Expanding the horizon of photoelectric investigations of the MIS system properties

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Outline

1. Introduction

2. Essentials and limitations of the classical theory of internal photoemission
   - Strong points - weak points of the classical theory
   - Why classical theory breaks down at low electric fields

3. Our model for photocurrents at low electric fields
   - Mathematical skeleton and comparison with experiments
   - Importance of diffusion current

4. Our method to extract the magnitude and the behavior of the diffusion currents

5. Measurement methods based on application of our models

6. Summary
1. Introduction

Band diagram of a Metal-Insulator-Semiconductor (MIS) system

Typical setup for photoelectric measurements of a MIS structure

Photoemission yield: \( Y = \frac{\text{Number of electrons emitted from emitter}}{\text{Number of photons absorbed by emitter}} \)

\[
Y = \frac{I \ h\nu}{P} \quad I - A \quad h\nu - eV \quad P - W
\]

Rzeszów June 26, 2019
2. Classical theory: history and essentials

Milestones of the history of photoemission

1. 1931. R.H. Fowler, external photoemission from metal: \( Y = A(\nu - E_B)^2 \)
2. 1960-70, E.O. Kane, J.M. Ballantyne: important theoretical studies on external photoemission from metals
3. 1962 G.W. Gobeli, F.G. Allen theoretical and experimental studies on external photoemission from silicon: \( Y = A(\nu - E_B)^3 \)

\[
Y = A(\nu - E_B + mV_{1/2})^p \exp(-z_0/L)
\]

Backbone of classical theory

\( A \) - constant, \( \nu \) – photon energy, \( E_B \) - potential barrier height
\( m \) - coefficient, constant for a given MOS structure: \( m = \sqrt{\frac{q}{4\pi\varepsilon_0 d}} \)
\( V_1 \) – potential drop on the dielectric, \( p \)–exponent=2 for metal=3 for semiconductor
\( z_0 \) – distance between the emitter surface and top of barrier: \( z_0 = \sqrt{\frac{qd}{16\pi\varepsilon_0 V_i}} \)
\( L \) – scattering length of electrons in the image force potential well


Research group at NIST (USA) led by N.V. Nguyen which published a number of papers advancing the understanding the MIS system photoelectric properties

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Rzeszów June 26, 2019
2. Classical theory: failure at $E \rightarrow 0$

- Significant differences between classical theory and experiment at low electric fields in the dielectric
- The voltage coordinate of the zero photocurrent point depends on the wavelength of light illuminating the sample.
- The shape of the $I$ vs. $V_i$ characteristics depends on the wavelength of light

\[ j = q \mu n_c E + \mu kT \frac{dn_c}{dx} \]

\[ \text{drift} \quad \text{diffusion} \]

At one wavelength of light

\[ \lambda = 220 \text{ nm}, \lambda = 230 \text{ nm}, \lambda = 240 \text{ nm}, \lambda = 250 \text{ nm}, \lambda = 260 \text{ nm} \]

Photocurrent $I$ vs. voltage drop in the dielectric $V_i$.
Focus on region where photocurrent changes sign.

Lot Fims3
Sample W5

- Rzeszów June 26, 2019
2. Classical theory: physics of failure at $E \to 0$

$J = q\mu n_c E + \mu kT \frac{dn_c}{dx}$

- $J \text{ [A/cm}^2\text{]}$ – photocurrent
- $q \text{ [C]}$ – electron charge
- $\mu \text{ [cm}^2\text{/Vs]}$ – mobility
- $n_c \text{ [cm}^{-3}\text{]}$ - concentration of electrons
- In the conduction band
- $kT \text{ [VC]}$ – diffusion potential
- $E \text{ [V/cm]}$ - electric field
- $X \text{ [cm]}$ – coordinate perpendicular to dielectric interfaces

Fractions of light power absorbed by 25nm Al gate and by silicon substrate in function of the light wavelength $\lambda$ (Effect of interference)

$t(\text{SiO}_2)=140\text{nm}$
3. Our theory of photocurrent at low electric fields

Mathematical formulation, solution and comparison with experiment

Solution for \( J=0 \)

\[
j = q\mu n_c(x)E(x) + \mu kT \frac{dn_c}{dx}
\]

\[
\frac{\varepsilon}{q} \frac{dE}{dx} = -n(x)
\]

\[
n_c = \Theta n
\]

\[
\frac{d^2 y}{dz^2} + \frac{1}{2} (J_z + C_z) y = 0
\]

\[
V_G^0 = \frac{kT}{q} \left[ \ln \frac{A(\lambda)}{T(\lambda)} + \ln \frac{(h\nu - E_{BG})^{p_s}}{(h\nu - E_{BS})^{p_s}} \right] + C
\]

