed curve is approximately a straight line. It is parallel to the Mott's V^2 law but considerably displaced from it as discussed in the literature [2].

We now derive the condition under which humps are observed in the J–V curves. Dash dotted curve in Fig. 1 represents the J–V curve for E_{t1} = 0.3 eV, E_{t2} = 0.2 eV, E_{t3} = 0.1 eV and their corresponding trap densities are the same as in case of dashed curve. Calculations for intermediate difference in the three energy levels were also made (not shown here). It is found that as the difference in the trap energies decreases, the heights of the humps decrease. For a small difference of 0.1 eV in the trap energies the humps seem to disappear (dash dotted curve). However a shallow hump is observed at high voltages. Therefore the observation of the humps in the J–V characteristics depends on the separation of the trap energy levels. For large difference in the trap energies the humps will be observed as many as the number of trap energy levels. For very low difference of trap energies only one hump will be observed in the J–V characteristics. If the difference in the trap energy is reduced to zero all the traps exists at one single level. However the density of the traps will be the sum of the trap densities in the individual energy level. The dotted curve represents the case of a sample containing traps in single level of energy equal to 0.7 eV and trap density equal to $H_a + H_b + H_c = 1.2 \times 10^{16}$ cm^{-3}. As expected only one hump in the J–V characteristic is observed. The low voltage straight line portion of the curve depends on the trap depth.

We now discuss Fig. 2 and show that if the positions of humps are considered to be the trap filled limit for traps at the corresponding energy level as assumed by Shen et al. [7] and Eq. (1) is used to calculate the trap concentration, wrong values of the trap concentrations are obtained. The error arises because of interaction between the two sets of traps. It is difficult to determine the exact position of trap filled limit for each hump from the observed curves. Following by Shen et al. the position of the first hump may nearly give the correct value of trap density at deepest trap energy level but the trap concentration determined from the second hump will fail to give the correct trap density at the second energy level. Similarly the trap densities determined from the subsequent hump would not give the correct density of traps at third energy level. The mathematical simulation presented here explains these discrepancies and gives the correct values of trap densities at each energy level.

Fig. 2 gives interesting results. The description of each curve is given in the caption of the figure. The dotted curve shows that the hump in the short dashed curve is the same as the hump due to trap filled limit in the dotted curve. The low voltage straight line portion of the short dashed and the dotted curves coincide. Their positions depend uniquely on trap depths. The low voltage curve is approximately parallel to the Mott's V^2 law as predicated by the approximate single level trap theory [2]. The dash dotted curve is calculated using the single level theory but effective trap concentration is $H_a + H_b$. The trap depth used in the calculations is 0.7 eV lower than that for the dotted curve. The low voltage straight line part of the curve is therefore higher and again is parallel to the Mott's V^2 law. The most important new result is that the second hump is not only due to traps at the second level but due to the sum of the traps at the first and second levels. The long dashed curve is calculated for the single level traps with the trap concentration $H_a + H_b + H_c$. The energy used for this curve is still smaller E_t = 0.4 eV. The low voltage part of the curve is therefore the highest among the three curves. It is also parallel to the Mott's V^2 law (dash double dotted curve). All the curves approach Mott's law at higher voltages asymptotically. The reason for this is given in Ref. [9]. V_1, V_2 and V_3 in Fig. 2 represent the trap filled limit for the cases represented by dotted, dash dotted and long dashed curves respectively. The most important conclusion drawn from these calculations is that the position of any one hump in the J–V curve does not give the correct trap density at the level corresponding to the positions of the humps as erroneously assumed by earlier workers [3,6,7]. In fact the number of traps determined from the position of the hump and using Eq. (1) is the sum of all the traps that exist at that level and deeper levels. It is therefore clear that the final hump can be used to determine the total concentration of the traps in the whole sample. However the correct trap densities and the trap energies can be obtained only by curve fitting using the theory given in Section 2.

To elucidate certain features of the J–V curves we have plotted the curves for four samples in Fig. 3. The solid J–V curve of Fig. 3 is for the sample 1, which contains traps at three different energy levels E_{t1} = 0.9 eV, E_{t2} = 0.7 eV and E_{t3} = 0.4 eV. The concentration of traps at each level is the same, i.e. 4×10^{15} cm^{-3}. This curve is identical to the dashed curve in Fig. 1. The dotted curve is for the sample 2, which contain $H_a = 4 \times 10^{15}$ cm^{-3} traps. Long dashed curve is for the sample 3, which contains traps with density two times of H_a. Finally short dashed curve is for the sample 4 containing $3 \times H_a$ traps. The trap depth in the samples 2–4 is equal to 0.9 eV. Dash double dotted curve is the Mott's curve. The new features of the curves in Fig. 3 are given below.

