Elements in the simulation with

NEGF applied to quantum transport model

1	**ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED**	
1.1	**ASPECT OF THE USER CASE TO BE SIMULATED AND HOW IT FORMS A PART OF THE TOTAL USER CASE**	*Calculation of quantum transport of electrons and holes in semiconductor devices based on nanostructure. Electrical properties such as current density and charge densities are to be calculated taking into account applied bias and material and geometrical properties of the device. These properties will be used to calculate the flow of electrons through the device.*
1.2	**MATERIAL**	*Nano-scale transistor with InGaAs channel.*
1.3	**GEOMETRY**	*<Picture to be included in final document >*
1.4	**TIME LAPSE**	*Not applicable*
1.5	**MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS**	$f^{B}(E, E_{fB})$ *Fermi-Dirac distribution function of the electrons in contact B with the Fermi level* E_{fB}*. The applied bias determines the shift of the contact Fermi levels with respect to their equilibrium position.*
1.6	**PUBLICATION**	

2	**GENERIC PHYSICS OF THE MODEL EQUATION**		
2.0	**MODEL TYPE AND NAME**	*Non-Equilibrium Green's Function Model for Transport of Electrons (1.4 in RoMM)*	
2.1	**MODEL ENTITY**	*The entity in this materials model is electrons expressed by Green's functions.*	
2.2	**MODEL PHYSICS/ CHEMISTRY EQUATION PE1**	**Equation**	***Green's function equations*** *(E-H)G(E)=I* *This equation applied for quantum transport is often combined with the MR given below. But here we give the most generic form of the PE.*
		Physical quantities	*E Electron energy* *H Hamiltonian matrix representing the device* *S Overlap matrix between all involved atomic orbitals*
2.2.1	**MATERIALS RELATION 1 MR1 TO PE1**		

Kommentar [AdB1]: I am not sure whether this appears in the most generic form of the Green's Function Equation.

		Physical quantities/ descriptors	*Hamiltonian in NEGF described using localised basis states in a matrix equation; with on-diagonal elements H_{ii} giving basis state on-site energy (interaction between one atom and itself), including external potential, off-diagonal elements H_{ij} (interactions with neighbours) giving energy interaction between basis states and S_{ij} describing overlap between states;* $H_{ij} = \langle\phi_i\|H\|\phi_j\rangle; S_{ij} = \langle\phi_i\|\phi_j\rangle$ *where ϕ_i are localised basis states over which H defined.* *The generic PE is often combined with the MR given below and then reads* *Retarded Green function:* $[ES - H - \Sigma^{RB}(E) - \Sigma^{RS}(E)]G^R(E) = I$ *Lesser/Greater Green's Functions:* $G^{\gtrless}(E) = G^R(E).\left(\Sigma^{\gtrless B}(E) + \Sigma^{\gtrless S}(E)\right).G^A(E)$ $\Sigma^{RB}(E)$ *Boundary retarded self-energy* $\Sigma^{RS}(E)$ *Scattering retarded self-energy* $\Sigma^{\gtrless B}(E)$ *Boundary lesser/greater self-energy* $\Sigma^{\gtrless S}(E)$ *Scattering lesser/greater self-energy* $G^R(E)$ *Retarded Green's Function* $G^A(E)$ *Advanced Green's Function* $G^<(E)$ *Lesser Green's Function* $G^>(E)$ *Greater Green's Function* *Here the advanced Green's function is defined as :* $G^A(E) = (G^R(E))^\dagger$ *Note that retarded and advanced solutions correspond to outgoing and incoming waves in contacts.* *The Green's functions dependencies are:* $G^R(E) - G^A(E) = G^>(E) - G^<(E)$ Difference between the retarded and advanced Green's functions is equal to the difference between the greater and lesser Green's functions From current conservation the following relations are derived ***First relation between the boundary self-energies*** $\Sigma^{RB}(E) - \Sigma^{AB}(E) = \Sigma^{>B}(E) - \Sigma^{<B}(E)$ Difference between the boundary retarded and advanced self-energies is equal to the difference between the boundary greater and lesser self-energies ***Advanced boundary self-energy:*** $\Sigma^{AB}(E) = (\Sigma^{RB}(E))^\dagger$ *Conjugate of boundary retarded self-energy $\Sigma^{RB}(E)$ is boundary advanced self-energy $\Sigma^{RA}(E)$* ***Second relation between the boundary self-energies:*** $\Sigma^{<B}(E) = -\left(\Sigma^{RB}(E) - \Sigma^{AB}(E)\right) \cdot f_c(E)$ $\Sigma^{>B}(E) = -\left(\Sigma^{RB}(E) - \Sigma^{AB}(E)\right) \cdot (f_c(E)\text{-}1)$ *$f_c(E)$ Fermi distribution function of the electrons in the contact C. It requires the knowledge of the corresponding*

Kommentar [AdB2]: Ok?

Fermi level E_{Fc}.