\( V_G^0 \) – gate potential for zero voltage drop in dielectric

\( V_G \) – gate potential for zero photocurrent

\( n_c \) – density of electrons in the conduction band

\( n \) - total density of electrons

\( j \) – photocurrent density

\( J \) – normalized photocurrent density

\( E_{BG} \) - barrier height at gate dielectric interface

\( E_{BS} \) - barrier height at semiconductor-dielectric interface

\( p \) – exponent equal 2 for metal equal 3 for semiconductor

\( C \) - constant

\( z \) – normalized distance

\( y \) - function of voltage drop in dielectric

\( \varepsilon \) – electrical permittivity

For \( J=0 \)

\[
q = \text{electron charge}
\]

\[
\mu = \text{electron mobility}
\]

\[
h\nu = \text{photon energy}
\]

\[
A(\lambda) = \text{fraction of light power absorbed by the gate}
\]

\[
T(\lambda) = \text{fraction of light power absorbed by the substrate}
\]

\[
\Theta = \text{proportionality factor}
\]
4. Our theory of photocurrent at low electric fields

Mathematical formulation, solution and comparison with experiment

Solution for \( j \neq 0 \):

Airy equation

\[
d^2 y + u y = 0
\]

Solution of Airy equation

\[
y = A[Ai(u) + C_2Bi(u)]
\]

\[
Ai^I(u_0)Bi^I(u_1) - k_1Ai^I(u_0)Bi(u_1) - k_0Ai(u_0)Bi^I(u_1) + k_0k_1Ai(u_0)Bi(u_1) = \\
= Ai^I(u_1)Bi^I(u_0) - k_0Ai^I(u_1)Bi(u_0) - k_1Ai(u_1)Bi^I(u_0) + k_0k_1Ai(u_1)Bi(u_0)
\]

E.g. \( j = f([u_0-u_1]^3] \)

\( Ai(u) \) – Airy Ai function of \( u \), \( Bi(u) \) – Airy Bi function of \( u \)
\( Ai^I(u) \) – Airy Ai Prime function of \( u \), \( Bi^I(u) \) – Airy Bi Prime function of \( u \)
\( k_0 \) and \( k_1 \) are the known functions of electron densities at both interfaces of the dielectric. \( A \) and \( C_2 \) are constants

Main differences between the classical and our theory

Classical

\( j = q\mu n_c E \)

No space charge in the insulator

Our theory

\( j = q\mu n_c E + \mu kT \frac{dn_c}{dx} \)

space charge limited current

\( \varepsilon/q \frac{dE}{dx} = -n(x) \) and \( n_c = \theta n \)

5. Expanding the horizon: Magnitude of diffusion current

\[ j = q \mu n_c E + \mu kT \frac{dn_c}{dx} \]

- \( j_E \): drift component
- \( j_D \): diffusion component

On the \( \lambda = 210 \) nm characteristic at \( V_G = V_{G0} \), \( j = j_D = 3.53 \times 10^{-11} \text{ A/cm}^2 \)

On the \( \lambda = 260 \) nm characteristic at \( V_G = V_{G0} \), \( j = j_D = -4.42 \times 10^{-11} \text{ A/cm}^2 \)
5. Expanding the horizon: Magnitude of diffusion current

Photocurrent \( j \) and its drift – \( j_E \) and diffusion - \( j_D \) components vs. Electric field in the dielectric – \( E_i \)

for \( \lambda = 210 \) nm

\[
J = 3.5041E-11 + 7.52088E-15*E_i + 4.88021E-20*E_i^2
\]

\( j_E = 7.52088E-15*E_i \)

\( j_D = 3.5041E-15 + 4.88021E-20*E_i^2 \)

Photocurrent \( j \) and its drift – \( j_E \) and diffusion - \( j_D \) components vs. Electric field in the dielectric – \( E_i \)

for \( \lambda = 260 \) nm

\[
J = 4.0432E-11 + 4.75014E-15*E_i - 8.38256E-20*E_i^2
\]

\( j_E = 4.75014E-15*E_i \)