(i) Just after the trap filled limits, the distance of the dotted curve from the Mott's curve is the smallest and in the short dashed curve is the largest. This is because in the first case the $p_t = H_a$ is small and therefore its contribution to electric field in Poisson's equation is also small. It is due to this electric field that the J–V curve does not meet immediately the Motts V^2 law even though all the traps are filled. On the other hand the contribution of trapped carriers to electric field is large in the sample 4 containing three times as many traps.

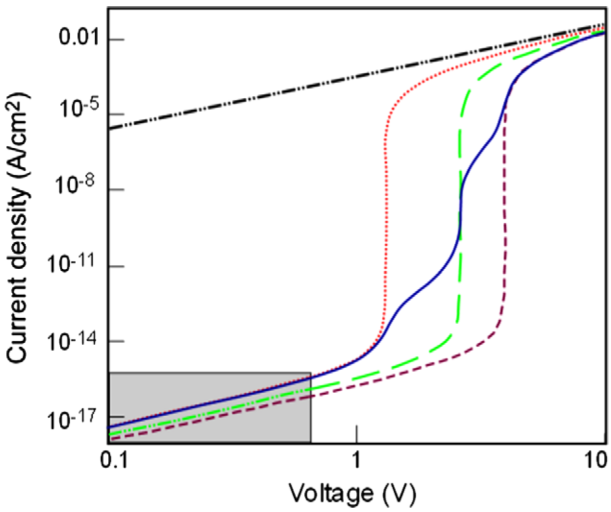

Fig. 3. Space charge limited current of four samples. Solid line is for sample 1 which contains three trap levels at E_{t1} = 0.9 eV, E_{t2} = 0.7 eV, E_{t3} = 0.4 eV. The trap concentrations at all these levels are same, i.e. 4×10^{15} cm^{-3}. The dotted curve is for sample 2 which contains the traps at E_{t1} = 0.9 eV and $H_a = 4 \times 10^{15}$ cm^{-3}. Long dashed curve is for sample 3 and contains traps twice of that in sample 2, i.e. $2 \times H_a$. Finally the short dashed curve is for sample 4 which contains three times traps, i.e. $3 \times H_a$. Dash double dotted curve is the Mott's curve as same in Fig. 2.

(ii) The heights of the humps after trap filled limit are weakly dependent on the concentration of traps.

(iii) At low voltages the J–V curves depend strongly on the trap depths but weakly on the trap concentrations. The low voltages plots in Fig. 3 are shown within the shaded area. The dependence on the energy and trap concentration is given by,

$$J_{Mott} - j_{Ha} = J_{Mott} \cdot (1 - \theta_1), \tag{11}$$

where θ1 is defined earlier. It has been verified by numerical calculations that Eq. (11) is valid for these low voltages plots. The conclusion we can draw from Fig. 2 and 3 is that the J–V curves provide a powerful method to determine trap concentrations and trap depths in the semi-crystalline semiconductors.

The above results can be understood more clearly from Fig. 4. The Fermi levels $E_f(V_1)$, $E_f(V_2)$ and $E_f(V_3)$ corresponding to V_1, V_2 and V_3 have just been plotted schematically for better understanding. At the voltage V_1 only traps H_a exiting at 0.9 eV are filled. Therefore the number of traps calculated from the position V_1 is correct that exists at E_{t1} and are shown by the lowest filled circle.

The height of the first hump in Fig. 2 is considerably suppressed because of the partial filling of the traps H_b and H_c located at 0.7

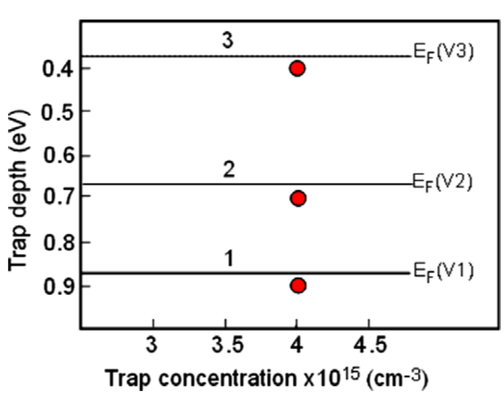

Fig. 4. Trap depths vs. trap concentrations are shown by filled circles. Horizontal lines show schematic Fermi levels for the trap filled limits V_1, V_2 and V_3 for each set of traps.

