Modelling of Surface Traps Effect on Semiconductor Nanowires

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Outlines

- Effect of *Surface Traps on NW Photoconductivity*

- NW conduction type p-n-switching due to surface traps

- The effect of interface traps on electrical characteristics of NW junctionless (JL) FETs
Due to high surface to volume ratio, **Nanowires (NWs)** are the most affected by surface traps topologies.

The effect of surface traps on device performance especially is pronounced while considering NWs as photoconductors.

Surface traps result from the interruption of the periodic lattice structure at the surface of a crystal.
The surface recombination of nonequilibrium electron-hole pairs through the surface states is the prevailing mechanism in NW PC

Minority carriers recombination with the trapped majority carriers.

bulk recombination through middle band-gap recombination centers: (t~ps)

surface recombination through the surface states: (t~minutes)

electrons and holes generated in conduction and valence band, respectively.

The contrast in time domain was used to obtain information about the energy density of trap states.

The model of photoconductivity

When the light is on the dynamics of PC is determined by rate equation written for the surface density of electrons $n_s$:

$$\frac{dn_s}{dt} = -(\frac{dn_s}{dt})_{\text{therm. act.}} + (\frac{dn_s}{dt})_{\text{capt. el.}} - (\frac{dn_s}{dt})_{\text{capt.holes}}$$

$$\frac{dn_s}{dt} = s \nu n(R)(N_S - n_s(t)) - (\frac{dn_s}{dt})_{\text{capt.holes}} - v s N_C n_s(t) e^\frac{E_S}{kT}$$

$N_S$ - is the density of surface traps,

$n_s$ - is the surface density of electrons,

$\nu$ - is the thermal velocity,

$s$ - is the electron capture cross section by surface traps,

$N_C$ - is the effective density of states in the conduction band,

$n(R)$ - is the volume density of electrons at the surface.

Comparison of analytical model and experimental data:

N.A. Stanford, P. T. Blanchard, K.A. Bertness et al.

Photocurrent over time graph illustrated in the scale of milliseconds.

The PC decay after turning the light off.

GaN NW

Photocurrent / dark current

Markers - Experimental data [11]
Lines - Analytical model

$N_D = 9 \times 10^{16} \text{ cm}^{-3}$
$P = 3.6 \text{ mW cm}^{-2}$,
$R = 160 \text{ nm}$
$L = 3.4 \mu \text{m}$

$\begin{align*}
P &= 0.05, 0.1, 0.2, 0.3 \text{ (mW/cm}^2) \\
\end{align*}$
Conclusion:

- The developed model explains both the dark conductivity and dynamics of PC transients.

- The kinetics of the photoconductivity is characterized by long-period relaxation processes. The persistent PC can be observed even at room temperatures.

- At small intensities we calculate very high photoconductive gain ($10^8$-$10^9$). Gain follows an inverse power law $G_n \sim P^{-k}$, where $k=0.9$. Also, one may expect that such a ultra-high gain could allow reaching even single-photon detection in a NW based photoconductor.

- **Surface traps play crucial role in NW PC!**
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The effect of surface traps on a single NW

Let’s consider n-type s/c NW and acceptor type surface traps

Upon depending on NW parameters: radius (R), the doping density (ND) and the density of surface states (Ns) the NW can be:

- **Partially depleted** (only part of the electrons are trapped on the surface)
- **Fully depleted** (all the electrons are removed from the volume)
- **Inverted** (electrons from valance band are captured by surface traps and holes become majority)
Surface traps ultimate effect on NW: the conduction type switching

- Inversion due to the surface traps when decreasing the NW radius

**Experimental**

Where we can ignore the inversion and where not?

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \varphi}{\partial r} \right) = -\frac{q}{\varepsilon_{sc}} (N_D - n(r) + p(r))
\]

\[
\left. \frac{\partial \varphi}{\partial r} \right|_{r=0} = 0 \quad \left. \frac{\partial \varphi}{\partial r} \right|_{r=R} = -q N_s f(E_t) / \varepsilon_{sc}
\]

Numerical “exact” solution

✓ When the NW is highly doped the inverted charge is negligible even at very small radii (5 nm) and high density of surface traps.
For lightly doped NWs the inversion takes place already at 40nm radius.

