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Bipolar Charge Transport Model of Insulator for HVDC Applications

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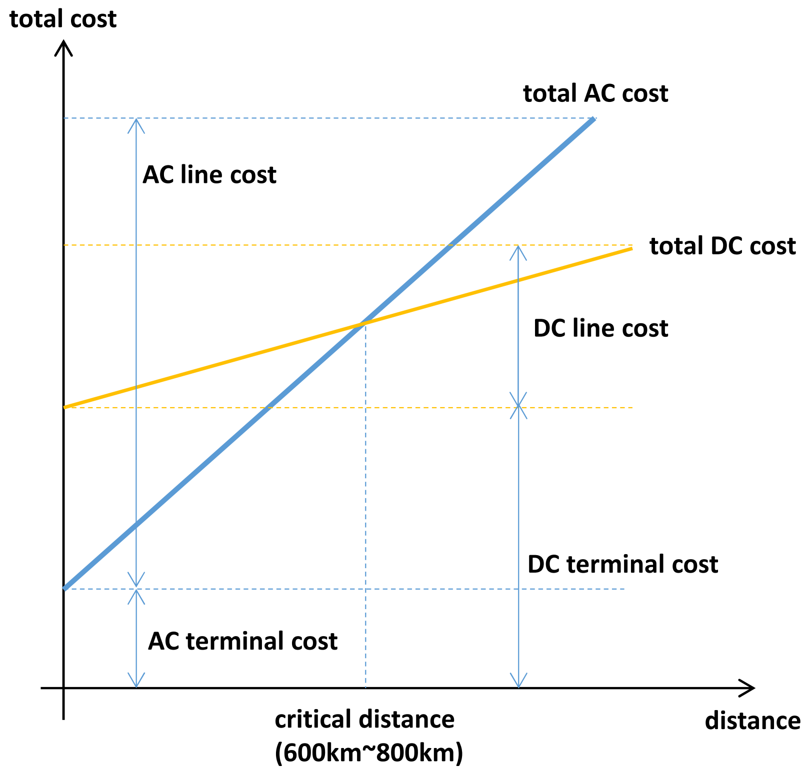
Outline

- HVDC Overview
- Insulation of HVDC System
- Microscopic Structure of Insulator
- Numerical Model of Insulator
- In Conclusion

High Voltage Direct Current (HVDC)

- A high voltage, direct current (HVDC) electric power transmission system (also called a power super highway or an electrical super highway) uses direct current for bulk transmission of electrical power, in contrast with more common alternating current (AC) systems.
  - For long-distance transmission, HVDC systems may be less expensive and suffer lower electrical losses.
  - For shorter distances, the higher cost of DC conversion equipment compared to an AC system may still be justified, due to other benefits of direct current links.
- The modern form of HVDC transmission uses technology developed extensively in the 1930s in Sweden and in Germany.
  - Early commercial installations included one in the Soviet Union in 1951 between Moscow and Kashira, and a 100kV, 20MW system between Gotland and mainland Sweden in 1954.
  - The longest HVDC link in the world is the Rio Madeira link in Brazil, which consists of two bipoles of ±600kV, 3150MW each, connecting Porto Velho in the state of Rondônia of the Säo Paulo area. The length of the DC line is 2,375km.



https://en.wikipedia.org/wiki/High-voltage_direct_current

Requirements for HVDC System

- The trends towards *more compact systems* in power engineering, leading to an increase in the power density
  - Polymers will be pushed towards their limits and there is an industrial concern for developing tools to define engineering safety limits.
- The trends towards *higher reliability* of electrical systems, due to their use in critical applications.
- The development of *new materials* for electrical application with tailored properties.
  - Chemical doping or matrix doping by micro- and nano-fillers.

Difficulties in Developing HVDC Insulation

- **Unpredictable Electric Field Distribution due to *Space Charge***
  - **Accumulation of localized electric charges cause electric field enhancement and electrical breakdown.**
  - **It makes difficult to predict field due to the space charge which is a function of temperature, field and time.**

$$\nabla \cdot \mathbf{E}(\mathbf{r}, t) = \frac{\rho(T, |\mathbf{E}|)}{\epsilon}$$

- **Non-linear behavior of *Conduction Current***
  - **Conduction current mainly depends on material conductivity which is non-linear under electric field strength and temperature.**
  - **High conduction current of insulation can cause thermal runaway.**

$$\mathbf{J}(r, t) = \sigma(T, |\mathbf{E}|)\mathbf{E}(\mathbf{r}, t)$$

Why Space Charge Distorts Electric Field?

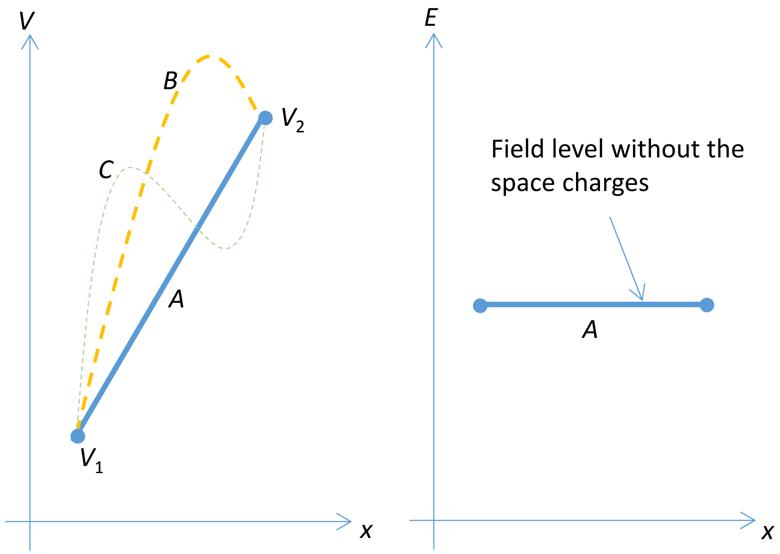
- **Electric Field Enhancement by Locally Distributed Charges**

If there are ***no space charges***, the potential and electric field obeys Laplace's equations.

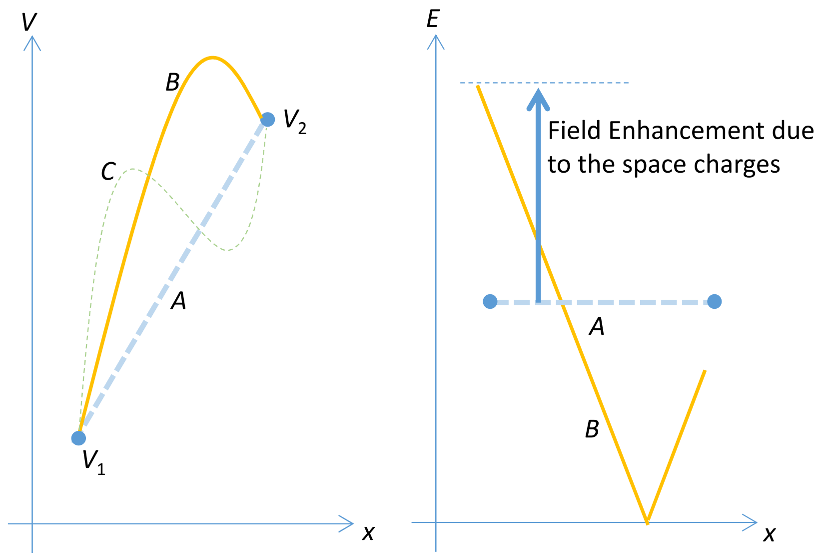
$$\nabla^2 V = 0$$

If there exists ***space charges***, the potential and electric field obeys Poisson's equations.

