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Analysis and Simulation of Heterostructure Devices

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To Dessi, Lili & Christine

Contents

List of Acronyms

AC	...	Alternating Current
ADS	...	Advanced Design System
BB	...	Band-to-Band tunneling
BCB	...	Benzocyclobutene
BGN	...	Bandgap Narrowing
BICMOS	...	Bipolar CMOS
BJT	...	Bipolar Junction Transistor
BV	...	Breakdown Voltage
CAD	...	Computer Aided Design
CML	...	Current-Mode Logic
CMOS	...	Complementary Metal Oxide Semiconductor
CQFL	...	Continuous Quasi-Fermi Level
CVD	...	Chemical Vapor Deposition
CW	...	Continuous wave
DC	...	Direct Current
DD	...	Drift-Diffusion
DHBT	...	Double Heterojunction Bipolar Transistor
DOS	...	Density of States
ECL	...	Emitter-Coupled Logic
ET	...	Energy Transport
FET	...	Field Effect Transistor
GSH	...	Global Self Heating
HBT	...	Heterojunction Bipolar Transistor
HD	...	Hydrodynamic
HEMT	...	High Electron Mobility Transistor
HFET	...	Heterostructure Field Effect Transistor
IC	...	Integrated Circuit
II	...	Impact Ionization
MAG	...	Maximum Available Gain
MBE	...	Molecular Beam Epitaxy
MC	...	Monte-Carlo
MDS	...	Microwave Design System
MESFET	...	Metal Semiconductor Field Effect Transistor

MIC	...	Microwave Integrated Circuit
MMIC	...	Monolithic Microwave Integrated Circuit
MOCVD	...	Metal Organic Chemical Vapor Deposition
MODFET	...	Modulation Doped FET
MOS	...	Metal Oxide Semiconductor
MOSFET	...	Metal Oxide Semiconductor FET
MSG	...	Maximum Stable Gain
NID	...	Non-Intentionally Doped
PAE	...	Power-Added Efficiency
PHEMT	...	Pseudomorphic HEMT
RF	...	Radio Frequency
RST	...	Real Space Transfer
SH	...	Self Heating
SHBT	...	Single Heterojunction Bipolar Transistor
SOI	...	Silicon on Insulator
SIMS	...	Secondary Ion Mass Spectroscopy
SIESTA	...	Simulation Environment for Semiconductor Technology Analysis
SRH	...	Shockley-Read-Hall
TBB	...	Trap-Assisted Band-to-Band Tunneling
TCAD	...	Technology CAD
TE	...	Thermionic Emission
TFE	...	Thermionic Field Emission
VISTA	...	Viennese Integrated System for TCAD Applications
WKB	...	Wigner-Kramers-Brillouin

List of Symbols

Δ ... step, difference, change

ΔE_{V},ΔE_{C} ... difference of the valence/conduction band at a heterointerface between two segments

ΔE_g ... total difference of the bandgaps at a heterointerface between two segments

Γ ... tunneling probability

Γ_{n}, Γ_{p} ... field enhancement factors

α,β ... general exponent

α ... general temperature coefficient

α ... in HBT compact model: amplification

α,β ... in the bandgap model: temperature coefficients

α_ν ... auxiliary quantity in the Hänsch mobility model for carrier type ν

α_ν ... quantity in the impact ionization model for carrier type ν

β_F ... inverse Fermi screening length

β_{n}, β_{p}, β_ν ... exponents in mobility models for electrons, holes, and general carrier type

γ ... exponent in mobility models

δE_ν ... barrier height lowering

ε ... permittivity

ε_{s}, $\varepsilon_{\mathrm{ins}}$ ... permittivity of semiconductor, insulator

ε_{r} ... relative permittivity

$\varepsilon_{\mathrm{ox}}$ ... relative permittivity of the oxide in the polysilicon contact model

ϕ_{B} ... barrier height

ϕ_{Fm} ... Fermi potential in the metal

ϕ_{ms} ... metal workfunction difference potential

ϕ_{Fn} ... quasi-Fermi potential for electrons in the semiconductor

$\phi_{\mathrm{Fn,1}}$ ... quasi-Fermi potential for electrons in the semiconductor 1

