Nonequilibrium Green's function method: Algorithm for regular and irregular leads

Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis
Network for Computational Nanotechnology,
Purdue University, West Lafayette, Indiana, USA, 47906
e-mail: wang1613@purdue.edu

INTRODUCTION

State of the art semiconductor devices face coherent quantum effects such as confinement and tunneling, as well as incoherent scattering with device imperfections and phonons. Over the last decade, the non-equilibrium Green's function method (NEGF) became the standard approach to model open nanoscale devices [1]. In this method, leads are either considered to be homogeneous or periodic [2,3]. In reality, however, leads have irregularities in their geometry, doping and alloy structure. Therefore, a method for solving regular as well as irregular leads is introduced in this work.

METHOD

The electronic transport has been solved with the atomistic tight binding NEGF implementation of the multipurpose nanodevice simulation tool NEMO5 [4]. All devices in this abstract are nanowires represented in the atomistic tight binding basis. Nevertheless, this method is applicable on any band structure model, geometry and periodicity (verified within NEMO5). Random alloys results have been averaged over 50 samples of discrete random distributions of the alloy atoms. The surface Green's functions of the leads are solved in a recursive Green's function (RGF) method [5,6]. Hereby, the lead portion that is considered explicitly in the RGF routine is determined by convergence of the lead surface Green's functions. This standard iterative approach is combined with an imaginary damping potential in leads that grows exponentially with increasing distance from the lead/device interface [6]. This damping potential allows limiting the numerical lead size to a few nanometers and is therefore essential for an efficient lead method.

All devices in this abstract are nanowires given in tight binding representation. Observables in the device such as the transmission and the density are obtained with the standard NEGF formula.

RESULTS AND DISCUSSION

To first verify the new lead algorithm, NEGF calculations with the iterative lead method are compared with NEGF calculations with leads solved in the well established transfer matrix method. Atomistic tight-binding NEGF simulations of a homogeneous Si 0.6nm × 0.6nm nanowire of 4.3 nm length with homogeneous Si leads have been performed using NEMO5. Figure 1 shows that the transmission coefficients resulting in both lead methods agree to a very high precision. Small deviations of the new iterative method are due to imperfect converged lead results typically close to band edges.

The new method can handle leads with arbitrary geometries. Figure 2 illustrates a benchmark device of a 12 nm long, 2 by 0.5 nm wide nanowire. The leads become wider with increasing distance to the device. The transmission of this device is calculated twice: first, only the homogeneous wire section is explicitly considered, while the rest is treated as leads (Fig.2 a). Second, a portion of the leads are explicitly included in the device. Since no bias is applied to the structure, the transmission coefficients of both situations have to agree – as confirmed by the results in Fig.3.

The new lead method can handle leads with random distribution of alloy atoms. Figure 4 shows the transmission in a GaAs nanowire with a 1.1 nm × 1.1 nm cross section and a length of 5 nm for 3 material configurations: pure GaAs in leads and wire, $In_{0.1}Ga_{0.9}As$ random alloy only in the wire, and $In_{0.1}Ga_{0.9}As$ alloy in the wire and the leads. NEGF results with randomness are averaged over 50 samples. The reduction of the transmission shows the large impact of alloy scattering in device and leads.

978-3-901578-26-7

CONCLUSION

A new algorithm is introduced for contact self-energies of general leads in the NEGF formalism. In contrast to existing methods, this method allows to model leads that include randomness fluctuations, such as random alloys and (not shown) random impurities.

ACKNOWLEDGEMENT

This work is support by nanoHUB.org computational resources and by the SRC task 2141.

REFERENCES

[1] S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge University Press, Cambridge (2005).

[2] M. Luisier, A. Schenk, W. Fichtner, G. Klimeck, *Atomistic simulation of nanowires in the sp3d5s* tight-binding formalism: from boundary condictions to strain calculations*, Phys. Rev. B 74, 205323 (2006).