$$\nabla^2 V = \frac{\rho}{\varepsilon}$$



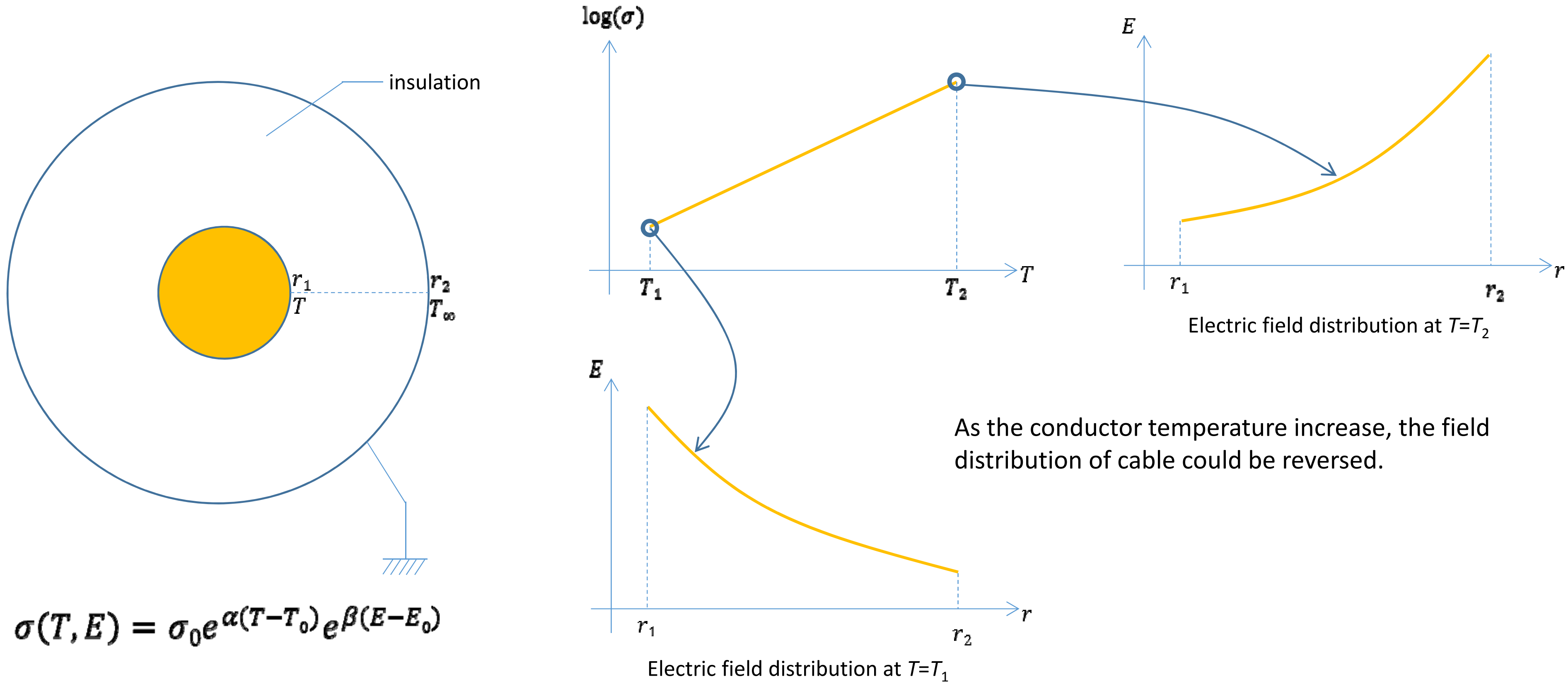
Laplace's equation can not yield solution B or C which has local maxima or minima between boundaries V_1 *and* V_2.



Poisson's equation can yield solutions B or C which has local maxima or minima between boundaries V_1 *and* V_2. Therefore, the electric field – a derivative of electric potential – could be enhanced according to curve B.

Why Conduction Current Distorts Electric Field?

- **Electric Field Reversal due to Temperature and Field Dependent Conduction**



$$\sigma(T,E) = \sigma_0 e^{\alpha(T-T_0)} e^{\beta(E-E_0)}$$

As the conductor temperature increase, the field distribution of cable could be reversed.

Microscopic to Macroscopic Approaches

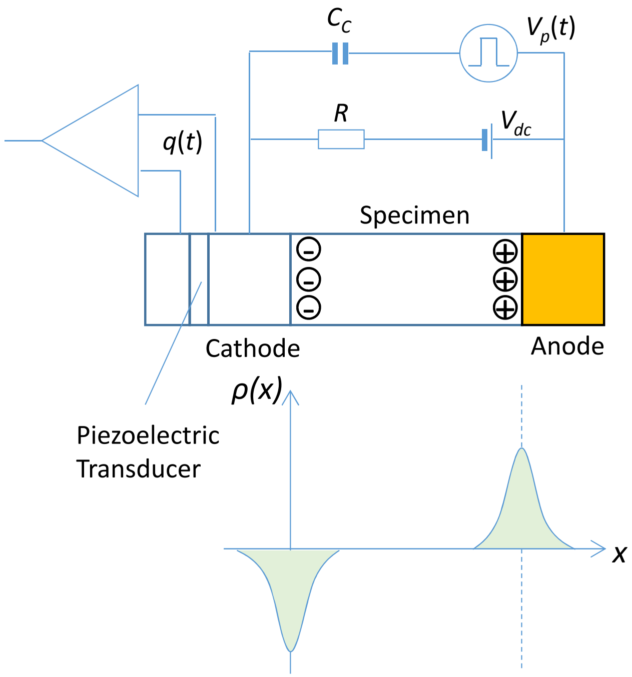
- **Macroscopic phenomena of *charge accumulation and non-linear DC conduction*, is strongly related with microscopic structure of insulation such as mobility of carriers, traps and their structures.**
- **In past years, modeling macroscopic phenomena is difficult due to the lack of microscopic information.**
- **Nowadays, two technologies make it easy to build a macroscopic model.**
  - ***Ab-initio methods* (1st principle calculation) to simulate microscopic structures**
  - **Direct observation of space charge distribution by *pulsed electro-acoustic method***

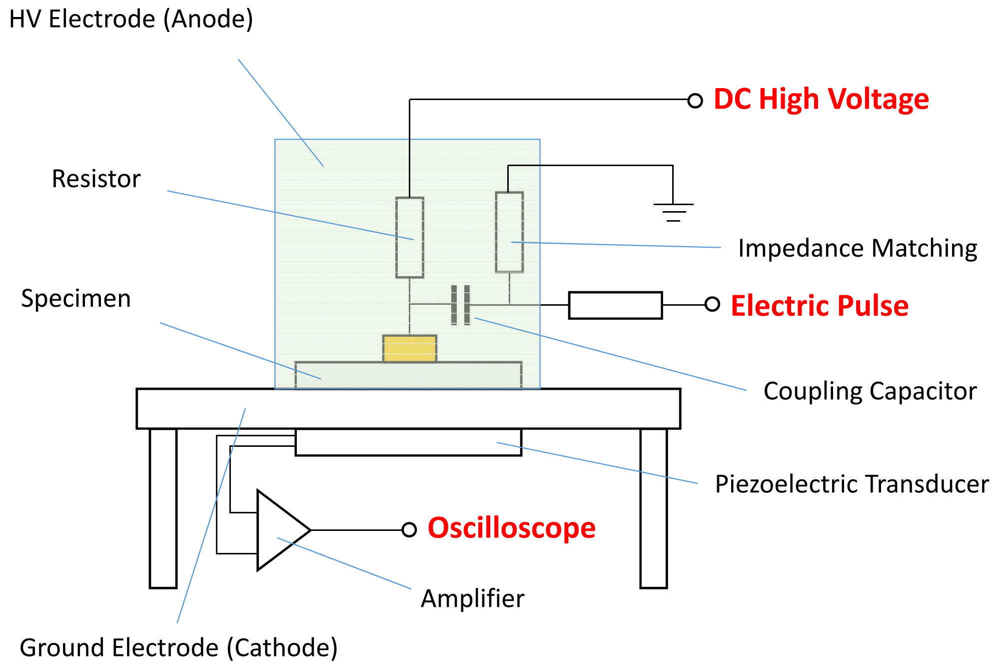
Ab-initio Methods

- Ab-initio methods - which is use only elementary physical information not empirical one - are computational chemistry methods based on quantum chemistry. The term ab-initio was first used in quantum chemistry by Robert Parr and coworkers.
- DFT (Density Functional Theory): based on quantum mechanics
- MD (Molecular Dynamics): based on classical mechanics

PEA (Pulsed Electro-Acoustic) Method

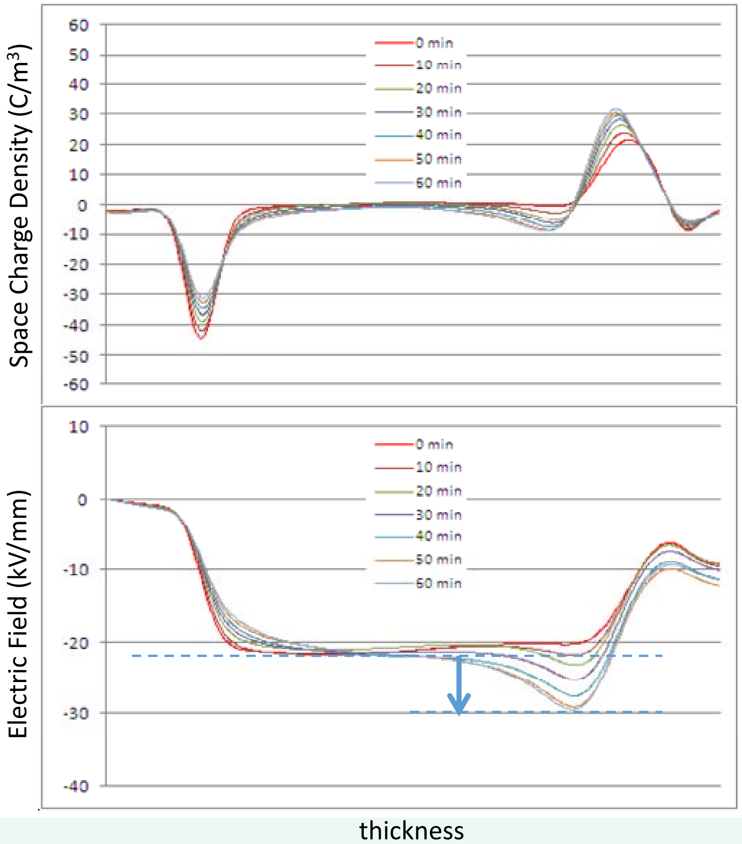
- **Introduction of PEA Method for Space Charge Measurement**

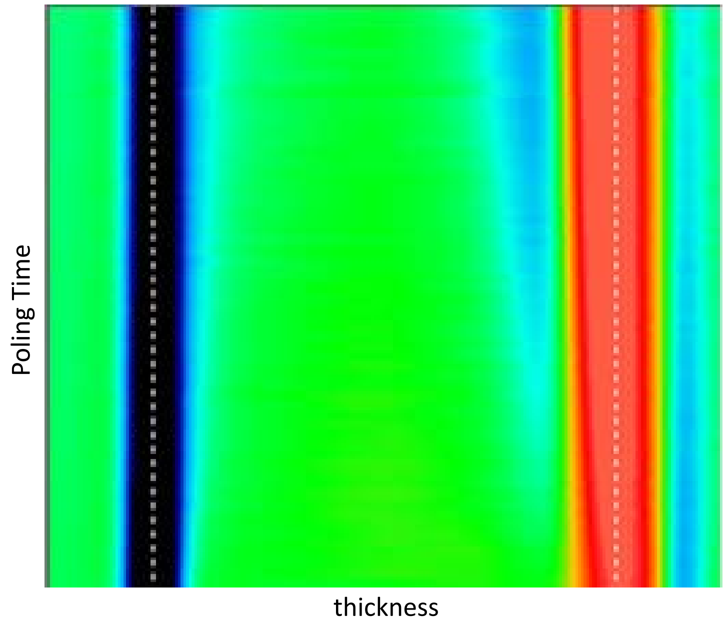




PEA (Pulsed Electro-Acoustic) Method

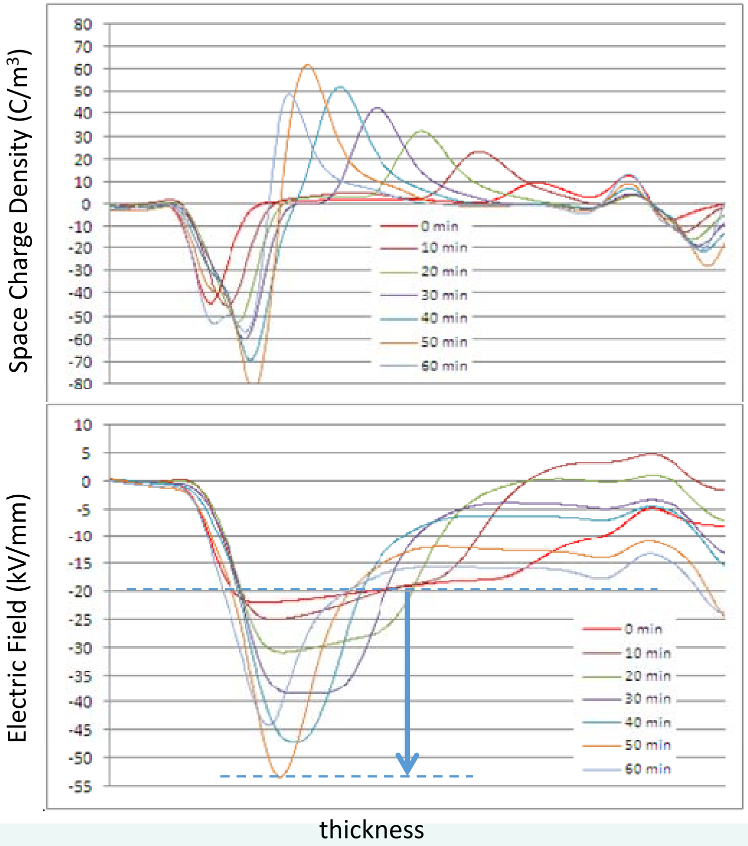
- **Examples of Space Charge Measurements**

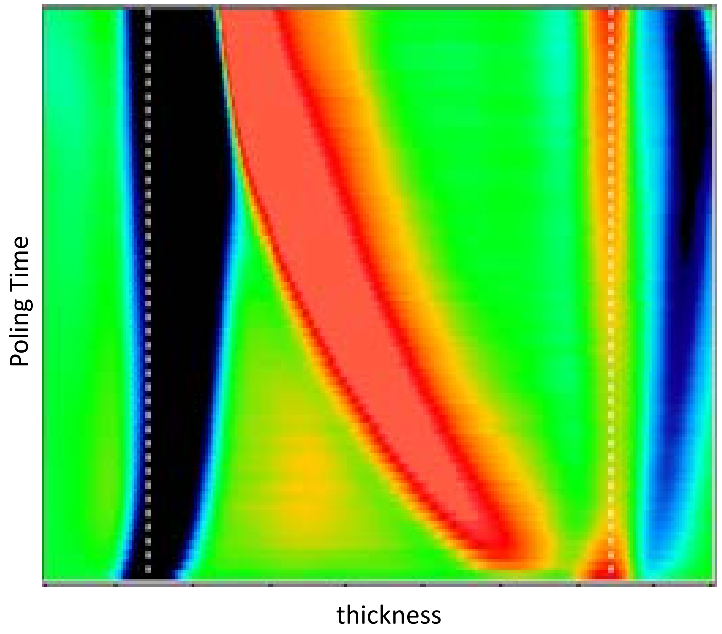




PEA (Pulsed Electro-Acoustic) Method

- **Examples of Space Charge Measurements**





Microscopic Structure of Insulator

- **Microscopic structure of insulator is strongly related with chemical defects, physical disorder and impurities or by-products**
- **Meunier and Quirke[1] studied the depth of trapped charges in insulating materials which is related to the presence of physical and chemical defects by quantum chemical calculation.**
- **Dakada[2] also studied the charge-trapping site of insulator such as LDPE, ETFE and polyimide by using DFT calculations.**

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[1] M. Meunier and N. Quirke, "Molecular Modeling of Electron Trapping in Polymer Insulator", Journal of Chemical Physics, Vol. 113, No.1, pp. 369 (2000)
[2] T. Takada, H. Kikuchi, H. Miyake and Y. Tanaka, "Determination of charge-trapping sites in saturated and aromatic polymers by quantum chemical calculation", IEEE Trans. On Dielectrics and Electrical Insulation, Vol. 22, Issue 2, pp. 1240-1249 (2015)

Microscopic Structure of Insulator

- **Quantum Mechanics: Schrödinger Equation**

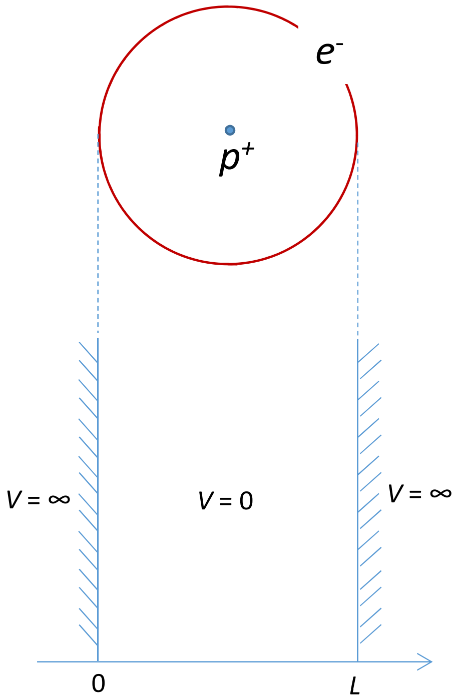
$$i\hbar \frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

- **Time-Independent Schrödinger Equation: Eigenvalue Problem**

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Microscopic Structure of Insulator

- **Eigenvalue Problem – Infinite Potential Well**



Infinite Potential Well - The simplest model of atom

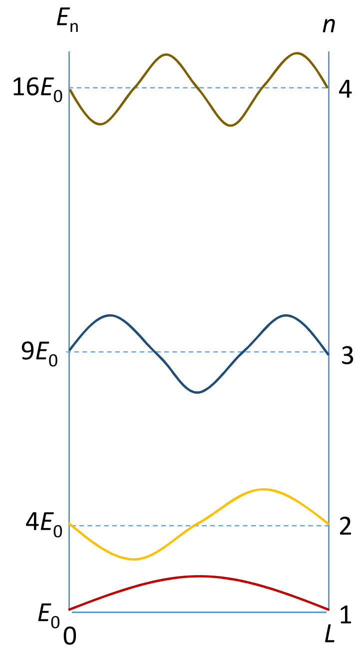
- **Time-Independent Schrödinger Eq. (1-D)**

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

- **Solution of Schrödinger Equation**

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

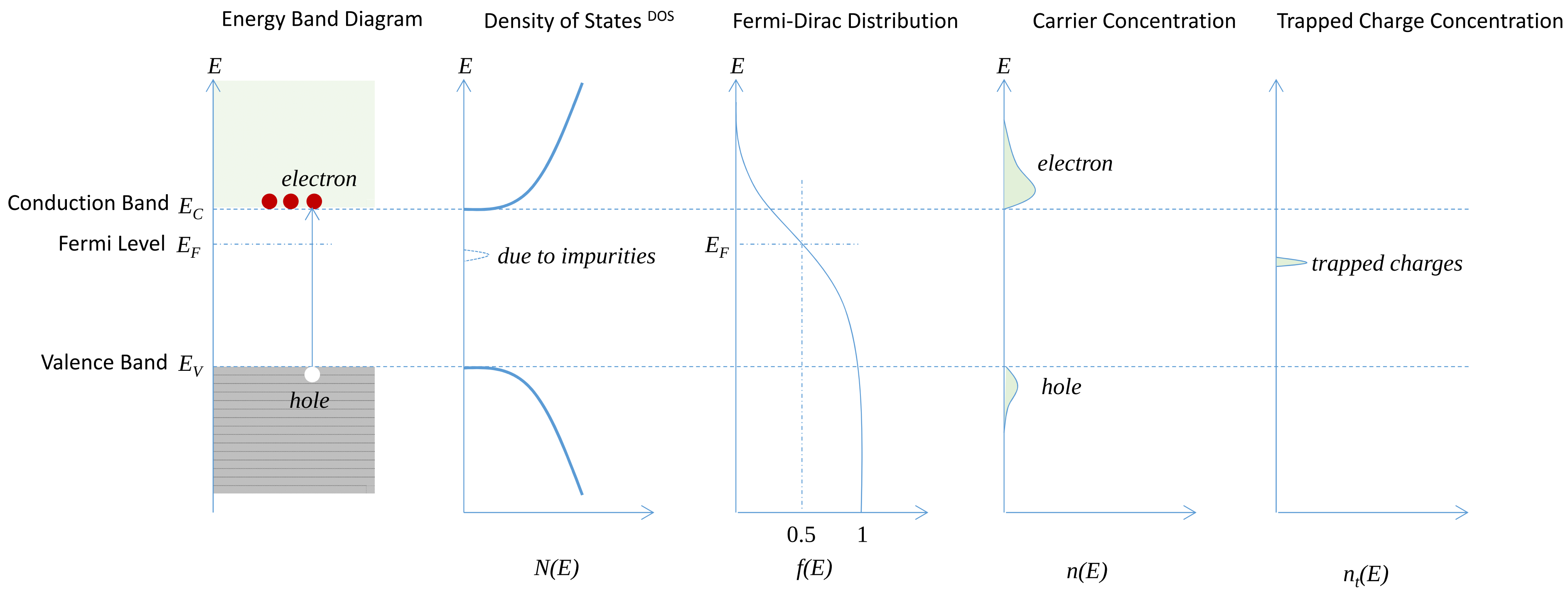
$$E_n = \frac{\hbar\pi^2}{2mL^2}n^2$$



Electrons only exist discrete energy levels

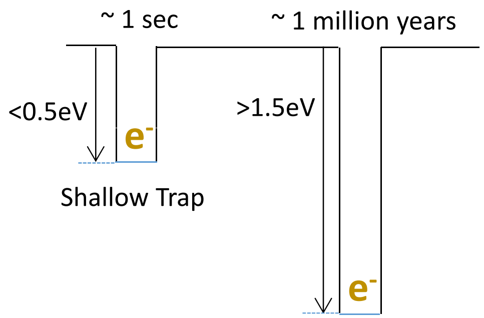
Microscopic Structure of Insulator

- **Carrier and Trapped Charge Concentration**



Microscopic Structure of Insulator

- **Shallow and Deep Traps**
  - **Shallow Traps: Traps above Fermi level, typically less than 0.5eV at RT**
  - **Deep Traps: Traps below Fermi level, typically larger than 0.5eV at RT**



Traps	Shallow Trap	Deep Trap
Depth	less than 0.5eV@RT	larger than 0.5eV@RT
Transport	Hopping conduction	Trap-limited conduction and space charge formation
Detrapping	A few seconds	A few hours
Cause	Physical disorder	Chemical defects and impurities

Shallow traps contribute the transportation of charges by hopping mechanism, however deep traps contribute that by trap-limited conduction and space charge accumulation.

Numerical Model of Insulator

- **Bipolar Charge Transport Model**
  - **Alison and Hill [J. Phy., 1994] have proposed a bipolar model in which the charge density available for injection is the difference between a constant source density and the charge density trapped adjacent to the injection electrode in order to describe XLPE behavior.**
  - **Charge transport is modeled numerically using an effective mobility, deep traps for electron and hole are represented as a single trap level with no detrapping.**
  - **Recombination is accounted for by a recombination coefficient for each pair of positive and negative species.**
  - **Results have been favorably compared to those obtained by Li and Takada.**

G. Teyssedre and C. Laurent, Charge Transport Modeling in Insulating Polymers: From Molecular to Macroscopic Scale, IEEE Transactions on Dielectrics and Electrical Insulation Vol. 12, No. 5; Oct. 2005

Numerical Model of Insulator

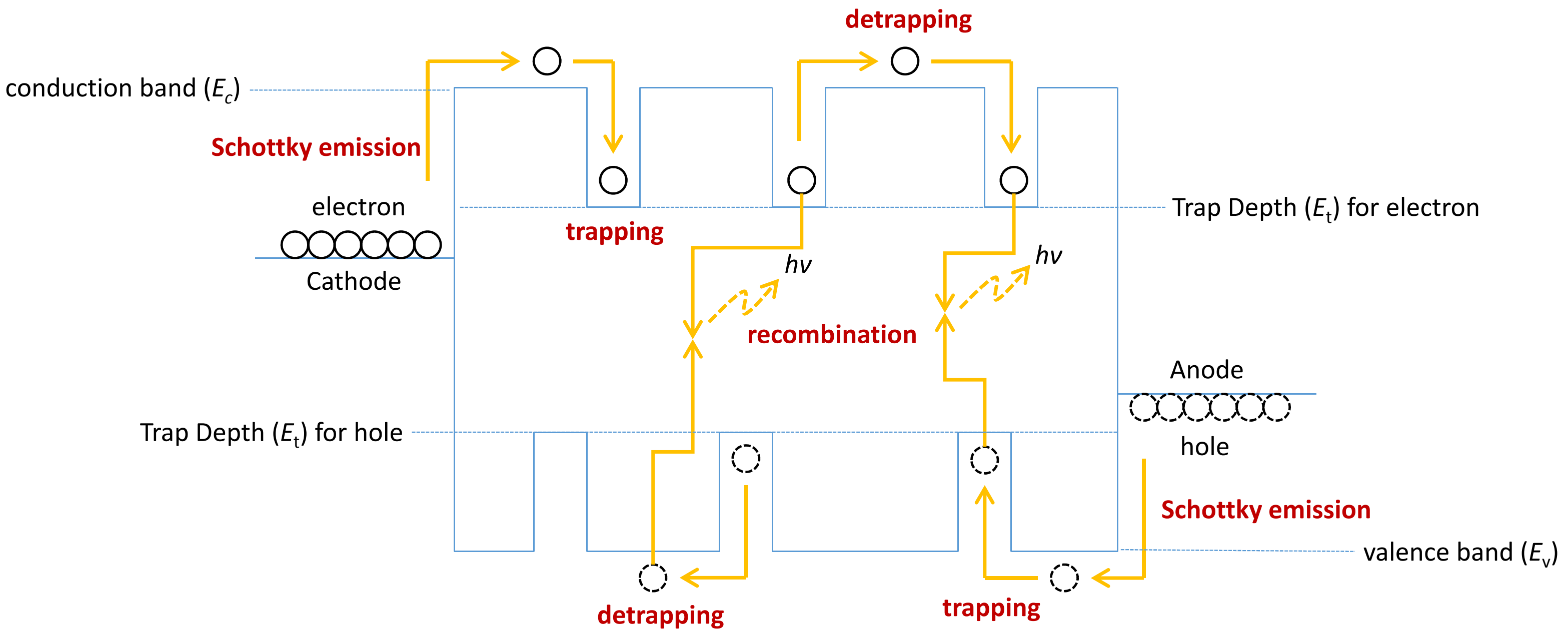
- **Features of the Principal Bipolar Charge Transport Models**

Reference	Alison and Hill (1994)	Fukuma et al. (1994)	Kaneko et al. (2001)	LeRoy at al. (2004)
Charge Generation	**Constant source at both electrodes**	**Schottky injection at both electrodes**	Schottky injection at both electrodes	Schottky injection at both electrodes
Charge Extraction	Non-blocking electrodes	Extraction barriers	Non-blocking electrodes	Non-blocking electrodes
Charge Transport	**Constant effective mobility**	Hopping conduction between sites of the same energy	Hopping conduction between sites of the same energy	Constant effective mobility
Charge Trapping	One deep trapping level, no detrapping	One deep trapping level, no detrapping	No deep trapping	**Trapping on one deep level with detrapping**
Charge Recombination	**For mobile and trapped charges**	For mobile carriers	For mobile carriers	For mobile and trapped charges
Other		Joule effects accounted for initial bulk charges		Initial bulk charges

G. Teyssedre and C. Laurent, Charge Transport Modeling in Insulating Polymers: From Molecular to Macroscopic Scale, IEEE Transactions on Dielectrics and Electrical Insulation Vol. 12, No. 5; Oct. 2005

Numerical Model of Insulator

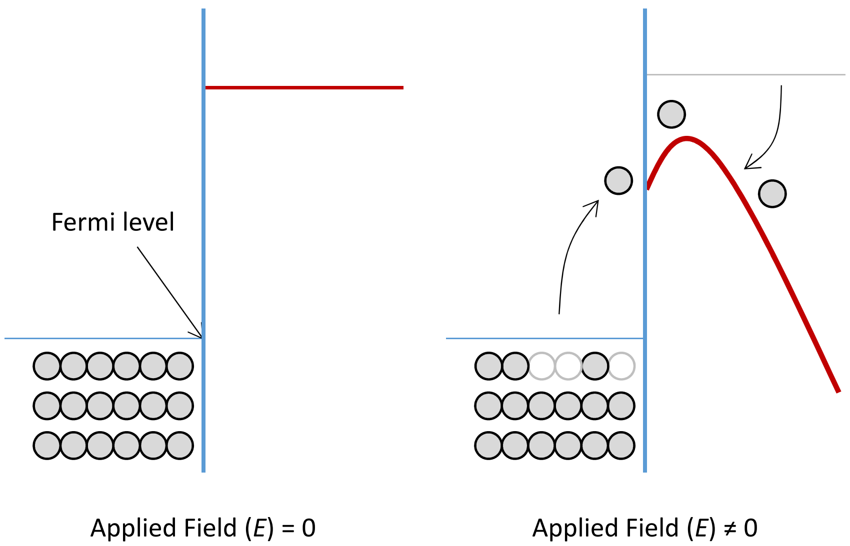
- **Charge Injection, Trapping and Recombination**



Numerical Model of Insulator

- **Charge Injection – Schottky Emission**

[Schottky Emission]



At cathode:

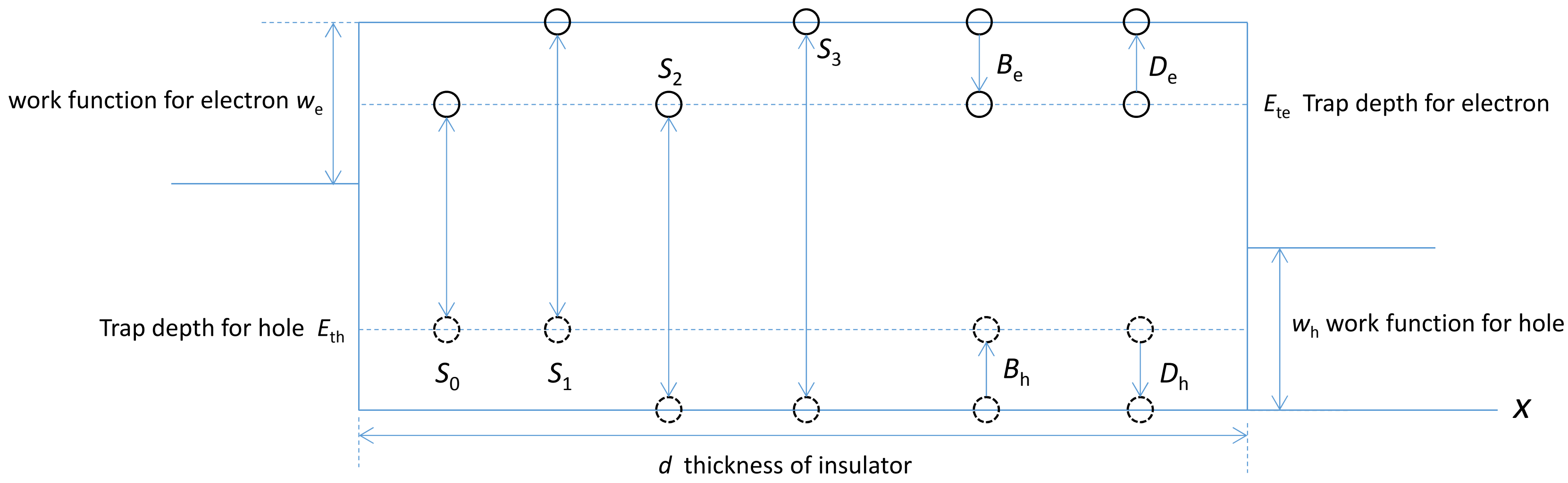
$$j_e(x=0,t) = \lambda_R \frac{4\pi m_e k^2 e}{h^3} T^2 e^{-\frac{w_e}{kT}} e^{\sqrt{\frac{e^3 E(x=0,t)}{4\pi\varepsilon kT}}}$$

At anode:

$$j_h(x=d,t) = \lambda_R \frac{4\pi m_h k^2 e}{h^3} T^2 e^{-\frac{w_h}{kT}} e^{\sqrt{\frac{e^3 E(x=d,t)}{4\pi\varepsilon kT}}}$$

Numerical Model of Insulator

- **Trapping, Detrapping and Recombination**



$$s_1 = \frac{\partial n_{e\mu}}{\partial t} = -B_e n_{e\mu}\left(1 - \frac{n_{et}}{n_{et,0}}\right) + D_e n_{et} - S_1 n_{ht} n_{e\mu} - S_3 n_{h\mu} n_{e\mu}$$

$$s_2 = \frac{\partial n_{et}}{\partial t} = B_e n_{e\mu}\left(1 - \frac{n_{et}}{n_{et,0}}\right) - D_e n_{et} - S_2 n_{h\mu} n_{et} - S_0 n_{ht} n_{et}$$

$$s_3 = \frac{\partial n_{h\mu}}{\partial t} = -B_h n_{h\mu}\left(1 - \frac{n_{ht}}{n_{ht,0}}\right) + D_h n_{ht} - S_2 n_{et} n_{h\mu} - S_3 n_{h\mu} n_{e\mu}$$

$$s_4 = \frac{\partial n_{ht}}{\partial t} = B_h n_{h\mu}\left(1 - \frac{n_{ht}}{n_{ht,0}}\right) - D_h n_{ht} - S_1 n_{ht} n_{e\mu} - S_0 n_{ht} n_{et}$$

Numerical Model of Insulator

- **Governing Equations**

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon}$$

Gauss' Law (Poisson's Equation)

$$\mathbf{J} = \sigma \mathbf{E} = \mu q n \mathbf{E}$$

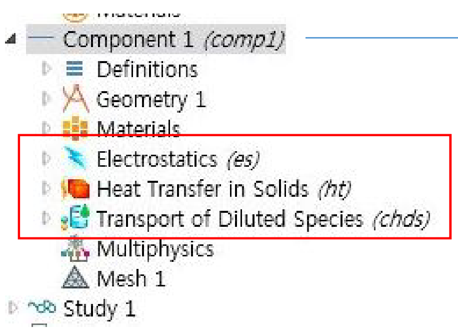
Ohm's Law (Transport Equation)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = s_i$$

Charge Conservation Law (Conservative Equation)

Numerical Model of Insulator

- **COMSOL Multiphysics® Implementation**



Electrostatics
- Electric Potential - V
- Ground
- Space Charge Density
  : $F_0 (n_{eu}+n_{hu}+n_{et}+n_{ht})$

Heat Transfer in Solid
- Temperature - T

Transport of Diluted Species
- Flux - J/F_0
- Reactions - s_1~s_4
- Charge Concentration – n_{eu}, n_{hu}, n_{et}, n_{ht}

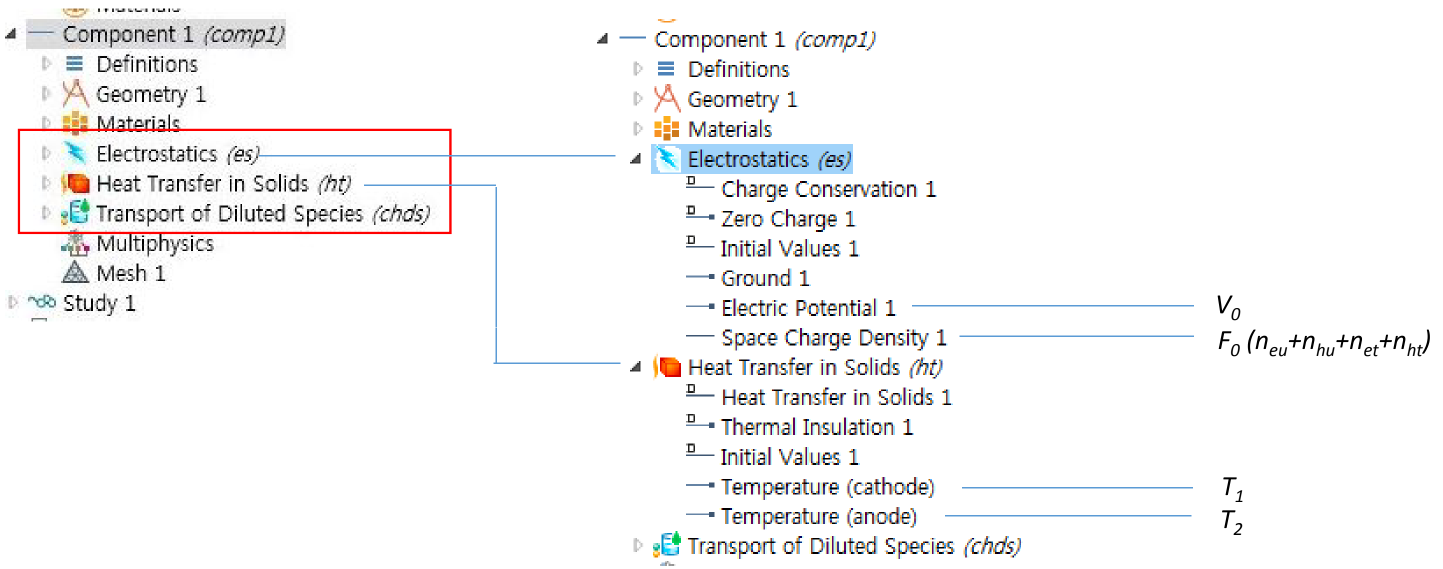
Materials
- Permittivity - ε
- Thermal Conductivity - k
- Heat Capacity - C_p
- Density - ρ

Geometry
- Interval (1D)

