General Retarded Contact Self-energies in and beyond the Non-equilibrium Green’s Functions Method

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Abstract. Retarded contact self-energies in the framework of nonequilibrium Green’s functions allow to model the impact of lead structures on the device without explicitly including the leads in the actual device calculation. Most of the contact self-energy algorithms are limited to homogeneous or periodic, semi-infinite lead structures. In this work, the complex absorbing potential method is extended to solve retarded contact self-energies for arbitrary lead structures, including irregular and randomly disordered leads. This method is verified for regular leads against common approaches and on physically equivalent, but numerically different irregular leads. Transmission results on randomly alloyed In_{0.5}Ga_{0.5}As structures show the importance of disorder in the leads. The concept of retarded contact self-energies is expanded to model passivation of atomically resolved surfaces without explicitly increasing the device’s Hamiltonian.

1. Introduction

The characteristic length scale of modern semiconductor nanodevices is typically smaller than the coherence length of electrons. In this length domain, details of the lead bandstructure and geometry influence the device transport characteristics [1]-[5]. The non-equilibrium Green’s function method (NEGF) [6] is accepted to model transport scenarios most consistently that face coherent and incoherent effects. The NEGF method allows to model devices with open boundary conditions and it describes coherent quantum effects such as confinement, interferences and tunnelling as well as incoherent scattering on phonons, and device imperfections (such as roughness, defects and impurities). In the NEGF framework, open boundary conditions of the device are described in terms of contact self-energies. These self-energies represent the charge injection and extraction effects of the leads and allow modelling specific density of states in the leads. The distinction of contacts and central device allows limiting the explicit NEGF calculation to the central device area and thereby reducing the numerical load [6] significantly. The majority of algorithms that solve the contact self-energies rely on ideal (periodic or homogeneous) leads [7][8]. There are well-known algorithms to solve self-energies for ideal leads, such as the Sancho-Rubio method [9] and the transfer matrix method [10][11]. However, both methods are based on the assumption of semi-infinite, periodic leads. Realistic leads are not ideal and often have non-linear geometries [3] or imperfections like alloy disorder or defects and impurities. Instead, the complex absorbing potential (CAP) [12]-[17] can be extended to irregular leads including e.g. disorder effects or nontrivial geometries. In this work, the CAP algorithm is described and applied on several nonideal leads as they commonly appear in experiments.

Contact self-energies can also be used for numerical passivation of dangling bonds: An atomistic resolution of nanoscale devices is inevitable to realistically describe bandstructures and transport.
properties. Atomistic representations of electronic structures typically face dangling bonds at atoms with insufficient bonding neighbours. This typically happens for atoms located at surfaces. This is particularly true for the wide spread empirical tight binding method. Likewise in experiments, those dangling bonds require saturation with Hydrogen atoms. Often, this saturation is modelled by explicitly including passivation atoms in the numerical discretization of the device. Depending on the ratio of dangling bonds versus actual device atoms, this explicit treatment of Hydrogen atoms can significantly increase the rank of the device Hamiltonian. This is insofar problematic since the computational load of NEGF equations scales cubically with the number of degrees of freedom in the Hamiltonian. In this work, it is shown how self-energies can be used to model the saturation of dangling bonds without increasing the number of explicitly discretized degrees of freedom.

In the following method section, the general retarded contact self-energy and the passivation self-energy are presented. The contact self-energies are applied within the NEGF method on regular leads to compare with the established transfer matrix method. The application to trumpet shaped leads proofs its applicability to non-periodic leads. Results of a Ga$_{0.5}$In$_{0.5}$As random alloy device show the relevance of non-ideal leads for quantitative device performance predictions. The passivation self-energy is used throughout those examples, but its effect is also explicitly discussed with an electronic bandstructure calculation of a GaAs quantum well at the end of the results section. The paper ends with a summarizing conclusion.

2. Method

The electronic transport results shown in the next section are produced with the recursive non-equilibrium Green’s function implementation of the multipurpose nanodevice simulation tool NEMO5 [18][19]. Electronic bandstructure data that illustrate the impact of passivation are results of NEMOS’s Schrödinger equation solver. Electrons are represented within atomistic tight binding with a varying number of orbital representations [20][21]. For random alloys, the atomic structure is relaxed following the Keating strain model [22]. Strain induced changes of the electronic Hamiltonian are considered following the model of Boykin et al. [23]. All IV characteristics are solved including charge self-consistency of the NEGF equations with the Poisson equation. For transmission and bandstructure results only, a constant potential profile was assumed.