[3] M. P. L. Sancho and J. M. L. Sancho, *Quick iterative scheme for the calculation of transfer matrices: Application to Mo (100)*, J. Phys. F, Met. Phys. 14, 5 (2000).

[4] S. Steiger, M. Povolotskyi, H.-H. Park, T. Kubis, and G. Klimeck, *NEMO5: A Parallel Multiscale Nanoelectronics Modeling Tool*, IEEE Trans. on Nano. 10, 1464 (2011).

[5] R. Lake, G. Klimeck, R. C. Bowen, D. Jovanovic, *Single and multiband modeling of quantum electron transport through layered semiconductors devices*, J. Appl. Phys. 81, 7845 (1997).

[6] T. Kubis, *Quantum transport in semiconductor nanostructures*, Verein zur Förderung des Walter Schottky Instituts der Technischen Universität München e.V., Garching (2009).

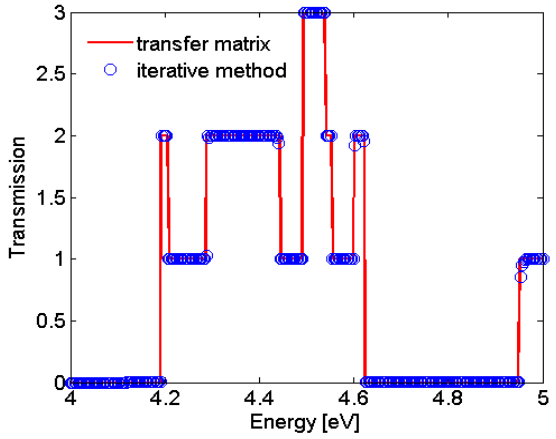

Fig. 1. Transmission coefficient of a homogeneous Si nanowire calculated in the transfer matrix (line) and the new iterative method (symbols).

Fig. 2. 12nm Si nanowire with a 2nm × 0.5nm cross section and conical leads when (a) only the wire is the active device (dark region) and (b) 2.7 nm of the leads are explicitly included.

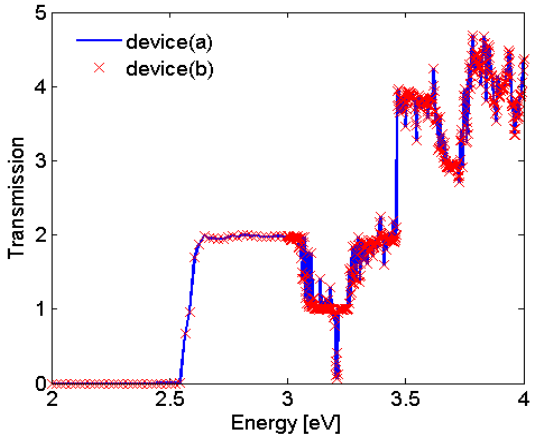

Fig. 3. Comparison of the transmission coefficient of the devices in Fig. 2 (a) (line) and Fig. 2(b) (symbols)..

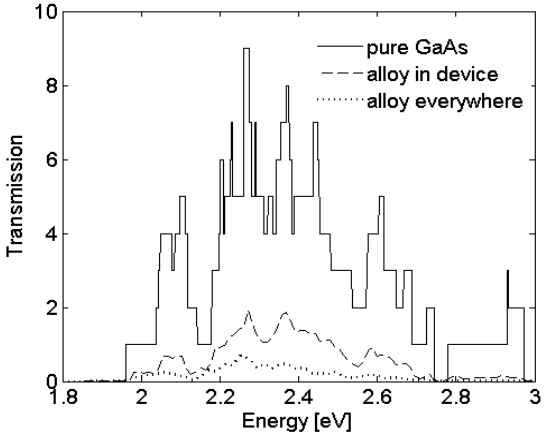

Fig. 4. Comparison of transmission in the pure and alloyed nanowire described in the main text.