Scattering self-energies *(description of alloy disorder, roughness, impurity, electron-phonon, and carrier-carrier scattering)*

$\Sigma^{RS}(E) = \mathcal{L}_R$*(scattering mechanisms)*

$\Sigma^{<S}(E) = \mathcal{L}_<$*(scattering mechanisms)*

$\Sigma^{>S}(E) = \mathcal{L}_>$*(scattering mechanisms)*

$\mathcal{L}_R$ *Function relating any scattering mechanism to the retarded self-energy* $\Sigma^{RS}(E)$

$\mathcal{L}_<$ *Function relating any scattering mechanism to the lesser self-energy* $\Sigma^{<S}(E)$

$\mathcal{L}_>$ *Function relating any scattering mechanism to the greater self-energy* $\Sigma^{>S}(E)$

First relation between the scattering self-energies

$$\Sigma^{RS}(E) - \Sigma^{AS}(E) = \Sigma^{>S}(E) - \Sigma^{<S}(E)$$

Difference between the scattering retarded and advanced self-energies is equal to the difference between the scattering greater and lesser self-energies

Advanced scattering self-energy:

$$\Sigma^{AS}(E) = (\Sigma^{RS}(E))^{\dagger}$$

Conjugate of boundary retarded self-energy $\Sigma^{RB}(E)$ *is boundary advanced self-energy* $\Sigma^{RA}(E)$

Second relation between the scattering self-energies:

$$\Sigma^{RS}(E) = -i\frac{\Gamma(E)}{2} + \wp\int\frac{dE'}{2\pi}\frac{\Gamma(E')}{E-E'}$$

$\Gamma(E) = i(\Sigma^{>S}(E) - \Sigma^{<S}(E))$ *Broadening function*

$\wp$ *Cauchy principal integral value* ***Boundary self-energies*** *(coupling of device with its contacts)*

$$\Sigma^{RB}(E) = \mathcal{F}_R(H_{DC})$$

$$\Sigma^{<B}(E) = \mathcal{F}_<(H_{DC}) \bullet f^B(E, E_{fB})$$

$$\Sigma^{>B}(E) = \mathcal{F}_>(H_{DC}) \bullet (f^B(E, E_{fB}) - 1)$$

where:

H_{DC} *Hamiltonian matrix describing the coupling between the device (D) and its contacts (C)*

$\mathcal{F}_R$ *Function relating* H_{DC} *and the boundary retarded self-energy. Several models exist.*

$\mathcal{F}_<$ *Function relating* H_{DC} *and the boundary lesser self-energy. Several models exist.*

$\mathcal{F}_>$ *Function relating* H_{DC} *and the boundary greater self-energy. Several models exist.*

And values for the parameters in the above PE <to be filled in>

2.4	**SIMULATED INPUT**	*HAMILTONIAN matrix from model1, including details of open contacts*
2.6	**PUBLICATION ON THIS ONE SIMULATION**	

3	COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	*Matrix Algebra*	
3.2	SOFTWARE TOOL	*Within DEEPEN, two in-house tools are used: OMEN (from ETHZ) and TiMeS (from Tyndall) (neither currently supported for external users, but other NEGF codes also available)*	
3.3	GRID SIZE	*Matrix size determined by number of atoms included in calculation times number of basis states used per atom.*	
3.4	TIME STEP	*None*	
3.5	COMPUTATIONAL REPRESENTATION *refers to how your computational solver represents the material, properties, equation variables,…..*	PHYSICS EQUATION	*TISE, Green's function and self-energy equations all expressed in a matrix format.*
		MATERIAL RELATIONS	*Green's function, self-energy and Hamiltonian matrix elements calculated by iterative solution of coupled equations.*
		MATERIAL	*Hamiltonian, Green's function and self-energy data all stored as floating point values. Both single and double precision are supported but double precision recommended.*
3.6	PUBLICATION	*The approach taken in OMEN is overviewed in M. Luisier, "Atomistic simulation of transport phenomena in nanoelectronic devices", Chem. Soc. Rev., 2014,43, 4357-4367. The approach taken in TiMeS is overviewed in D. Sharma, L. Ansari, B. Feldman, M. Iakovidis, J. C. Greer and G. Fagas "Transport properties and electrical device characteristics with the TiMeS computational platform: Application in silicon nanowires", J. Appl. Phys.* ***113****, 203708 (2013)*	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	• *Distribution of electron states with respect to energy -with open boundary conditions* • *Spatially- and energetically-resolved density-of-states (DOS)* • *Energy-resolved transmission probability* • *Carrier density* • *Current flow* *Electrostatic potential all of these are calculated for finite volumes to be used in the continuum model 3.*
4.2	METHODOLOGIES	• *Electrostatic potential from the carrier density through the Poisson equation* $\nabla.\varepsilon\nabla V = -q(p - n + \sum_i[\delta(\boldsymbol{r}_{Di} - \boldsymbol{r})] - \sum_j[\delta(\boldsymbol{r}_{Aj} - \boldsymbol{r})])$ *with* ε *Dielectric constant* $\boldsymbol{r}_{Di}$ *Position of* i^{th} *donor atom* $\boldsymbol{r}_{Aj}$ *Position of* j^{th} *acceptor atom* *Spatially- and energetically-resolved density-of-states (DOS) calculated through energy integration,* $n = -\frac{i}{2\pi}\int dE\ G^{<}(E)\,;\,p = \frac{i}{2\pi}\int dE\ G^{>}(E)$; *with carrier densities n (p) and potential V* *The electrostatic potential is determined from the carrier density through the Poisson equation* • *Energy-resolved transmission probability from Green's or Wave Function* • *Current flow from the transmission probability, through energy integration*
4.3	MARGIN OF ERROR	• *Generation of energy grid that captures the DOS features, can lead to significant error in the carrier density.* • *Convergence of Poisson equation, needed: <0.1% variations in the*

		electrostatic potential. If not, possible changes in the current by >10%.