\( j_D = -4.0432E-11 - 8.38256E-20*E_i^2 \)

\[
j = q \mu n_C E + \mu kT \frac{dn_C}{dx}
\]

H.M. Przewłocki - Unpublished
6. Practical applications of the considerations presented

6.1 The photoelectric method of the $\phi_{MS}$ factor determination

$\phi_{MS}$ – the effective contact potential difference in the MIS system

In general

$$V_G = V_I + \phi_S + \phi_{MS}$$

At flat band in dielectric ($V_I = 0$)

$$V_{G0} = \phi_{S0} + \phi_{MS}$$

- $V_{G0}$ can be very accurately determined from the straight line characteristic of photocurrent $j$ vs. Electric field $E$

- $\phi_{S0}$ can be found from independently measured $C(V)$ characteristic

- $\phi_{MS}$ can be determined with the accuracy of $\pm 10$ mV

This makes it the most accurate of the existing $\phi_{MS}$ determination methods

6. Practical applications of the considerations presented

6.2 The method of quantitative monitoring of the processing operations which generate trapping centers in the insulator

\[ j = q\mu n_C E \]

or in other words

\[ j = qn\mu \theta E \]

where \( \theta = \frac{n_C}{n} \)

Reduction of slope \( q\mu n_C \) of the straight line characteristic resulting from e.g. plasma treatment

Initial slope: \( qn\mu \theta = 2.2192 \times 10^{-14} \frac{A}{\text{Vcm}} \)

Changes with the intensity of processing

\[ j = q\mu n_C E + \mu kT \frac{d\nu_C}{dx} \]
7. Summary

- Classical theory of internal photoemission in the MIS system was outlined and its limitations pointed out

- Mathematical formulation of our model which eliminates the deficiency of classical theory was presented and results of its application compared with experiment

- Physical details of the model were discussed with the emphasis on the role of diffusion currents

- A simple method of extracting the diffusion component from the experimental characteristics was demonstrated

- Examples of useful measurement methods based on our model were given
Thank you
4. Why classical theory breaks down at low electric fields
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\[ j = q\mu n_c(x)E(x) + \mu kT \frac{dn_c}{dx} \]

\[ \frac{\varepsilon}{q} \frac{dE}{dx} = -n(x) \]

\[ n_c = \theta n \]

\[ \frac{d^2y}{dz^2} + \frac{1}{2} (J_z + C_1) y = 0 \]

\[ V_G^0 = \frac{kT}{q} \left[ \ln \frac{A(\lambda)}{T(\lambda)} + \ln \frac{(h\nu - E_{BG})^{p_s}}{(h\nu - E_{BS})^{p_s}} \right] + C \]
The graph shows the relationship between current density ($j$) and electric field ($E_i$) with the equation:

$$j = 3.5041 \times 10^{-11} + 7.52086 \times 10^{-15} E_i + 4.88021 \times 10^{-20} E_i^2$$

The residual sum of squares is $3.19662 \times 10^{-22}$, and the adjusted R-square is 0.99924.
Photocurrent $j$ and its drift – $j_E$ and diffusion - $j_D$ components vs. Electric field in the dielectric - $E_i$

Equation:
$$y = \text{Intercept} + B1 \times x^1 + B2 \times x^2$$

Weight: No Weighting

Residual Sum of Squares: 3,19662E-22

Adj. R-Square: 0.99924

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Standard Error</th>
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<tr>
<td>Intercept</td>
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<tr>
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<tr>
<td>B2</td>
<td>4.88021E-20</td>
<td>2.36963E-21</td>
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$$j = \text{Intercept} + 7.52086E-15 \times E_i + 4.88021E-20 \times E_i^2$$

$R^2 = 0.99924$

## Photocurrent $j$ and its drift – $j_E$ and diffusion - $j_D$ components vs. Electric field in the dielectric - $E_i$

$$j = -4.04328E-11 + 4.75014E-15 \times E_i - 8.38256E-20 \times E_i^2$$

$R^2 = 0.99921$

Equation:
$$y = \text{Intercept} + B1 \times x + B2 \times x^2$$
Recent advances in photoelectric characterization technique

Advantages of GIS vs. MIS capacitors

**MIS capacitor**

**GIS capacitor**

![Graphene-SiO_{2}-Si](image)