Study
- Time Dependent

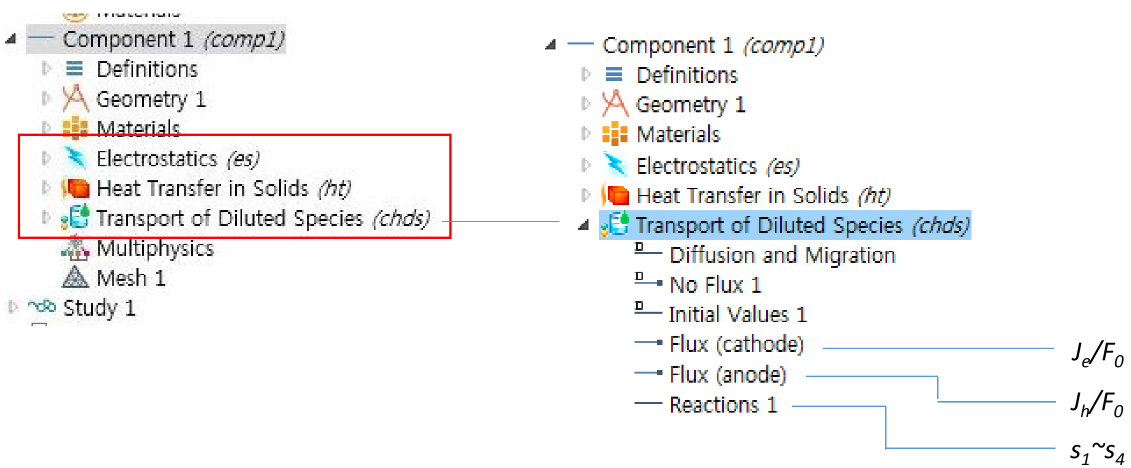
Numerical Model of Insulator

- **Boundary Conditions – Electrostatics and Heat Transfer in Solids**



Numerical Model of Insulator

- **Boundary Conditions – Transport of Diluted Species**



Numerical Model of Insulator

- **Variables and Material Coefficients Definition**

Symbol	Unit	Description
n_{eu} / n_{et}	mol/m^3	Concentration of mobile / trapped electron
n_{hu} / n_{ht}	mol/m^3	Concentration of mobile / trapped hole
n_{0et}	mol/m^3	Concentration of deep trap density of electron
n_{0ht}	mol/m^3	Concentration of deep trap density of hole
μ_e	m^2/V/s	Effective mobility of electron
μ_h	m^2/V/s	Effective mobility of hole
B_e	1/s	Trapping coefficient for electron
B_h	1/s	Trapping coefficient for hole
D_e	1/s	Detrapping coefficient for electron
D_h	1/s	Detrapping coefficient for hole
S_0	m^3/C/s	Recombination coefficients between trapped electron and hole
S_1	m^3/C/s	Recombination coefficients between mobile electron and trapped hole
S_2	m3/C/s	Recombination coefficients between trapped electron and mobile hole
S_3	m3/C/s	Recombination coefficients between mobile electron and mobile hole

Numerical Model of Insulator

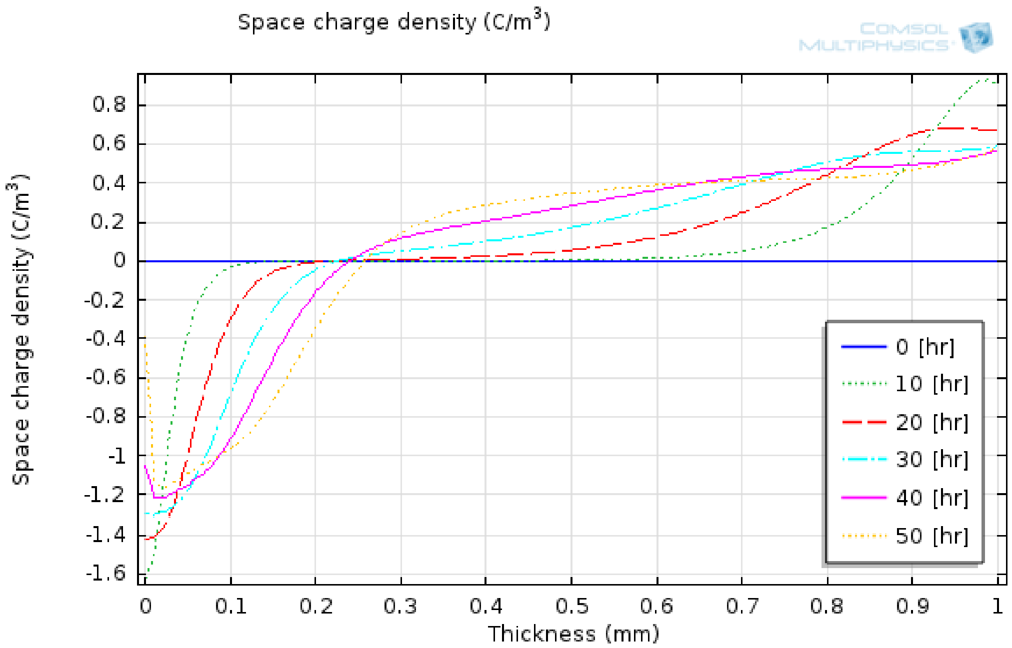
- **Physical Constants and Simulation Parameters**

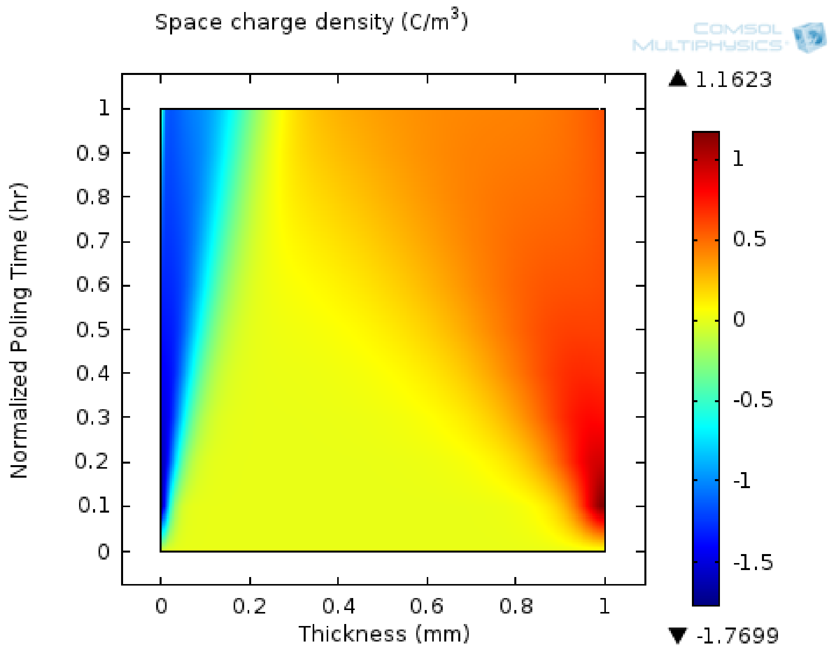
Parameters

Name	Expression	Value	Description
A	0.5*1200[mA/(mm^2*K^2)]	6.0000E5 A...	Richardson constant
wei	1.30[eV]	2.0828E-19 J	Injection barriers for electron
whi	1.27[eV]	2.0348E-19 J	Injection barriers for hole
mu_e	1e-14[m^2/V/s]/F0	1.0354E-19 ...	Effective mobility for electron
mu_h	2e-14[m^2/V/s]/F0	2.0707E-19 ...	Effective mobility for hole
Be	0.2[1/s]	0.20000 1/s	Trapping coefficients for hole
Bh	0.1[1/s]	0.10000 1/s	Trapping coefficients for hole
n_oet	100[C/m^3]	100.00 C/m³	Deep trap densities for electron
n_oht	100[C/m^3]	100.00 C/m³	Deep trap densities for hole
S0	1e-5[m^3/C/s]	1.0000E-5 ...	Recombination coefficients
S1	1e-5[m^3/C/s]	1.0000E-5 ...	Recombination coefficients
S2	1e-5[m^3/C/s]	1.0000E-5 ...	Recombination coefficients
e	1.602e-19[C]	1.6020E-19 C	elementary charge
F0	96584[C/mol]	96584 s·A/...	Faraday's number
k	1.38e-23[J/K]	1.3800E-23 ...	Boltzmann constant
ep0	8.854e-12[F/m]	8.8540E-12 ...	Permittivity of vacuum