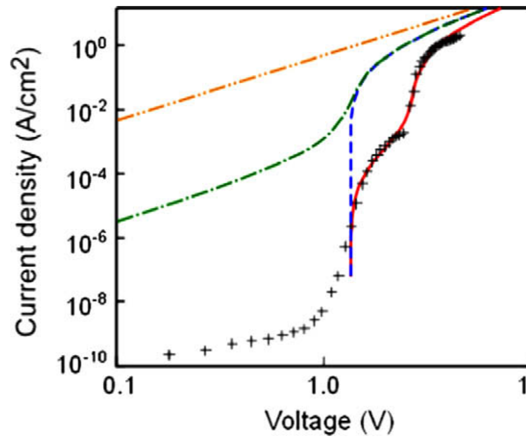

Fig. 5. The experimental data [7] shown by '+' symbols is compared with our theory (solid line). The value of H_a, H_b, E_{t1}, E_{t2} for which best fit is obtained are $H_a = 4.2 \times 10^{15}$ cm^{-3}, $H_b = 4.2 \times 10^{15}$ cm^{-3}, E_{t1} = 0.75 eV and E_{t2} = 0.39 eV. The J–V curve expected from single trap level E_{t1} is shown by the dash curve and that for the trap level E_{t2} is shown by the dash dotted line. These two curves show that the trap density at E_{t1} and E_{t2} are practically the same. The dash double dotted line shows the Mott V^2 law. The values of other parameters used are $\varepsilon = 10$, $\mu = 8 \times 10^{-2}$ cm^2 V^{-1} s^{-1} and $N_v = 10^{19}$ cm^{-3}.

and 0.4 eV. This happens because Boltzmann statistics is being used for trapping and detrapping. The Fermi level, when the traps H_b are filled is shown by the line $E_f(V_2)$. Note that for this position of the Fermi level both the traps H_a and H_b must be filled. This explains why the total number of traps, which give rise to the second hump, is equal to $H_a + H_b$. This also explains why the position of the second hump coincides with the dash dotted curve in Fig. 2. Similar arguments show that for the Fermi level $E_f(V_3)$ traps at all the three levels must be filled. Third hump corresponds to the trap filled limit of the $H_a + H_b + H_c$. This is why the long dashed curve coincides with the position of third hump in Fig. 2.

We now compare our theory with experimental results reported by Shen et al. [7]. The Schottky diodes studied by Shen et al. were grown by low-pressure metalorganic chemical vapour deposition (MOCVD) on basal plane sapphire substrates. They prepared three samples. We compare the result of the sample with the thickness of 0.6 μm. Their experimental data for this sample are shown by '+' symbols in Fig. 5. A plot of the theory given in Section 2 is shown by the solid curve. The best fit with the theory was obtained for the values of parameters given in caption of Fig. 5. Dash double dotted line is for Mott's V^2 law. Surprisingly the trap concentrations in the two energy levels obtained by the curve fitting are the same, $H_a = 4.2 \times 10^{15}$ cm^{-3} and $H_b = 4.2 \times 10^{15}$ cm^{-3}. The two humps appear because the trap depths for the two sets are different and the second hump corresponds to a trap concentration equal to $H_a + H_b$. The dash dotted curve and dashed curve in Fig. 5 are calculated using theory of Section 2 for single level traps. The trap concentrations used are the same, i.e. 4.2×10^{15} cm^{-3} for both the curves. The trap energies used are 0.75 eV for dashed curve and 0.39 eV for dash dotted curve. The value of the trap concentration for the second hump obtained by Shen et al. [7] does not agree with the value obtained by us in Fig. 5. The trap concentration corresponding to the first hump (the deepest level) also shows some disagreement with our value. It will be helpful to determine the trap concentration by using optical techniques such as PL and electroluminescence.

4. Limitations of the regional approximations

We now discuss the limitations of the regional approximations used extensively in 1970s. In those days computers were not

