
# CURRENT FLOW AT THE INTERFACE OF COPPER AND POLYETHYLENE IN HIGH-VOLTAGE APPARATUS

By

**Eng. Mohammed Ahmed El-Shahat Abo-Saleh**

A Thesis Submitted to the
Faculty of Engineering at Cairo University
In partial Fulfillment of the
Requirements for the Degree of

**DOCTOR OF PHILOSOPHY**
**In**
**Electrical Power and Machines Engineering**

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Under the Supervision of

**Prof. Dr. Hussein I. Anis**

**……**

Electrical Power and Machines Department
Faculty of Engineering, Cairo University

**Dr. Ahmed A. Huzayyin**

**……..……**

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Approved by the Examining Committee:

| | |
|---|---|
| **Prof. Dr. Hussein I. Anis** | Thesis main Advisor |
| **Prof. Dr. Hany A. Elghazaly** | Internal Examiner |
| **Prof. Dr. Mohamed A. Izzularab** | External Examiner |

(Professor in Shbeen ELkoom Engineering at Monoufia University)

FACULTY OF ENGINEERING, CAIRO UNIVERSITY
GIZA, EGYPT

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**Engineer:** Mohammed Ahmed El-Shahat Abo-Saleh.
**Date of Birth:** 01 / 10 / 1988
**Nationality:** Egyptian.
**E-mail:** elbagalaty_2010@yahoo.com.
**Phone:** 01007537277
**Address:** Building 907 /distinct 4/ 6 October City / Giza.

**Registration Date:** 01/ 03 / 2014
**Awarding Date:**
**Degree:** Doctor of Philosophy.
**Department:** Electric Power and Machines Engineering.
**Supervisors:** Prof. Dr. Hussein I. Anis.
Dr. Ahmed A. Huzayyin.
**Examiners:** Prof. Dr. Hussein I. Anis.
Prof. Dr. Hany A. Elghazaly
Prof. Dr. Mohamed A. Ezz Elarab
**(**Professor in Shbeen ELkoom Engineering at Monoufia University)

**Title of Thesis:**

Current flow at the interface of copper and polyethylene in high-voltage apparatus.

**Key Words:**
Polyethylene – copper – interface –barrier to injection – dielectric constant.

**Summary:**
Computational quantum mechanics in the framework of density functional theory (DFT) is used to develop the interface model between Cu (111) and PE (001). The "bulk plus band line up" method and the projected density of states (PDOS) analysis are combined to calculate the actual barrier to charge injection. This combination of methods lead to finding new states appearing between the Fermi level of Cu and the conduction band of PE, which lowered the barrier to electrons injection. These states are due to morphological deformation that takes place in both the metal and the polymer at the interface. The most common chemical impurities that are normally found in PE are studied in this thesis to understand their impact on conduction mechanism. These impurities, such as carbonyl, vinyl, and conjugated double bond, produce trap states between the conduction and valence bands of PE, which reduce the barrier height to around the experimental value of 1 eV. The lowered barrier height increases the charge injection, which then facilitates the conduction mechanism. Variations in the dielectric constant at the interface are also a significant factor. The present study investigates the change in dielectric constant of PE at the interface with Cu using the microscopic polarization theory. It is concluded that the calculated current density using Schottky injection mechanism under a certain electric field and temperature does not only depend on the barrier height, but also on the relative dielectric constant at the interface, which in turn changed the current density and the conduction process.

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# LIST OF SYMBOLS

| | |
|---|---|
| $\lambda$ | Trap separation |
| $q$ | Electronic charge |
| $E$ | Electric field |
| $J$ | Current density |
| $A$ | Richardson constant |
| $T$ | Temperature |
| $V_b$ | Barrier to charge injection height |
| $K$ | Boltzmann's constant |
| $\varepsilon$ | Dielectric constant |
| $\varepsilon_0$ | Free space dielectric constant |
| $\varepsilon_r$ | Relative dielectric constant |
| $h$ | Plank's constant |
| $m_T$ | Tunneling effective mass |
| $E_a$ | Electron affinity |
| $a, b, c$ | Lattice constant |
| $E_g$ | Band gap |
| $V_b^e$ | Electrons barrier height |
| $V_b^h$ | Holes barrier height |
| $WF$ | Work function |
| $m$ | Particle mass |
| $\nabla^2$ | Laplacian operator |
| $\Psi$ | Wavefunction |
| $E_T$ | Total energy |
| $E_p$ | Potential energy |
| $\hat{H}$ | Hamiltonian operator |
| $E_k$ | kinetic energy |
| $Z$ | Charge number |
| $r_i$ | Locations of electron i |
| $R_j$ | Locations of nucleus j |
| $\delta(\sigma_i, \sigma_j)$ | Kronecker-Delta function |
| $H_{HF}$ | Hartree-Fock Hamiltonian |
| $E_{P\,x}$ | Exchange potential |
| $E_{P\,Hartree}$ | Hartree potential |
| $E_{P\,c}$ | Correlation potential |
| $n(r)$ | Electron density |
| $E_{P\,ext}$ | External potential energy |
| $F[n]$ | Global functional |
| $E_{xc}$ | Exchange-correlation energy |
| $H_{KS}$ | Khon and Sham Hamiltonian |
| $E_{P\,KS}$ | Effective potential of KS |
| $\emptyset_k$ | Basis set functions |
| $C_k$ | Constant coefficients |
| $L$ | Size of a basis sets |
| $r_c$ | Cutoff radius |