Numerical Model of Insulator

- **COMSOL Multiphysics® Simulation**



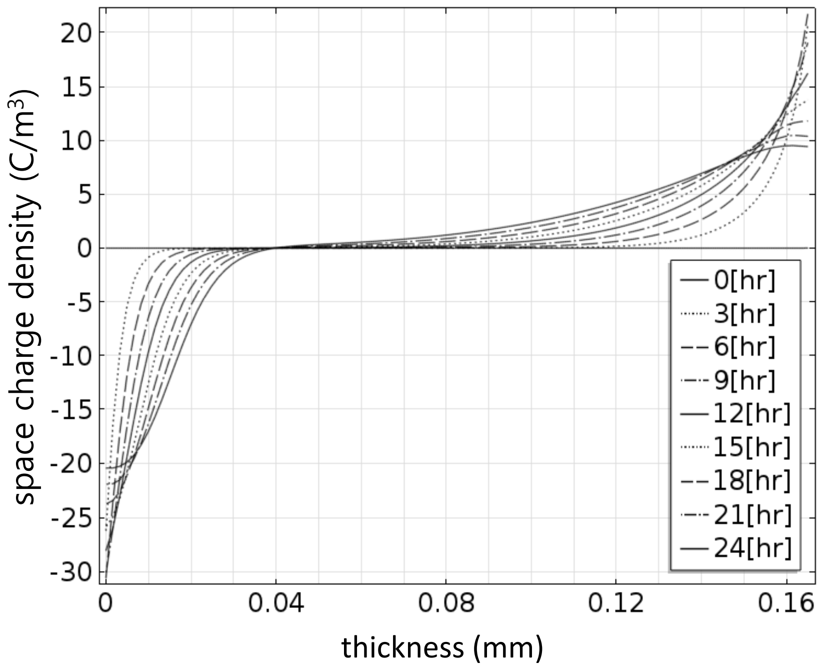


Numerical Model of Insulator

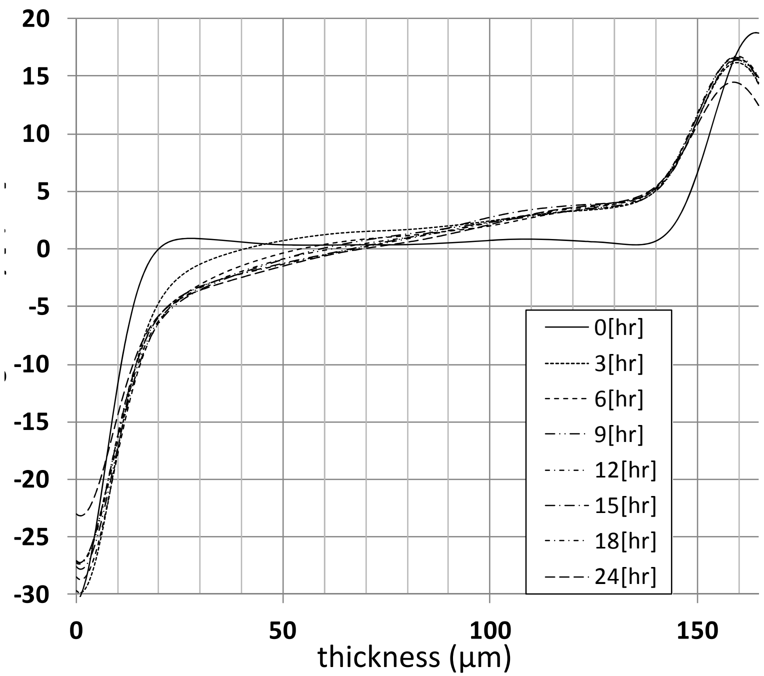
- **Numerical vs. Experimental Results – Space Charge Density**

Space Charge Distribution

Bipolar Charge Transport Model



Space Charge Measurement by PEA

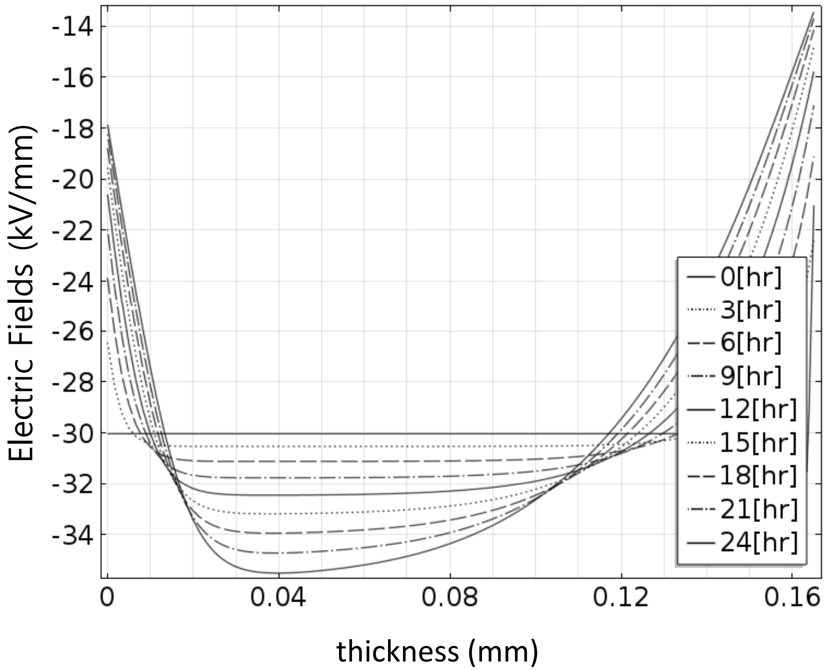


Numerical Model of Insulator

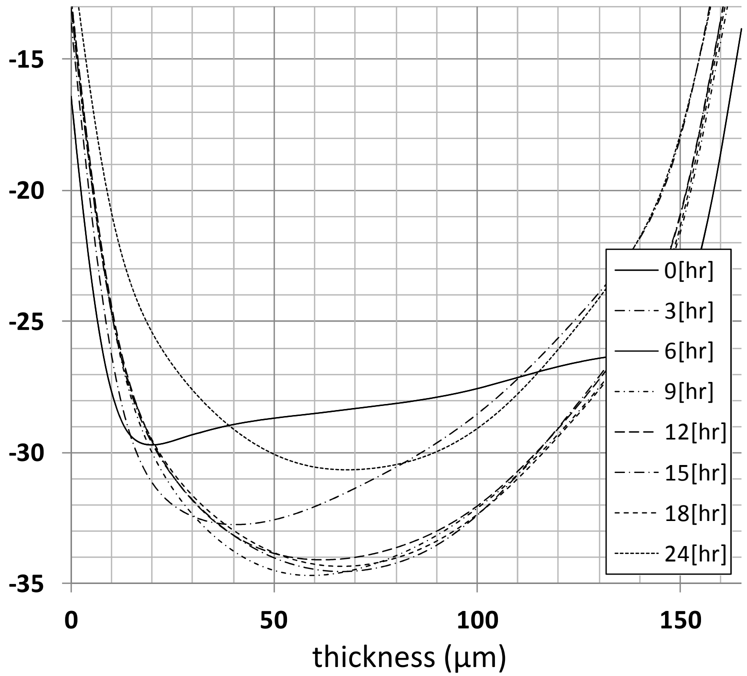
- **Numerical vs. Experimental Results – Space Charge Density**

Electric Fields Distribution

Bipolar Charge Transport Model



Space Charge Measurement by PEA



In Conclusion

- Charge transport behavior must be considered in developing HVDC design.
- In microscopic level, the space charge and conduction mechanisms are related with energy band-gap and shallow/deep trap distribution and these come from chemical defects, physical disorder and impurities or by-products.
- Macroscopic model is implemented by COMSOL Multiphyiscs® software.
    - Electrostatics, Transport of Diluted Species and Heat Transfer modules are used.
    - Single level deep trap, effective mobility and Schottky injection model are adopted.
    - Simulated space charge behavior of XLPE specimen are compared with observed one.
- The material properties required for macroscopic model of insulator can be obtained by quantum chemical calculation or experimental method.

Thank you

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