κ_{L} ... lattice thermal conductivity

κ_{n}, κ_{p}, κ_{ν}	...	thermal conductivity of electrons, holes, and general carrier type
κ_{300}^{A}	...	thermal conductivity at 300 K of material A
λ_0, λ	...	temperature dependent mean free path for the optical phonon
λ_B	...	De Broglie wave length
μ_{ν}	...	mobility of carrier type ν
μ_{ν}^{min}	...	minimum mobility
μ_{ν}^{sr}	...	surface mobility contribution of carrier ν at 300 K in the surface scattering model
μ_{ν}^{L}	...	mobility due to lattice scattering
μ_{ν}^{LI}	...	mobility due to lattice and impurity scattering
μ_{ν}^{LIS}	...	mobility due to lattice, impurity, and surface scattering
$\mu_{\nu}^{\mathrm{LISF}}$	...	mobility including lattice, impurity, surface scattering, and high-field reduction
$\mu_{\nu}^{\mathrm{LIST}}$	...	mobility including lattice, impurity, surface scattering, and high-temperature reduction
μ_{ν}^{LIT}	...	mobility including lattice, impurity, and high-temperature reduction
$\mu_{\mathrm{maj}}^{\mathrm{mid}}$, $\mu_{\mathrm{maj}}^{\mathrm{hi}}$	...	parameters of the majority mobility model
$\mu_{\mathrm{min}}^{\mathrm{mid}}$, $\mu_{\mathrm{min}}^{\mathrm{hi}}$	...	parameters of the minority mobility model
μ_{n}, μ_{p}	...	electron and hole mobilities
$\mu_{\nu,300}^{\mathrm{ref}}$	...	reference mobility of carrier ν at 300 K in the surface scattering model
ρ_{L}	...	mass density
$\sigma_{\mathrm{T,n}}$, $\sigma_{\mathrm{T,p}}$	...	trap capture cross sections for electrons and holes
σ_{ox}	...	oxide conductivity
σ_{s}	...	surface (interface) charge density
τ	...	phase term of the transconductance g_{m}
τ_{port}	...	port extension
$\tau_{\epsilon,\mathrm{n}}$, $\tau_{\epsilon,\mathrm{p}}$, $\tau_{\epsilon,\nu}$	...	energy relaxation times for electrons, holes, and general carrier type
$\tau_{\epsilon,0}$, $\tau_{\epsilon,1}$	...	parameters for the energy relaxation times model
$\tau_{\nu,\mathrm{dop}}$	...	doping dependent lifetime of carrier $\nu=$ n,p
$\tau_{\nu,\mathrm{max}}$	...	maximum lifetime of carrier $\nu=$ n,p
τ_{AUG}	...	carrier lifetime defined by *Auger* recombination
τ_{C}	...	bowing parameter energy relaxation time
τ_{DIR}	...	carrier lifetime defined by direct recombination
τ_{SRH}	...	carrier lifetime defined by SRH recombination
τ_{SURF}	...	surface contribution to carrier lifetime