✓ At low densities of surface traps the inversion doesn’t occur while reducing the NW radius for doping densities exceeding \( N_D = 5 \times 10^{16} \text{ cm}^{-3} \).
An analytical potential-based model to calculate the inverted charge in moderate or lightly doped NWs

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \varphi}{\partial r} \right) = - \frac{q}{\varepsilon_{sc}} (N_D - n(r) + p(r))
\]

\[
\left. \frac{\partial \varphi}{\partial r} \right|_{r=0} = 0 \quad \left. \frac{\partial \varphi}{\partial r} \right|_{r=R} = - q N_s f(E_t) / \varepsilon_{sc}
\]

A regional approach is applied. 3 electrostatic regions along the NW radius are considered and apply different simplifying assumptions for each region:

- inversion region close to the surface
- next follows the region of full depletion
- the electro-neutral region close to the center of NW

These regional approximations allow us to get the continuous potential distribution in radial direction throughout the whole NW.
Validation of analytical potential model with 3D Sentaurus TCAD

Potential and mobile charge radial distribution depicted respectively on left and right axes in NWs with 20 nm radius: a), and 10 nm radius: b).
Central and surface potentials for NWs with different radii. Lines: analytical model, circles: numerical calculations (Wolfram)

The dependences of floating \((x_0, x_1)\) points on NW radii at normalized radial axis: left axis, and at non-normalized axis: the inset
Inverted charge calculation

Charge neutrality equation:

\[ 2\pi R n_S = \pi R^2 N_D + 2\pi \left( \int_{x_i}^{x_0} p(r) r \, dr - \int_0^{x_0} n(r) r \, dr \right) \]

\[ Q_{mob} = q(2\pi R n_S - \pi R^2 N_D) \]

Total mobile charge in NW:

\[ \rho_m^* = \frac{Q_{mob}}{q\pi R^2} \]

\[ n_s = \delta N_{sm} \left[ \frac{N_D}{n_i} \exp \left( \frac{kT}{\delta} u(1) \right) - 1 \right] \]
Conclusion:

- We clarified the conditions when the surface traps effect can cause inversion in NW.

- The potential model was developed including both type of mobile charges in Poisson equation.

- The derived potential model provides a simple way to calculate the inverted charge density raised due to surface traps effect.

- The model accurately predicts the radius dependent conductivity type switching in semiconductor NWs which is important for optimal design of nanowire devices.
Outlines

- Effect of *Surface Traps on NW Photoconductivity*

- The ultimate effect of surface traps on NW conduction type, causing p-n-switching, analytical model

- The effect of interface traps on electrical characteristics of NW junctionless (JL) FETs
How strong is the impact of surface traps on NW based FETs?

- The CMOS technology uses dedicated processes to neutralize fixed-charges and surface traps, *the density of surface traps can be reduced to $N_s = 10^{10} \text{cm}^{-2}$.*

- However when NW FETs are used as an ‘open surface’ sensor elements then these sensors are subjects to host many more defects than the state of the art CMOS devices.

- For sensing applications junctionless (JL) FETs are the most used, as there are no junctions along the NW: conducting channel, source and drain have the same doping type and density, which makes easy the fabrication process.

- The effect of interface traps on JL FET characteristics was presented

Modeling self-depletion induced by traps in ungated highly doped NWs

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \varphi}{\partial r} \right) = -\frac{q}{\varepsilon_{sc}} (N_D - n(r)) \]

Charge neutrality requires a balance between charges in the semiconductor and charges at the interfaces

\[ Q_{sc} = -Q_{SS}^\text{c} = q \frac{N_s}{1 + \exp\left(\frac{E_t - i}{kT}\right) \exp\left(-\frac{\varphi_S}{U_T}\right)} \]

\[ \varphi_s = \frac{qR^2}{4\varepsilon_{si}} \left( n_i \exp\left(\frac{\varphi_0}{U_T}\right) - N_D \right) + \varphi_0 \]

\[ E_s^2 = \frac{qn_i U_T}{\varepsilon_{si}} \left[ \left( \frac{\varphi_s}{U_T} - \frac{\varphi_0}{U_T} \right) - \frac{N_D}{n_i} \left( \frac{\varphi_s - \varphi_0}{U_T} \right) \right] \]


The effect of interface traps on electrical characteristics of highly doped Si NWs

NW channel depletion in %

NW normalized mobile charge in linear and logscale

Markers – TCAD Synopsys Sentarus 3D simulations
Lines – physics-based compact analytical model

- Almost full trapping occurs in mid-gap states
- The exponential dependence is very well captured which would not be possible relying on full depletion approximation.
Charge based modeling of NW junctionless FETs with interface traps

\[ \varphi_s = \frac{qR^2}{4\varepsilon_{si}} \left( n_i \exp \left( \frac{\varphi_0 - V}{U_T} \right) - N_D \right) + \varphi_0, \]

\[ E_s = \left[ \frac{qn_i U_T}{\varepsilon_{si}} \left( e \frac{\varphi_s - V}{U_T} - e \frac{\varphi_0 - V}{U_T} \right) - \frac{N_D}{n_i} \left( \frac{\varphi_s - \varphi_0}{U_T} \right) \right]^{1/2}. \]

\[ Q_{ss}^- = -q \frac{N_s}{1 + \exp \left( \frac{E_{t-i}}{kT} \right) \exp \left( -\frac{\varphi_s - V}{U_T} \right)} \]

\[ Q_{sc} = -Q_G = -C_{ox} \left( V_G^* + \frac{Q_{ss}^-}{C_{ox}} - \varphi_s \right) \]

✓ We introduce the interface trapped charge effect in charge based model by adding \( \delta = \frac{Q_{ss}^-}{C_{ox}} \) shift to the effective gate voltage and avoid further modifications of explicit drain current model.

The effect of interface traps on electrical characteristics of NW junctionless (JL) FETs

An exponential distribution for the trap density with respect to the energy is considered

To make more visible the effect of surface traps, the drain current is also obtained for zero density of interface traps at $V_D = 1\, \text{V}$ and is depicted with black dashed-line.

Lines: analytical model
Circles: Synopsys Sentarus 3D TCAD
Inclusion of surface traps in nanowire topologies has been done on top of a charge-based model developed previously.

Different trap energies and densities were analyzed in detail.

The proposed model reproduces correctly the results obtained from TCAD simulations.

This research represents an interesting development which can be useful for the design of nanowire based biosensors where the free surface is used to sense biological solutions and chemicals.
Technologies in Armenia

- Micro-and nano-electronics
- Photonics
- Advanced Materials
- Nanotechnologies
- Biotechnology

- Well developed*
- Less developed

*) Approximate picture
IT services export

If we look to IT services export chart we see that with this index Armenia is placed at the top of CIS countries.

The chart is provided from World Bank publications 2012.
National and international collaboration

There are 360 R&D companies operating in Armenia. The chart below illustrates the distribution of R&D companies by local and foreign ownerships.

According to data (source EIF), 151 foreign companies operating in Armenia have the following distribution of ownership.

These charts are from Enterprise Incubator Foundation (EIF) “Armenian ICT Sector 2012 State of Industry Report.”
Usefull links to find more about the current situation in science and activities of research groups:

**Research & Development**

- Journal of Contemporary Physics, Publisher *Springer Verlag*
- Center of Semiconductor Devices & Nanotechnologies: [http://www.semicond.ysu.am/](http://www.semicond.ysu.am/)
- State Committee of Science: [http://scs.am/?hl=en_US](http://scs.am/?hl=en_US)

**Commercial-Technology oriented organizations**

- Enterprise Incubator Foundation (EIF): [http://www.eif.am/eng](http://www.eif.am/eng)

ESSDERC

MOS-AK, September 2017, Leuven
Cooperation of High Education with Private Businesses

- Armenian universities have close cooperation with private businesses.

  Example of such cooperation is:

  - Interdepartmental Chairs of “Microelectronic Circuits and Systems” established by Synopsys at SEUA, YSU, RAU since 2004.

    Synopsys has the heavy investment in local microelectronics education.

    Established a presence in Armenia in 2004 Synopsys currently is one of the largest IT employers in Armenia with more than 570 employees.

✓ These cooperation of business and high education provides Armenia with highly qualified and industry-ready IT specialists.
Research activities:

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- Thin film solar cells research
  ✓ Thin-film CIGS solar cells on non-conducting perlite

- Theoretical studies of nanowires and nanospheres

- Electronic Device Compact Modeling

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Thank you for your attention