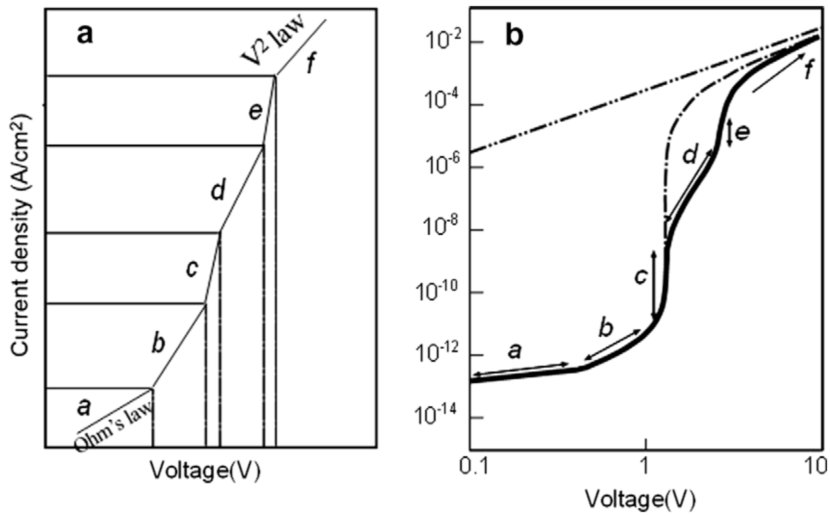

Fig. 6. (a) Represents different regions of *J–V* curve used in the regional approximation for a sample containing two sets of traps at two single energy levels. Regions *a–f* is described in the text. (b) Solid curve represents the exact *J–V* curve calculated using theory describes in Section 2. The dash double dotted curve represents the Mott's V^2 law. Dash dotted curve is for the semiconductors containing traps in single energy level at 0.7 eV with trap concentration of 4×10^{15} cm^{-3}. The regions *a–f* corresponds to the regions *a–f* in figure (a). The region *d* in figure (a) corresponds to the filling of shallow energy traps. In figure (a) the region *d* is solely determined by the shallow traps. Furthermore in figure (a) the V^2 law obtains immediately. In region *f* in figure (b) the *J–V* curve is significantly below the V^2 law in the *f* region and approaches the V^2 law at large values of the voltage. In figure (b) the region *d* is strongly affected by the deeper traps also. These features emphasize the limitation of the regional approximation.

available and it was difficult to make numerical computations. Since it was difficult to make an analytical model of the *J–V* curve for the entire range of voltage of interest, the applied voltage was divided into different regions and a different mathematical equation was used to describe each region. For example using the regional approximations the *J–V* characteristics of an insulator containing two electron trapping centers at two different energy levels are schematically shown (regions *a–f*) in Fig. 6a [6]. At low voltages Ohm's law was observed (region *a*) which was attributed to the presence of thermally generated charge carriers. As the voltage increases the trap filling region (region *b*) starts which were followed by the nearly vertical trap filled region (region *c*). The nearly vertical region *c* corresponds to the limit of filling of the deep level traps. The region *c* was than followed by the filling of shallow traps (region *d*). Again region *d* was followed by the nearly vertical trap filled region (region *e*). Once all the traps are filled the *J–V* characteristic follows the well known Mott's V^2 law (region *f*).

Equations for trap filling regions *b* and *d* and for the trap filled regions *c* and *e* are given in the literature [9]. Material parameters are adjusted so that the observed curve agrees approximately with the calculated curve. We have plotted in Fig. 6b the *J–V* curve (solid line) using the theory given in Section 2 for a similar sample containing traps distributed in two discrete energy levels at 0.7 and 0.4 eV with trap concentrations of 4×10^{15} and 4×10^{15} cm^{-3} respectively. The dash double dotted curve represents the Mott's V^2 law. Dash dotted curve is the calculated *J–V* curve if the semiconductor contains only one set of traps with density equal to $H_a = 4.0 \times 10^{15}$ cm^{-3} and energy $E_{t1} = 0.7$ eV. To compare our model with the regional approximations we have divided the solid curve into six different regions (designated as *a–f*) corresponding to those shown in Fig. 6a. In both figures region *a* corresponds to the Ohm's law. Instead of direct transition the region *b* rises gradually and merges with the region *c*. This gradual transition region cannot be included correctly in the regional approximations.

For the dash dotted curve, once all the traps are filled the curve approaches asymptotically to the Mott's V^2 law [9]. Note that the dash dot curve rising vertically does not go up to the V^2 law but remains significantly below it. In the regional approximation the region *d* is attributed wholly to the filling of shallow traps. This significant suppression of current due to the deeper traps is not correctly included in the *d* region in the regional approximations. Again the transition region from *d* to *e* is not correctly included in the in regional approximation. Region *e* in Fig. 6b corresponds to the trap filled region for the total traps in the insulator. Contrary to the results shown in Fig. 6a (region *f*) once all the traps are filled the *J–V* curves do not meet the V^2 law but reaches the V^2 law asymptotically at high voltages (region *f* in Fig. 6b). This happens because even though all the traps are filled, the free carrier concentrations is still not much larger than the trap filled carriers and the electric field contribution due to trapped carriers in the Poisson's Eq. (3) cannot be neglected [9]. It is therefore clear that the regional approximation is very limited. Our efforts to reproduce experimental curves of Shen et al. [7] using regional approximations fail.

5. Conclusions

The *J–V* characteristics of a sample, where traps are distributed in several discrete energy levels show humps as many as the number of trap levels. The trap concentration determined from the positions of the hump does not always correspond to the actual trap concentration for which the hump occurs, as erroneously assumed by earlier workers. A mathematical simulation has been presented for *J–V* characteristics of a sample containing three numbers of trap energy levels. The calculated *J–V* curves agree well with the existing published experimental results satisfactorily. A more accurate theory and its comparison with the observed *J–V* curve give $H_a = H_b = 4.2 \times 10^{15}$ cm^{-3}. It might appear surprising that two equal trap densities give humps at significantly different voltages. The two humps appear because the trap depths for the two sets are different and the second hump corresponds to a trap concentration equal to $H_a + H_b$.

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