τ_T	...	time constant, inverse of f_T
τ_b	...	base transit time
τ_c	...	collector transit time
$\tau_{\mathrm{cap},\nu}$	...	capture time constant for carrier ν
τ_eb	...	base emitter transit time
τ_ec	...	emitter collector transit time
$\tau_{\mathrm{em},\nu}$	...	emission time constant for carrier ν
τ_ext	...	time constant, inverse of extrinsic f_T
τ_i	...	intrinsic delay time
τ_n, τ_p	...	recombination lifetimes for electrons and holes
$\tau_{\mathrm{n},300}$, $\tau_{\mathrm{p},300}$, $\tau_{\nu,300}$	...	lifetime of carrier $\nu=$ n,p at $T_\mathrm{L}=$ 300 K
τ_sc	...	space charge transit time
τ_tot	...	total carrier lifetime
φ_m	...	metal quasi-**Fermi** level
φ_w	...	workfunction difference potential
ψ	...	electrostatic potential
ψ_bi	...	built-in potential
φ_s	...	semiconductor contact potential
ω	...	oscillation frequency
ω_0	...	oscillation frequency of phonon
A_ν	...	temperature coefficient saturation velocity for carrier $\nu=$ n,p
A_ν	...	coefficient for impact ionization for carrier $\nu=$ n,p
A^*	...	**Richardson** constant typical for thermionic emission process
A, B	...	general parameters in recombination models
B_ν	...	threshold energy in the impact ionization model
B_ν	...	parameter for the surface mobility in the **Lombardi** mobility model
BV_CE0	...	collector-emitter breakdown voltage
BV_GD	...	gate-drain diode breakdown voltage
BV_i	...	breakdown voltage
C_ε	...	permittivity bowing parameter
C_κ	...	thermal conductivity bowing parameter
C_μ	...	mobility bowing parameter
C_ν	...	parameter for the surface mobility in the **Lombardi** mobility model
$C^{\Gamma}_{\mathrm{vsat},\nu}$	...	bowing parameter of the saturation velocity of carrier type ν in Γ-valley
$C^{\mathrm{AUG}}_{\nu,300K}$	...	**Auger** coefficients for carrier ν at 300 K
C^{AUG}_{ν}	...	**Auger** coefficients for carrier ν
C^{DIR}	...	direct recombination coefficient

C_I	...	total impurity concentration
C_IN	...	parasitic input capacitance
C_OUT	...	parasitic output capacitance
C	...	bowing parameter in the energy relaxation time model for *alloy materials*
C_1, C_2, C_3	...	reference concentrations in the Masetti mobility model
C_0^AB	...	model parameter for *alloy materials* in the energy relaxation time model
C_bc	...	base collector capacitance
$C_\mathrm{bc,tot}$	...	total base collector capacitance
C_ds	...	drain-source capacitance
$C_\mathrm{eb,dep}$	...	emitter depletion capacitance
C_fb	...	feedback capacitance
C_fringe	...	fringe contribution to a capacitance
$C_\mathrm{g,tot}$	...	total gate capacitance
C_g	...	bandgap bowing parameter
$C_{\mathrm{g},\mathit{\Gamma}}$	...	bandgap bowing parameter $\mathit{\Gamma}$-valley
$C_\mathrm{g,X}$	...	bandgap bowing parameter X-valley
C_gd	...	gate drain capacitance
C_gs	...	gate source capacitance
C_i	...	i=1,..,4: parameter for the impact ionization model
C_i	...	i=0,..,3: parameter for the energy relaxation time model
C_i	...	i=1,2: parameter for the built-in potential
C_jc	...	collector junction capacitance
C_im	...	additional capacitance due to impact ionization
C_in	...	input capacitance
$C_{\mathrm{m},\nu}$	...	relative carrier mass bowing parameter
C_met	...	contribution to C_gd due to coupling of metal periphery
$C_\mathrm{maj}^\mathrm{mid}$, $C_\mathrm{maj}^\mathrm{hi}$	...	parameters of the majority mobility model
$C_\mathrm{min}^\mathrm{mid}$, $C_\mathrm{min}^\mathrm{hi}$	...	parameters of the minority mobility model
C_net	...	net concentration
C_pad	...	parasitic pad capacitance
C_pass	...	contribution to C_gd due to device passivation
C_pds, C_pgs, C_pgd	...	parasitic drain-source, gate-source, and gate-drain capacitances
C_ref	...	reference impurity concentration
C_spaceDC	...	contribution to C_gs due to the space charge region
C_traps	...	frequency dispersive contribution to C_gs