- Gate voltage $V_G$ [V]
  - R
  - T
  - A

- Photocurrent $I_F$ [pA]
  - 1
  - 2
  - 3
  - 4
  - 13
  - 15

- Photoelectric characterization technique

Bydgoszcz 2017.06.21
Recent advances in photoelectric characterization technique

Our measurement results of a Graphene – SiO$_2$ – Si structure

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<tr>
<th>Measurement no.</th>
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<th>$E_h$</th>
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<th>$E_{G(SiO_2)}$</th>
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<td>7</td>
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<td>Result of this work</td>
<td>4.34 ± 0.01</td>
<td>4.70 ± 0.03</td>
<td>1.12</td>
<td>7.92 ± 0.04</td>
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<td>Result of NIST</td>
<td>4.3 ± 0.1</td>
<td>4.6 ± 0.1</td>
<td></td>
<td>7.9 ± 0.2</td>
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</table>
Photocurrent $I$ vs. voltage drop in the dielectric $V_I$.

Focus on region where photocurrent changes sign.

Lot Fims3
sample W5

\[ j = q \mu n_c E + \mu kT \frac{dn_c}{dx} \]
Negative photocurrent

Positive photocurrent

Negative photocurrent

Positive photocurrent

$V_G$ $E_F$ $E_C$ $E_V$ $M$ $I$ $S$

$I = 0$?

$I = 0$?
4. Our theory of photocurrent at low electric fields: Practical application

A method to accurately determine the effective contact potential difference \( \phi_{MS} \) in the MIS system

In general

\[
V_G = V_I + \phi_S + \phi_{MS}
\]

At flat band in dielectric \( (V_I = 0) \)

\[
V_{G0} = \phi_{S0} + \phi_{MS}
\]

\( \phi_{S0} \) can be found from independently measured \( C(V) \) characteristic

\( \phi_{MS} \) can be determined with the accuracy better than ± 10 mV

This makes it a simple and most accurate of the existing \( \phi_{MS} \) determination methods

Thank you
Characteristics of the photocurrent $I$ vs. gate voltage $V_G$.
Focus on the region where photocurrent changes sign.
Photocurrent \( j \) and its drift – \( j_E \) and diffusion - \( j_D \) components vs. Electric field in the dielectric – \( E_i \) for \( \lambda=260 \text{ nm} \)

\[
j = -4.04328E-11 + 4.75014E-15 \cdot E_i - 8.38256E-20 \cdot E_i^2
\]

\( R^2 = 0.99921 \)

\[
J = -4.04328E-11 + 4.75014E-15 \cdot E_i - 8.38256E-20 \cdot E_i^2
\]

\[
j_E = 4.75014E-15 \cdot E_i
\]

\[
j_D = -4.04328E-11 - 8.38256E-20 \cdot E_i^2
\]
Fractions of light power absorbed by 25nm Al gate and by silicon substrate in function of the light wavelength $\lambda$. $t(\text{SiO}_2) = 140\text{nm}$

\[ j = q \mu n_c(x) E(x) + \mu kT \frac{dn_c}{dx} \]

\[ \varepsilon \frac{dE}{q dx} = -n(x) \]

\[ n_c = \varepsilon n \]

\[ V_G^0 = \frac{kT}{q} \left[ \ln \frac{A(\lambda)}{T(\lambda)} + \ln \frac{(h \nu - E_{BG})^{\mu_g}}{(h \nu - E_{BS})^{\mu_s}} \right] + C \]
Recent advances in photoelectric characterization technique

Photocurrent of electrons emitted from substrate at positive gate bias

Photocurrent of holes emitted from substrate at positive gate bias

Determination of the insulator band gap $E_{GI}$

$$E_{GI} = E_{belectrons} + E_{bholes} - E_{GS}$$
4. Why classical theory breaks down at low electric fields

- **a)** Negative photocurrent
- **b)** Positive photocurrent
- **c)** No photocurrent???

NOT NECESSARILY
A - constant, \(h\nu\) - photon energy, \(E_B\) - potential barrier height, \(m\) - coefficient, constant for a given MOS structure: 
\[m = \text{coefficient} \sqrt{\frac{q}{4\pi\varepsilon\varepsilon_0d}}\]

\(V_I\) - voltage drop on the dielectric, \(p\) - exponent 
\(p = 2\) for metal = 3 for semiconductor 
\(z_0\) - distance between the emitter surface and the top of barrier: 
\[z_0 = \sqrt{\frac{qd}{16\pi\varepsilon\varepsilon_0V_i}} \cdot L\]

- scattering length of electrons in the image force potential well