If not stated otherwise, the lead self-energies are solved with the CAP method [12]-[17]: The last few (~10) nanometres of the concrete lead structure that are closest to the device are considered in the lead calculation [24]. This lead portion is partitioned into segments to allow for a recursive solution of the surface Green’s functions $g_n$ of each segment $n$

$$
\sum_n = (E + i\eta_0 e^{-\lambda(n-1)} - H_{n,n} - \sum_n)^{-1}
$$

Here, $\sum_n$ is the corresponding contact self-energy and $H_{n,n}$ is the Hamiltonian of the lead segment $n$. The first segment’s contact self-energy is assumed to vanish ($\Sigma_0=0$). An imaginary damping potential $\eta_0$ with exponential shape is chosen as the CAP. It decays due to the decay parameter $\lambda$ with increasing $n$ smoothly to 0 when getting closer to the device. The initial damping potential $\eta_0$ is comparable with the energy $E$ and therefore large enough to blur the impact of the vanishing initial guess of $\Sigma_0$. The purpose of the CAP $\eta_n$ is mainly to improve the convergence behaviour [12]. A direct iteration of the equations (1) without the CAP suffers severely from bad convergence with $n$. Depending on the actual lead structure and geometry, the optimal $\eta_n$ can vary. For the devices in this work, $\eta_0 = -0.5eV$ and $\lambda = 0.1$ provide good convergence. For comparison and in the case of ideal leads only, the Sancho-Rubio method and transfer matrix method of NEMO5 are used to solve the contact self-energies. In these cases, the leads are considered periodic repetitions of a given unit cell.

If not stated otherwise, the electronic tight binding Hamiltonian $H_{SS'}$ between different surface atoms $S$ and $S'$ as well as the on-site one (i.e. $S'=S$) is given as
Here, $H_0$ is the original empirical tight binding Hamiltonian \[25,26\] with $N_H$ unsaturated surface bonds. The sum in equation (2) that models the saturation of dangling bonds has first been introduced by Lee et al. in Ref.\[27\] for sp3-hybridized semiconductors. One can extend the passivation model beyond the sp3-symmetry when the $\Sigma_{S'S',i}$ are given as

$$
\Sigma_{S'S',i} = H_{SH} (\varepsilon - H_{H})^{-1} H_{H,S'}
$$

Equation (3) agrees with the contact self-energy formula of the NEGF method in equation (1). However, the inverted term in equation (3) represents a single Hydrogen atom with a fixed energy parameter $\varepsilon$ and a Hydrogen Hamiltonian $H_{H}$ instead of the energy dependent Green’s functions of semi-infinite leads in equation (1). The passivation Hamiltonian of Ref.\[27\] can be identically reproduced with the parameters $\varepsilon = 1 \text{eV}, V_{ss} = -2.739 \text{eV}, V_{sp} = 4.743 \text{eV}, E_s = V_{sd} = V_{s*} = 0$ which is done within this work. It is worth to mention other passivation parameter sets can be used to mimic the saturation with various type of atoms (such as with SiO$_2$ as in Ref.\[28\]).

3. Results

The presented CAP lead method is first verified on a 3x3x10nm homogeneous Si nanowire in the sp3d5s* tight binding representation \[20\]. Since the lead consists of pure Si and is considered to be periodic, the common boundary self-energy methods are applicable here and can serve as a verification baseline. The electronic transmission is solved with the NEGF method and the contact self-energies calculated by the transfer matrix method \[10\] and the CAP method. In the CAP case, the numerical lead structure for the calculation includes 156 slabs in total. Figure 1 shows that the transmission of the CAP case agrees well with the reference. All observed deviations are very close to van-Hove singularities where convergence of the presented method is indeed the worst. These deviations are typically within a very small energy interval and become irrelevant in charge self-consistent calculations when the solution of the Poisson equation creates inhomogeneous potential profiles. In particular, for charge self-consistent IV characteristics, such deviations have been found to be negligible.

![Figure 1. Transmission in valence and conduction band of a Si nanowire described in the text solved with contact self-energies of the transfer matrix method (solid line) and self-energies of the CAP method (symbols).](image-url)
20nm long, 10nm thick graphene nanoribbon (GNR) illustrated in Fig.2 (a). Here, electrons are represented within the pd tight-binding model [21]. The leads are GNRs with a width that increases constantly with increasing distance to the nanoribbon channel. To verify the modelling, the transmission of this structure is solved in two ways, i.e. with two numerically different devices: In the case of device1, the active region where the NEGF equations are solved is limited to the central nanoribbon with constant width of 10nm. In the case of device2, the region where all NEGF equations are solved extends 5nm beyond the central ribbon into the trumpet shaped leads as shown in Fig.2 (a). Obviously, the lead/device interface width differs in the two cases. However, the ballistic transmission describes electronic propagation from minus to plus infinity along the transport direction. Since the devices 1 and 2 are physically equivalent, their transmissions have to agree – as confirmed in Fig.2 (b).

Random disorder as it appears in random alloys can also be covered by the presented method. A common treatment of alloy disorder scattering in the NEGF framework involves a perturbative treatment [19][8]. The unperturbed configuration in that case is then given by the virtual crystal approximation that was shown to potentially miss some band bowing effects [29]. A full 3D atomistic modelling capability of a non-perturbative alloy disorder scattering treatment in the lead is available with the presented CAP method.

