The Journal of CPRI,
Vol. 12, No. 1, March 2016 pp. 145-150

Steady-state DC conductivity of low density polyethylene with deep chemical impurity

Upadhyay A K* and Reddy C C**

This paper presents the effect of deep chemical impurities on the conductivity of insulating polymers. Although plenty of literature available to give conductivity model for insulating polymers but still there is a need of more accurate model. The authors try to propose a new theoretical model for mobility of electrons in order to understand the behaviour of electron towards deep chemical impurities at atomic level using quantum mechanical approach. Our model shows that chemical impurity plays an important role on conductivity of polyethylene.

Keywords: *HVDC Cables, LDPE, chemical impurities, time independent schrodinger wave equation, mobility.*

1.0 INTRODUCTION

From the beginning of usage of High Voltage Direct Current (HVDC) cables for transmission of power, there is a continuous problem from insulating material in extruded cables such as leakage current, charge accumulation and breakdown. Insulating material like Low Density Polyethylene (LDPE) is one of the most common and versatile polymer, with ease of obtaining high uniformity, which is used as insulating material in extruded cables.

Among problems encountered in LDPE, space charge got important attention to the researchers as it affects the breakdown strength and amount of leakage current. As far as leakage current is concerned it majorly depends upon different parameters related to charge carrier behaviour within the insulators. Most of the concepts used to define the physics behind behaviour of charge carriers are already present in literature [1, 2].

In order to fulfil the requirement of perfect insulation and suppression of space charge LDPE has gone through many chemical changes. One of the very common changes for making effective improvement is introduction of inorganic nanoparticles like MgO, SiO_2, Al_2O_3 in LDPE. [3-5]. It has also been explained that there is decrement in space charge in polyethylene due to presence of several physical and chemical impurities, using Density Function Theory (DFT) theory. Also the effect of chemical and physical trap depths on residence time, for any particular trap, is examined. [6, 7].

It is well established from the reputed literature [6, 7] that charge carriers get trapped in chemical and physical impurities in LDPE but the method adopted by charge carriers for transportation within LDPE is still not clear.

The authors have recognized this problem and have attempted to propose a semi theoretical

*Research Scholar, Electrical Engineering, IIT Ropar, Punjab - 140001. E-mail: avnish.upadhyay@iitrpr.ac.in, Mobile: +91 9876327779
**Associate Professor, Electrical Engineering, IIT Ropar, Punjab - 140001, E-mail: reddy@iitrpr.ac.in

approach to define the mobility of free charge carriers as a function of trap depth, using quantum mechanics, since it is no longer independent from the presence of deep chemical impurities.

2.0 ANALYSIS OF TRAP GENERATED FROM DEEP CHEMICAL IMPURITY

Any deep chemical impurity can be modelled as an electric dipole with fixed value of parameters (charge and distance) [3]. So in order to illustrate potential distribution due to chemical impurity we are using the parameters of carbonyl group as an example, since it is assumed as one of the deep impurity with considerable concentration, as shown in Figure 1.

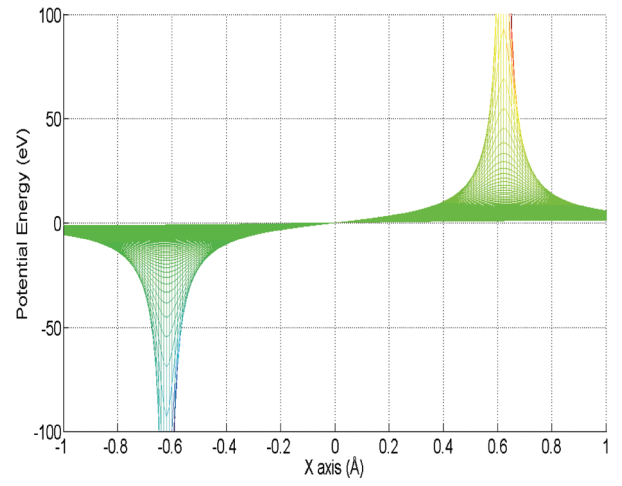

FIG. 1 ONE DIMENTIONAL POTENTIAL ENERGY VARIATION OF ELECTRICAL DIPOLE

If we restrict our self between ±1 eV in Figure 1, we will get an approximated potential well having rectangular shape with width of 2 Angstrom.