C_vsat	...	bowing parameter of the saturation velocity
$\mathbf{D}$	...	dielectric flux
D_ν	...	parameter for the surface mobility in the **Lombardi** mobility model
D_n	...	effective diffusivity in the base
E_ν^crit	...	critical field for impact ionization for carrier ν
E_crit	...	critical field for the onset of saturated behaviour in compact models
E_F	...	**Fermi** energy
E_Fm	...	**Fermi** energy in the metal
E_Fn	...	**Fermi** energy for electrons in the semiconductor
E_Fp	...	**Fermi** energy for holes in the semiconductor
E_T	...	trap energy
$\mathbf{E}$	...	local electric field
E_C	...	conduction band energy
E_g	...	bandgap energy
E_gate	...	effective field at the gate
$E_{\mathrm{g},\mathit{\Gamma}}$	...	bandgap energy in $\mathit{\Gamma}$-valley
$E_\mathrm{g,X}$	...	bandgap energy in X-valley
$E_\mathrm{g,0}$, $E_\mathrm{g,300}$	...	bandgap energy at 0 K, and at 300 K
E_i	...	bandgap modeling parameters
E_i	...	threshold energy
$E_{\mathrm{i},\nu}$	...	threshold energy of carrier ν
$\mathbf{E}_\mathrm{ins}$	...	local electric field in insulator
E_off	...	energy offset
$E_{\perp 2}$	...	electric field orthogonal to the interface
$E_\mathrm{r,0}$	...	energy loss per scattering at reference temperature
$\mathbf{E}_s$	...	local electric field in semiconductor
E_V	...	valence band energy
E_w	...	workfunction energy difference
E_0	...	minimum energy in the traps-assisted model
F	...	field in impact ionization model
F_min	...	minimum noise figure
F_n, F_p, F_ν	...	driving force for electrons and holes
$F_c^\pm$	...	critical field strengths in the direct band to band tunneling model
F_o	...	steady-state occupancy function
F_0	...	critical driving force at which overshoot in the velocity-field characteristics occur
G_n, G_p	...	electron and hole emission rate
G_n, G_p, G_ν	...	generation rate of carrier $\nu=$ n,p
G_ν^{II}	...	impact ionization generation of carrier ν

$\boldsymbol{G}_{\text{tun}}$	local generation rate associated with the tunneling
H	heat generation
I_{B}, I_{C}, I_{E}	base, collector, emitter currents
I_{Con}	current through a contact
I_{D}	drain current
I_{Dmax}	maximum drain current
I_{DS}	drain source current
I_{G}	gate current
I_{II}	impact ionization contribution to the gate current
I_{TFE}	thermionic field emission contribution to the gate current
$\mathbf{J}_{\text{n}}$, $\mathbf{J}_{\text{p}}$	electron and hole current densities
J_{tun}	current density of tunneling currents
K_i	temperature coefficients for *Auger* recombination
L_{D}, L_{G}, L_{S}	drain, gate, and source inductances
MAG	maximum available gain
M_{C}	valley degeneracy factor of the conduction band
ME	modulation efficiency
MSG	maximum stable gain
N_{A}	acceptor doping concentration
N_{C}	effective density of states for electrons
$N_{\text{C},0}$	effective density of states for electrons evaluated at reference temperature T_0
N_{D}	donor doping concentration
$N_{\text{ref},\nu}$	reference doping concentration for carrier $\nu=$ n,p
N_{T}	concentration of traps
N_{V}	effective density of states for holes
$N_{\text{V},0}$	effective density of states for holes evaluated at reference temperature T_0
P_ν	pressing forces for the carrier ν
P_ν^{ref}	reference pressing forces for the carrier ν
P_{L}	ratio of the Γ and L valley populations in the multivalley mobility model
Q_s	total charge in the device
R	net recombination rate
R^{AUG}	Auger recombination rate
R_{B}	parasitic base resistance
R^{BB}	band to band tunneling recombination rate
R_{Con}	contact resistance

