Electron-phonon scattering from green's function transport combined with molecular dynamics: Applications to mobility predictions

T Markussen[1], M Palsgaard[1,2], D Stradi[1], T Gunst[2], M Brandbyge[2] and K Stokbro[1]

[1]QuantumWise A/S, Denmark, [2]Technical University of Denmark, Denmark

The interaction between electrons and phonons is an important scattering effect limiting the mobility of carriers in nanoscale materials. Phonon-limited mobilities can be rigorously calculated at the atomistic level, using established electronic structure methods such as density functional theory (DFT) or tight- binding, coupled to either the Boltzmann transport equation (BTE) [1] in the case of bulk materials, or to Non-equilibrium Green's function (NEGF) theory [2,3,4] in the case of devices.

Nevertheless, in practical applications the evaluation of the electron-phonon coupling (EPC) matrix is numerically challenging, and approximations have to be applied. The most common one in both the BTE and the NEGF approaches is to treat the phonons within the harmonic approximation, thereby neglecting anharmonic effects, which might play an important role at finite-temperatures. Further approximations are also used in NEGF-based approaches to make the computation of the EPCs based on perturbation theory feasible [3,5,6].

In this contribution, we present an alternative approach combining NEGF theory and the Landauer approach with molecular dynamics (MD) [7] to calculate phonon-limited mobilities at the atomistic level [8]. In a device geometry with a central region coupled to two electrodes, we perform MD simulations for central regions of increasing length, and extract the resistivity and eventually the mobility from the slope of the resulting resistance vs. length curves. Compared to previous approaches for the phonon- limited mobility, the present method is conceptually simple, it naturally includes finite-temperature and anharmonic effects, and allows for simulations of mobilities in non-crystalline and defected materials. We validate our approach by comparing to mobilities and conductivities obtained using the BTE for different bulk and one-dimensional systems, and compare successfully against experimental values for bulk silicon and gold. All the calculations have been performed using the Atomistix ToolKit software [9].

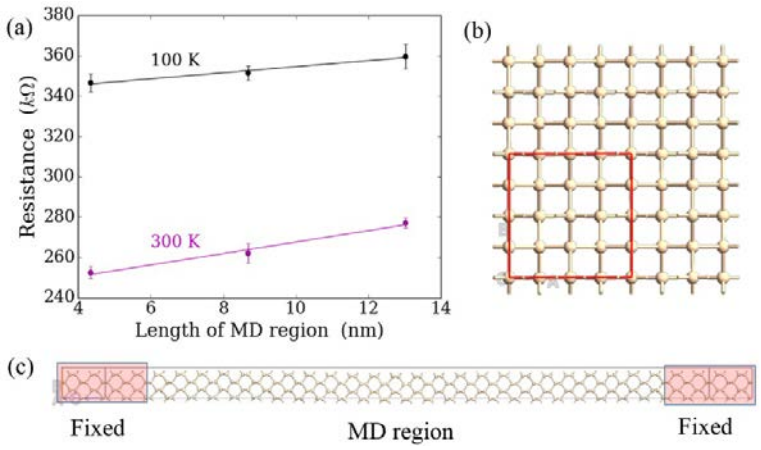

Figure: (a) Resistance vs. length curve for bulk silicon at temperatures T = 100 K (upper curve) and T = 300 K (lower curve). (b) Cross section of the simulation cell. (c) