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Unified tunnelling-diffusion theory for Schottky and very thin MOS structures

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ABSTRACT

We derive general formulae for calculating the transport of free charge carriers in a MOS structure with a thin insulating layer. In particular, we obtain relationships for boundary concentrations of free charge carriers on the insulator–semiconductor interface and for the current densities flowing through the MOS structure. Our direct tunnelling-diffusion approach makes the well known thermionic emission–diffusion theory for the Schottky interface applicable also to metal–insulator–semiconductor barriers with a very thin insulator layer. We demonstrate how direct tunnelling through the insulating layer and drift–diffusion of free charge carriers in the semiconductor affect the *I–V* and *C–V* curves and the boundary concentrations needed to numerically solve the continuity equations.

1. Introduction

MOS FET structures with a thin high-κ oxide layer and a metallic gate represent a new generation of unipolar integrated circuits [1]. Analysis of the physical phenomena in the MOS structures, particularly in the 1–2 nm scale of insulator thickness, requires deep knowledge of the processes taking place in the oxide layer, in the underlying working region of the semiconductor and at their interface. At this length scale, quantum-mechanical tunnelling through the gate dielectric causes a significant leakage current which raises numerous problems with static power dissipation [2] and reliability of the dielectric [3]. Therefore, accurate modelling of the tunnelling current through the gate dielectric and subsequent predictive simulation is inevitable for a proper device and circuit design. Many papers dealing with this hot topic were presented within the last few years [4–8]. A comprehensive review and detailed comparison of existing models is given in [9].

The formulae we present generalize the well established thermionic emission–diffusion theory for metal–semiconductor barriers derived by Crowell and Sze [10] and later by Simmons and Taylor [11] and Tung [12]. Simulation of *I–V* and *C–V* characteristics contributes to a thorough understanding of the phenomena taking place in the MOS structure with the thin high-κ oxide gate layers.

2. Theory

The theory charge transfer through the MOS structures is based on 1-D self-consistent solution of the Schrödinger and Poisson equations and of the continuity equations for electrons and holes in a metal/dielectric/silicon stack. The Schrödinger equation is solved by the effective mass approximation applying closed boundary conditions, the final result being the tunnelling probability.

Our model is 1-D, it does not consider a 2-D MOSFET structure. Therefore, the transport of charge carriers is not affected by the current flowing in the transistor structure between the source and drain. The theory takes into account direct tunnelling of charge carriers through the insulating layer and drift–diffusion, as well as tunnelling mechanisms of charge transport in the semiconductor. The continuity equations along with the formulae for boundary electron and hole concentrations on the insulator-to-semiconductor interface constitute the basic set of equations. For the sake of simplicity we will distinguish the quantities related to electrons and holes by indices. For example, electron and hole concentrations are denoted as c^{e} and c^{h}, respectively. Similarly, the upper sign in the equations belongs to electrons, the lower sign to holes.

The Poisson equation takes the form

$$-\frac{d}{dx}\left(\kappa\frac{d\psi}{dx}\right)=\frac{q}{\varepsilon_0}\left(c^{h}-c^{e}+N_D-N_A\right) \tag{1}$$

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Nomenclature

C	capacitance of the MOS structure ($F\,m^{-2}$)
C_{ox}	capacitance of the sandwich oxide layer ($F\,m^{-2}$)
C_S	differential capacitance of the semiconductor ($F\,m^{-2}$)
$c^{e,h}$	density of free electrons or holes in the semiconductor (m^{-3})
$c_S^{e,h}$	density of free electrons or holes at the place of the insulator–semiconductor interface (m^{-3})
$c_{S0}^{e,h}$	density of free electrons or holes at the place of the insulator–semiconductor interface under TDE (m^{-3})
$c_{T\_GR}^{e,h}$	quantity having a dimension of concentration (m^{-3})
$c^{e,h}(L)$	density of free electrons or holes at the right boundary of the semiconductor substrate (at $x = L$) (m^{-3})
D_S	integral surface charge density in the insulator (m^{-2})
$E_{C,V}$	bottom of the conduction band or top of the valence band (eV)
E_F	Fermi energy level in the metal (eV)
$E_F^{e,h}$	quasi-Fermi energy levels in the semiconductor (eV)
$E_{\perp}$	energy perpendicular to the surface (eV)
$E_{\parallel}$	energy parallel to the surface (eV)
E	total energy of free charge carriers (eV)
E_g	energy band gap (eV)
$F_{1/2}$	Fermi integral of the order of 1/2 (–)
G	net generation of electron and holes in the semiconductor by all mechanisms ($m^{-3}\,s^{-1}$)
$J_D^{e,h}$	drift–diffusion current densities of electrons or holes in the semiconductor ($A\,m^{-2}$)
$J_{G,RDT}^{e,h\_1,2}$	generation G or recombination R direct tunnelling current density of electrons or holes in region 1 or 2 ($A\,m^{-2}$)
$J^{e,h}$	total electron or hole current density ($A\,m^{-2}$)
$J_{R-G}^{e,h}$	recombination–generation current density of free charge carriers in the semiconductor ($A\,m^{-2}$)
$J_{DT}^{e,h\_1,2}$	direct tunnelling current density of electrons or holes in region 1 or 2 ($A\,m^{-2}$)
$J_{RDT}^{e,h\_1,2}$	recombination direct tunnelling current density of electrons or holes in region 1 or 2 ($A\,m^{-2}$)
$J_{GDT}^{e,h\_1,2}$	generation direct tunnelling current density of electrons or holes in region 1 or 2 ($A\,m^{-2}$)
$K^{e,h}$	empirical function for electrons or holes used in approximating the Fermi integral of order 1/2 (–)
k	Boltzmann constant ($J\,K^{-1}$)
L	right boundary of the semiconductor substrate (–)
$m^*_{e,h}$	effective electron or hole mass (kg)
$m_t^{e,h}$	effective tunnelling mass of electron or hole (kg)
m_t	transversal electron mass (kg)
m_l	longitudinal electron mass (kg)
m_0	rest electron mass (kg)
m_{lh}	mass of light holes (kg)
m_{hh}	mass of heavy holes (kg)
$N_{C,V}$	effective density of states in the conduction or valence band (m^{-3})
N_i	intrinsic density of charge carriers (m^{-3})
$N_{A,D}$	donor or acceptor impurity density (m^{-3})
n_{ie}	modified intrinsic density (–)
n_{ie}^*	twice modified intrinsic density using correction factors $\gamma^{e,h}$ (m^{-3})
Q_f	effective fixed charge of the insulator ($C\,m^{-2}$)
Q_{SC}	total integral charge in the semiconductor ($C\,m^{-2}$)
q	elementary charge (m^{-3})
R	net recombination of electron and holes in the semiconductor by all mechanisms ($m^{-3}\,s^{-1}$)
T	absolute temperature (K)
t_{ox}	total oxide thickness (m)
V_a^S	voltage drop on the semiconductor (V)
V_a^I	voltage drop on the insulation layer (V)
V_a	applied voltage (V)
V_{step}	applied voltage step (V)
V_{step}^S	voltage step applied to the semiconductor (V)
V_{step}^I	voltage step applied to the insulation layer (V)
$V_{bi}^{S\_TDE}$	built-in potential in the semiconductor under TDE (V)
x	x-coordinate normal to the metal–insulator–semiconductor interfaces (m)
x_{it}	position of the insulator–semiconductor interface (m)
x_t	place in the semiconductor, where tunnelling vanishes (m)
$\hbar$	reduced Planck constant (J s)
χ_S	electron affinity of the semiconductor (eV)
ΔE_g	band gap narrowing (eV)
ϵ_0	permittivity of vacuum ($F\,m^{-1}$)
Φ_B	Schottky barrier height on n-type semiconductor (eV)
Φ_M	work function of the metal (eV)
$\Gamma^{e,h}$	electron or hole tunnelling coefficient (–)
$\gamma^{e,h}$	correction factors for Fermi integral of order 1/2 (–)
$\varphi^{e,h}$	quasi-Fermi potentials (V)
κ	relative permittivity (–)
$\kappa_{S,I}$	relative permittivity of the semiconductor or insulator (–)
κ_{Ii}	relative permittivity of the ith layer in the insulator (–)
$\mu^{e,h}$	electron or hole mobility in the semiconductor ($m^2\,V^{-1}\,s^{-1}$)
$v_{RDT}^{e,h}$	recombination velocities of direct tunnelling for electrons and holes ($m\,s^{-1}$)
$v_{GDT}^{e,h}$	generation velocities of direct tunnelling for electrons and holes ($m\,s^{-1}$)
$v_D^{e,h}$	diffusion velocity of electrons or holes ($m\,s^{-1}$)
$\tau^{e,h}$	lifetime of electrons or holes in the semiconductor (s)
ψ	electrostatic potential (V)
$\psi^{e,h}$	modified electrostatic potentials for electrons or holes (V)

and is solvable satisfying the insulator-to-semiconductor interface condition

$$\varepsilon_0 \kappa_S \frac{d\psi}{dx}\bigg|_S - \varepsilon_0 \kappa_I \frac{d\psi}{dx}\bigg|_I = Q_f, \tag{2}$$

where the x-coordinate is perpendicular to the metal–insulator–semiconductor interface, ψ is the electrostatic potential, N_D and N_A are donor and acceptor doping densities, κ_S and κ_I are relative permittivities of the semiconductor and insulator, respectively, and Q_f is the effective fixed charge of the insulator, $Q_f = qD_S$. Here, D_S is the integral surface charge density in the insulator. Note that a similar condition holds for all interfaces present in the structure, thus also for the interface between the high-κ insulator and the interface layer, see Fig. 1.

Distribution of free charge carriers in the semiconductor is obtained by solving the quasi-stationary continuity equations for electrons and holes

$$\frac{dJ_D^{e,h}}{dx} = \pm q(R - G) \pm \frac{d\left(J_{RDT}^{e,h\_2} - J_{GDT}^{e,h\_2}\right)}{dx}, \tag{3}$$

where $J_D^{e,h}$ are the drift–diffusion current densities of electrons and holes in the semiconductor expressed as