Approximate disordered nanowire bandstructures have been compared for AlGaAs wires [30] indicating the relationship between tunneling turn-on and the approximate bandstructure. These results also indicated that the atomistically disordered wire confines localized states which can result in resonant-like transport. In those simulations, however it cannot be concluded if the localization is induced by the centrally disordered device or the attached homogenous leads that form a
herostructure with the central device. With the approach described in this work one can treat quantum transport with disordered contacts.

Figure 3 (a) shows two In$_{0.5}$Ga$_{0.5}$As nanowires with squared cross-sections of 3x3nm. The electrons are represented in sp3d5s* tight binding model [20]. The first device consists of In$_{0.5}$Ga$_{0.5}$As in the central region only and ideal InAs leads surrounding it while the second device consists of In$_{0.5}$Ga$_{0.5}$As in both device and leads. The In and Ga atoms in all In$_{0.5}$Ga$_{0.5}$As areas are randomly distributed within the atomically resolved structure. All results that are subject to random atom distributions are averaged over 50 samples.

The transmission coefficients for the alloy cases and their error bars are shown in Fig.3(b) for devices with lengths of 18nm and 6nm. Figure 3(b) illustrates for the case of pure InAs leads that the transmission through a 6nm long device is significantly larger than that of a 18nm long device. In contrast, leads with random alloy yield virtually device length independent transmission coefficients. This indicates the tunneling of pure InAs lead electrons through the random alloy In$_{0.5}$Ga$_{0.5}$As devices: the longer the device, the more pronounced is the dispersion mismatch between alloyed devices and ideal leads and the less likely is tunneling through the device. Similar lead/device reflections were reported when incoherent scattering was included in the active device, but ballistic leads were attached [31]. In contrast, when leads and device face the same effective random alloy the density of states between the leads and the device match and lead electrons face less reflection. As a result, the transmission remains the same when the device length changes. The small reduction of the device transmission with alloyed leads in the 18nm long device compared to 6nm long one (Fig. 3b) is due to a more pronounced weak localization in longer randomly alloyed devices.

**Figure 3.** (a) Schematic of randomly alloyed In$_{0.5}$Ga$_{0.5}$As nanowires with pure InAs leads and leads with In$_{0.5}$Ga$_{0.5}$As random alloy. (b) Calculated transmission coefficients for the alloy randomness structures as shown in (a), with device lengths of 18nm and 6nm, respectively.

Contact self-energies can be used to model the impact of dangling bond passivation without increasing the numerical load. This is illustrated in the following with solutions of the Schrödinger equation. All results and statements are transferable to the NEGF method as well.
Figure 4. (a) Bandstructure of a 4.3 nm GaAs quantum well grown in (111) direction in 10-band atomistic tight binding representation. Without any special treatment of the surface atoms the bandstructure shows states within the bandgap of GaAs (0-1.4 eV). (b) Bandstructure of the quantum well in (a) including the passivation self-energy of equation (3). The band gap is free of states.

Figure 4 (a) shows the bandstructure of a 4.3 nm thick GaAs quantum well without any special treatment of the surface atoms. The quantum well band gap should be larger than the GaAs material band gap, since the conduction (valence) band edge gets increased (lowered) by the confinement energy of the first confined valence and conduction band states. The effective (indirect) band gap of the unpassivated GaAs quantum well in Fig. 4(a), however, is smaller than the one of GaAs (~1.4 eV). For comparison, Fig. 4 (b) shows the same bandstructure when the passivation self-energies of equation (3) are added to the Hamiltonian. In that case, no states lie within the GaAs band gap.
Figure 5. Absolute squared of the wave functions at the Gamma point of Figs. 4. A typical surface state at energy $E=0.15\text{eV}$ in Fig.4(a) is shown with a solid line and a typical volume state (at $E=-0.02\text{eV}$ in Fig.4(b)) is given by a dash-dotted line. Oscillations between anions and cations that superpose the exponential decay of the surface state and the first confined state envelope of the volume state are common in atomistic representations.

Figure 5 compares the absolute squared wave function of one of the dangling bond states in Fig. 4 (a) at the Gamma point at an energy of $0.15\text{eV}$. This state is clearly located at the quantum well surface. In contrast Figure 5 also shows a typical state of the passivated quantum well of Fig. 4 (b) at the Gamma point and with an energy of -0.02eV.

4. Conclusion

It is demonstrated in this work how contact self-energies of irregular lead structures can be solved with the CAP method. It is also shown how contact self-energies can be used to efficiently model surface atom passivation. The CAP method is verified against conventional approaches for regular leads. The transmission of two numerically different, but physically equivalent irregular lead-structures agrees identically and verifies this method for irregular leads as well. Random alloy disorder in the leads is successfully modelled. It is shown that the typical assumption of ideal leads gives significant deviations from the disordered lead setup.

Atomistic tight binding calculations require to saturate dangling bonds of surface atoms. In this work it is shown how the concept of contact self-energies can be used to include passivation with Hydrogen atoms without increasing the system’s electronic Hamiltonian.

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6. References

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