R_{C}	parasitic collector resistance
R^{DIR}	direct (radiative) recombination rate
R_{E}	parasitic emitter resistance
R_{H}	Huang-Rhys factor
R^{II}	contribution from impact ionization to the net generation/recombination rate
R_{SM}, R_{DM}	metal contribution to R_{S}, R_{D}
R^{SRH}	SRH net recombination rate
R_{S}, R_{G}, R_{D}	parasitic source, gate, drain resistances
$R_{\mathrm{Ssemi/alloy}}$, $R_{\mathrm{Dsemi/alloy}}$	semiconductor or alloy contribution to R_{S}, R_{D}
R_{TH}	thermal resistance
R_{bb}	base resistance
R_{ds}	drain-source resistance
$R_{\mathrm{eff},\nu}$	effective (net) recombination rate of carrier ν
R_{gap}	contribution to base resistance
R_{gd}	gate-drain resistance
R_{gs}	gate-source resistance
$R_{\mathrm{TH,glob}}$	global thermal resistance
R_{im}	resistance describing impact ionization in compact models
R_{maj},R_{min}	majority and minority Rydberg energies
R_{n}, R_{p}	recombination rate of carrier n,p
R_{pgd}	gate leakage resistance drain side
R_{pgs}	gate leakage resistance source side
R_{spread}	contribution to base resistance
$\mathbf{S}_{\mathrm{L}}$	lattice heat flux density
S_{ij}	scattering (S-) parameter, i,j=1,2
s_{n}, s_{p}	surface recombination velocities for electrons and holes
$\mathbf{S}_{\mathrm{n}}$, $\mathbf{S}_{\mathrm{p}}$	electron and hole energy flux density
T_{C}	contact temperature
T_{L}	local lattice temperature
T_{n}, T_{p}	electron and hole temperatures
T_{ν}	carrier temperature of carrier ν
$T_{\nu,i}$	carrier temperature of type ν in segment i
T_{sub}	substrate temperature
U	unilateral gain
V_{BE}, V_{CE}, V_{BC}	base-emitter, collector-emitter, and collector-base voltages
V_{Con}	voltage at a contact
V_{DS}, V_{GD}, V_{GS}	drain-source, gate-drain, and gate-source voltages
V_{bar}	equivalent potential barrier height

V_{ox}	...	voltage drop over the oxide at the polysilicon contact
V_{thr}	...	threshold voltage
W_{g}	...	gate width
X_{b}	...	effective base width
Y_{ij}	...	Y-parameter for i,j=1,2
Z_{ij}	...	Z-parameter for i,j=1,2
c_{L}	...	lattice specific heat
$c_{\mathrm{L,300}}$	...	lattice specific heat at T_{L}= 300 K
c_{eff}	...	effective capacitance
c_{n}, c_{p}	...	heat capacity of electron gas and hole gas
d	...	thickness, length
d_{eff}	...	effective gate-to-channel separation
d_{ox}	...	oxide thickness
d_{tun}	...	effective tunneling length
d_{R}	...	recess length
f_{T}	...	current gain cut-off frequency
$f_{\mathrm{T,ext}}$	...	extrinsic current gain cut-off frequency
f	...	frequency
f_{c}	...	frequency for k = 1
f_{max}	...	maximum frequency of oscillation
g_{ds}	...	output conductance
$g_{\mathrm{ds,ext}}$	...	extrinsic output conductance
g_{m}	...	transconductance
g_{mi}	...	intrinsic transconductance
g_{mim}	...	transconductance due to impact ionization
$g_{\mathrm{m,max}}$	...	maximum transconductance
h	...	Planck constant
$\hbar$	...	reduced Planck constant
k_{B}	...	Boltzmann constant
k	...	stability factor
l_{Co}	...	length contact to recess
l_{g}	...	gate length
$m_{\mathit{\Gamma}}$	...	relative carrier masses in $\mathit{\Gamma}$-valley
m_{ν}^{*}	...	effective tunneling mass band-to-band model
m_{L}	...	relative carrier masses in L valley
m_{0}	...	free electron mass
$m_{\mathrm{0,n}}$, $m_{\mathrm{0,p}}$	...	relative masses of electrons and holes at 0 K
m_{X}	...	relative carrier masses in X valley
m_{n}, m_{p}	...	relative masses of electrons and holes
$m_{\mathrm{1,n}}$, $m_{\mathrm{1,p}}$, $m_{\mathrm{2,p}}$	...	parameters for the temperature dependence of the relative masses of electrons and holes
m_{nt}	...	transversal electron mass