We can generalise this rectangular potential well for any deep chemical impurity after assuming potential depth of U_0 and having width of '2a' as shown in Figure 2.

Our next aim is to find the possible bound energy states and scattering states for the generalised rectangular potential well after considering electron as a majority charge carrier for sake of simplicity.

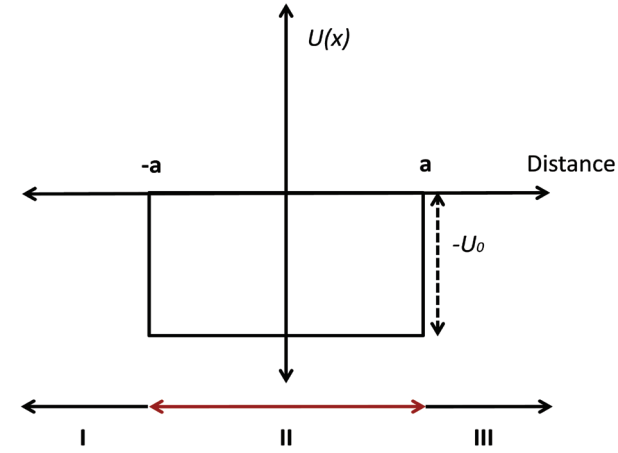

FIG. 2 APPROXIMATED POTENTIAL ENERGY TRAP OF ELECTRICAL DIPOLE.

2.1 Calculation for Bound Energy States

Proceeding with the basic assumption of bound state condition for electrons in equation (1) we are going to locate the exact location of bound states within the rectangular trap. We solved the Time independent schrodinger wave equation (TISWE)(2) for region I, II and III of Figure 2 in this section.

$$E < [U(-\infty)\ and\ U(\infty)] \quad \text{....(1)}$$

E is the total energy of electron and $U(\pm\infty)$ are infinite value of well.

General form of time independent schrodinger wave equation

$$-\frac{\hbar}{2m}\nabla^2\psi(x,y,z) + U(x,y,z)\psi(x,y,z) = E\psi(x,y,z) \quad \text{....(2)}$$

Here $\hbar = \frac{h}{2\pi}$ and h is plank's constant. $\Psi\ (x, y, z)$ is the wave function of electron.

U (x. y, z) is potential energy of electron.

E is the total energy of electron.

Solution of TISWE for bound energy state for given rectangular potential well is obtained and

shown in following equation (3) after assuming wave function as purely even function.

$$\psi(x) = \left(\begin{array}{c|c} Fe^{-kx} & x > a \\ Dcos(lx) & 0 < x < a \\ \psi(-x) & x < 0 \end{array}\right) \quad \text{....(3)}$$

Here F and D are arbitrary constants and

$$l = \sqrt{\frac{2m(E+U_0)}{\hbar^2}} \; and \; k = \sqrt{\frac{-2mE}{\hbar^2}}$$

Since wave function and its derivative must follow the continuity condition at the critical points that is at x=±a hence

$$k = ltan\,(la)$$

To reduce some complexity in calculation we adopted following simpler notation which is given as follows.

Let

$z \equiv la$ and

$z_0 = \frac{a}{\hbar}\sqrt{2mU_0}$ Finally

$$tan(z) = \sqrt{\frac{z_0^2}{z^2} - 1}$$

This is a transcendental equation for 'z' as function of 'z_0'. This equation will also give relationship between E and 'size' of the well. To solve this equation by using graphical method we plotted $\tan z$ and $\sqrt{\frac{z_0^2}{z^2}}$ on the same scale and calculated the intersection points as shown in Figure 3.

These intersection points will help us to calculate Bound energy states.

2.1 Calculation for Scattering Energy States

The basic condition of scattering state calculation for electrons is given in equation (4)

$$E > [U(-\infty) \; and \; U(\infty)] \quad \text{....(4)}$$

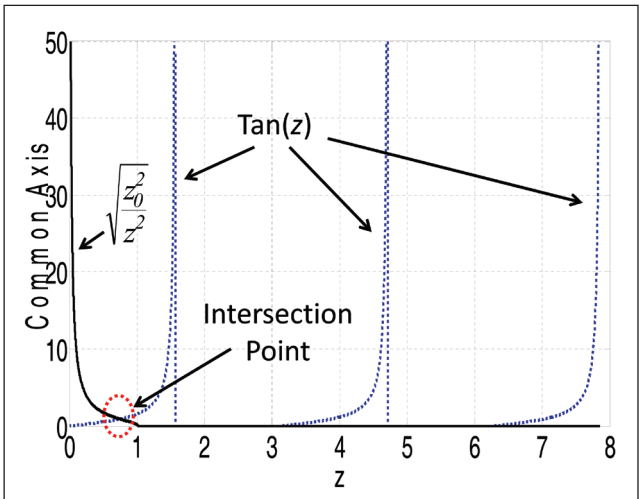

FIG. 3 GRAPHICAL SOLUTION FOR EVALUATING BOUND ENERGY STATES.

Solving TISWE for the given rectangular trap after taking care of scattering condition we have the following equation of wave function.

$$\psi(x) = \left(\begin{array}{c|c} Ae^{ikx} + Be^{-ikx} & x < -a \\ Csin(lx) + Dcos(lx) & -a < x < a \\ Fe^{-ikx} & x > a \end{array}\right) \quad \text{....(5)}$$

Here

$$l = \sqrt{\frac{2m(E+U_0)}{\hbar^2}} \; and \; k = \sqrt{\frac{2mE}{\hbar^2}}$$

Again considering the continuity of wave function and its derivative at x=±a we can find the value of arbitrary constants as follows

$$B = i\frac{sin(2la)}{2kl}(l^2 - k^2)F \quad \text{....(6)}$$

$$F = \frac{e^{-2ika}A}{cos(2la) - i\frac{(k^2+l^2)}{2kl}sin(2la)} \quad ....(7)$$

$T = \frac{|F|^2}{|A|^2}$ The transmission coefficient [8]

After putting the values from equation (6) and (7)

$$T^{-1} = 1 + \frac{{U_0}^2}{4E(E+U_0)} sin^2\left(\frac{2a}{\hbar}\right)\sqrt{2m(E+U_0)} \quad ....(8)$$

Now plot of transmission coefficient with respect to total energy, which is shown in Figure (3), will give us transparent states present in the scattering band which is depicted in Figure (4).

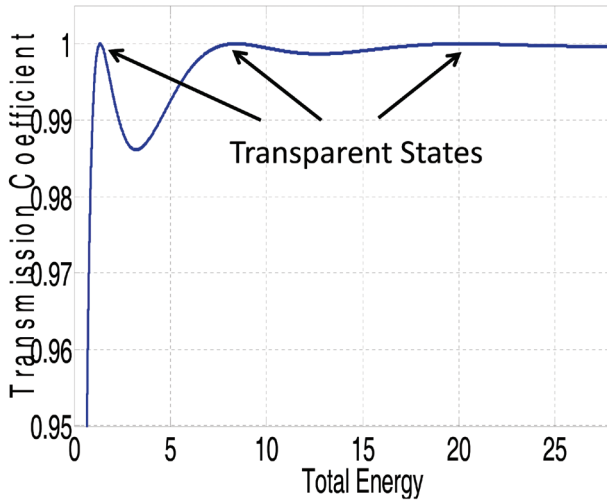

FIG. 4 PLOT OF TRANSMISSION COEFFICIENT WITH RESPECT TO TOTAL ENERGY

Above whole discussion on bound states and scattering states suggest that whenever electron fulfil the total energy criteria for scattering, given in equation (4), after collecting sufficient energy by any means, like thermal excitation, phonon interaction etc., it will get scattered from that potential well.