| | |
|---|---|
| $\mathbf{E_{vac}}$ | Vacuum level |
| $\mathbf{E_f}$ | Fermi level |
| $\mathbf{P}$ | Polarization |
| $\boldsymbol{\rho_{ind}}$ | Induced charge density |
| $\mathbf{E_{loc}}$ | Localized field |
| $\mathbf{E_{ext}}$ | External field |

# LIST OF ABBREVIATIONS

| | |
|---|---|
| **PDOS** | Projected density of states |
| **DFT** | Density Functional Theory |
| **CBM** | Conduction band minimum |
| **VBM** | Valence band maximum |
| **QE** | Quantum Espresso |
| **PE** | Polyethylene |
| **Cu** | Copper |
| **Ag** | Silver |
| **Al** | Aluminum |
| **Au** | Gold |
| **Pt** | Platinum |
| **Pd** | Palladium |
| **Si** | Silicon |
| **$SiO_2$** | Silicon oxide |
| **SCLC** | Space-Charge-Limited Conduction |
| **XPS** | X-ray Photoelectron Spectroscope |
| **EELS** | Electron Energy Loss Spectroscope |
| **LDA** | Local density approximation |
| **GGA** | Generalized gradient approximation |
| **HSE** | Heyd-Scuseria-Ernzerhof |
| **HF** | Hybrid functionals |
| **MCSCF** | Multi configuration self-consistent field |
| **CI** | Configuration interaction |
| **CC** | Coupled cluster |
| **MP** | Perturbation theory by MØller and Plesset |
| **HK** | Hohenberg and Kohn |
| **KS** | Kohn and Sham |
| **SCF** | Self-consistent field |
| **LCAO** | Linear Combination of Atomic Orbitals |
| **PW** | Plane Waves |
| **AS** | Atomic Sphere |
| **CG** | Conjugate gradient |
| **BFGS** | Broyden- Fletcher-Goldfarb-Shanno |
| **MD** | Molecular Dynamics |
| **DOS** | Density of states |
| **GDIIS** | Geometric direct inversion in the iterative subspace |
| **CP** | Car-Parrinello |
| **PWSCF** | Plane-Wave Self-Consistent Field |
| **PAW** | Projector Augmented Waves |
| **PBE** | Perdew-Burke-Ernzerhof |
| **FCC** | Face centered cubic |
| **PEA** | Pulsed electro-acoustic |

# ABSTRACT

Polymers are increasingly becoming the insulator of choice in various high voltage power apparatus, such as capacitors and cables. Under high operating fields conduction (leakage) currents in polymers contribute to the eventual breakdown of the insulator, thus determining its active life time. A barrier to charge injection at polymer/metal interface is a key to understanding the high field conduction in cables and supercapacitors. The conduction mechanism of injected currents is influenced by barriers to charge injection and also by possible variations in the dielectric constant at the interface. The present work investigates barriers to charge injection at the atomic level at the interface of copper and polyethylene (PE), one of the most dominant material combinations in the power industry. Emphasis is carried out in this work on morphological deformation.

Computational quantum mechanics in the framework of density functional theory (DFT) is used to develop the interface model between Cu (111) and PE (001) in the light of previous DFT studies on the interface of PE with Pt, Au, and Ag in terms of the absolute barriers to holes and electrons injection. The "bulk plus band line up" method and the projected density of states (PDOS) analysis are combined to calculate the actual barrier to charge injection, which was not well identified in similar studies. This combination of methods lead to finding new states appearing between the Fermi level of Cu and the conduction band of PE, which lowered the barrier to electrons injection. These states are due to morphological deformation that takes place in both the metal and the polymer at the interface. The present work stresses the importance of considering morphological deformation in lowering the barriers to charge injection in soft metal which is less considered as compared to chemical impurities.

The most common chemical impurities that are normally found in PE are studied in this thesis to understand their impact on conduction mechanism. These impurities, such as carbonyl, vinyl, and conjugated double bond, produce trap states between the conduction and valence bands of PE, which reduce the barrier height to around the experimental value of 1 eV. The lowered barrier height increases the charge injection, which then facilitates the conduction mechanism.
This work recognizes the fact that the barrier height is not the sole factor affecting conduction. Variations in the dielectric constant at the interface are also a significant factor. The present study investigates the change in dielectric constant of PE at the interface with Cu using the microscopic polarization theory. It is concluded that the calculated current density using Schottky injection mechanism under a certain electric field and temperature does not only depend on the barrier height, but also on the relative dielectric constant at the interface, which in turn changed the current density and the conduction process.