m_nl	...	longitudinal electron mass
m_ph	...	heavy hole mass
m_pl	...	light hole mass
m_t	...	effective tunneling mass heterojunction tunneling
n_0	...	equilibrium concentration at contact
$\mathbf{n}$	...	a normal vector
n	...	electron concentration
n_1	...	auxiliary concentration in the SRH model
n_c	...	reference charge
n_i	...	intrinsic electron concentration
n_s	...	surface concentration of electrons
n_sheet	...	channel sheet charge density
n_t	...	auxiliary concentration in the trap-assisted model
n_T	...	concentration of occupied traps
p	...	hole concentration
p_0	...	equilibrium concentration
p_1	...	auxiliary concentration in SRH model
p_i	...	intrinsic hole concentration
p_t	...	auxiliary concentration in the trap-assisted model
p_s	...	surface concentration of holes
q	...	elementary charge
r_s	...	density parameter for the BGN model
t	...	time
u	...	carrier energy relative to the threshold energy
v_eff	...	effective carrier velocity
v_n, v_p	...	velocity for electrons and holes
$v_\mathrm{em,n}$, $v_\mathrm{em,p}$	...	emission velocities for electrons and holes
$v_\mathrm{sat,n}$, $v_\mathrm{sat,p}$	...	saturation velocities for electrons and holes
$v_\mathrm{sat,n,300}$, $v_\mathrm{sat,p,300}$	...	saturation velocities for electrons and holes at 300 K
$v^{\mathit{\Gamma}}_\mathrm{sat,n}$, $v^\mathrm{L}_\mathrm{sat,n}$	...	saturation velocities for electrons in valley $\mathit{\Gamma}$, L
$v_\mathrm{th,n}$, $v_\mathrm{th,p}$	...	average thermal velocities for electrons and holes
$v_\mathrm{th,n,300}$, $v_\mathrm{th,p,300}$	...	thermal velocities for electrons and holes at 300 K
w_n, w_p	...	average electron/hole energy
x	...	material composition
y	...	distance
y^ref	...	surface reference distance

1. Introduction

Communication and information systems are subject to rapid and highly sophisticated changes. Currently semiconductor heterostructure devices, such as Heterojunction Bipolar Transistors (HBTs) and High Electron Mobility Transistors (HEMTs), are among the fastest and most advanced high-frequency devices. They satisfy the requirements for low power consumption, medium integration, low cost in large quantities, and high-speed operation capabilities in circuits. In the very high-frequency range, cut-off frequencies up to 500 GHz [557] have been reported on the device level. HEMTs and HBTs are very suitable for high-efficiency power amplifiers at 900 MHz as well as for data rates higher than 100 Gbit/s for long-range communication and thus cover a broad range of applications.

To cope with explosive development costs and the competition of today's semiconductor industry, Technology Computer-Aided Design (TCAD) methodologies are used extensively in development and production. As of 2003, III-V semiconductor HEMT and HBT micrometer and millimeter-wave integrated circuits (MICs and MMICs) are available on six-inch GaAs wafers. SiGe HBT circuits, as part of the CMOS technology on eight-inch wafers, are in volume production. Simulation tools for technology, devices, and circuits reduce expensive technological efforts. This book focuses on the application of simulation software to heterostructure devices with respect to industrial applications. In particular, a detailed discussion of physical modeling for a great variety of materials is presented.

Chapter 2 discusses the status of research regarding the most important electronic heterostructure devices, HBTs and HEMTs. It includes a review of state-of-the-art materials, devices, and driver applications. Device-specific optimization potentials are discussed systematically. Device simulators are reviewed and a discussion of the materials and material systems on which heterostructure devices are based is given.

Chapter 3 is dedicated to the derivation and application of physics-based analytical models, compiled in a comprehensive and carefully systemized collection. It contains models for the lattice, thermal, band-structure, and transport properties of various semiconductor materials, as well as models for important high-field and high-doping effects which occur in the devices. The quality of these models, in terms of their accuracy and simplicity, is decisive for the predictive capabilities

V. Palankovski et al., *Analysis and Simulation of Heterostructure Devices*