Transportation of charge carrier within insulating polymers is often described by a hopping mechanism in which carriers move from one trap to another trap by surpassing the potential barrier shown in Figure 5. For a single trapping level of depth U_0, the resulting mobility has the following form [9].

$$\mu = \frac{2\nu\Delta x}{E}\exp\left[\frac{-U_0}{KT}\right]\sinh\left[\frac{eE_f\Delta x}{2KT}\right] \quad ....(9)$$

where 'e' the elementary charge, 'ν' the phonon frequency, 'U_0'is trap depth, 'Δx' the inter-site distance, 'K' the Boltzmann constant, 'T' the temperature and 'E_f' the field.

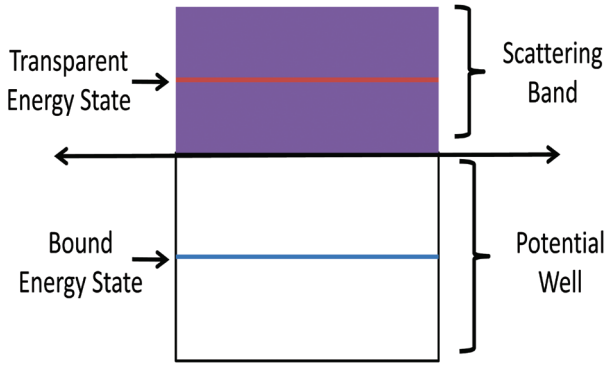

FIG. 5 DEPICTION OF TRANSPARENT STATES PRESENT IN THE SCATTERING BAND AND BOUND STATE.

3.0 CONCLUSIONS

We have developed a theoretical model for explanation of electron mobility in LDPE including the effect of trap depth, trap width, electric field and temperature. Mobility of free electrons is no longer independent from deep chemical impurities meanwhile it has decreased value due to presence of these impurities. Hence it plays an important role in calculation of conductivity of LDPE.

ACKNOWLEDGEMENT

We gratefully acknowledge the encouragement from CPRI for providing financial support through Grant CPRI / R&D / NPP / 2014 for carrying out this work.

REFERENCES

[1] T J Lewis, Nanometeric Dielectrics, IEEE Trans. Dielectr. Electr. Insul, Vol. 1, pp. 812-825, 1994

[2] R Bartnikas, Performance Characteristics of Dielectrics in the Presence of Space Charge, IEEE Trans. Dielectr. Electr. Insul, Vol. 4, pp. 544-557, 1997.

[3] T Takada, Y Hayase, Y Tanaka, and T Okamoto, Space Charge Trapping in Electrical Potential Well Caused by Permanent and Induced Dipoles for LDPE/ MgO Nanocomposite, IEEE Trans. Dielectr. Electr. Insul, Vol. 15, pp. 152-160, 2008.

[4] K Ishimoto, EtsuKanegae, Yoshimichi Ohki, Toshikatsu Tanaka, YoitsuSekiguchi, Yoshinao Murata and C C Reddy, Superiority of Dielectric Properties of LDPE/MgO Nanocomposites over Microcomposites, IEEE Trans. Dielectr. Electr. Insul, Vol. 16, pp. 1735-1742, 2009.

[5] W Jiandong, Y Yi, L Li, Wang Qiaohua, Li Xuguang, and Xiao Dengming, Space Charge Trapping and Conduction in Low-Density Polyethylene/Silica Nanocomposite, Jpn. J Appl. Phys, Vol. 51, 041602, 2012.

[6] M Meunier and N Quirke, Molecular modeling of electron trapping in polymer insulators, J Chem. Phys., Vol. 113, pp. 369-376, 2000.

[7] M Meunier, N Quirke and A Aslanides, Molecular modelling of electron traps in polymer insulators: Chemical defects and impurities, J. Chem. Phys., Vol. 115, pp. 2876-2881, 2001.

[8] D J Griffiths, Introduction to Quantum Mechanics, Pearson Education International, New Jersey, pp. 82, 2005

[9] S Le Roy, P Segur, G Teyssedre and C Laurent, Description of bipolar charge transportin polyethylene using a fluid model with a constant mobility: model prediction, J. Phys. D: Appl. Phys., Vol. 37, pp. 298–305, 2004.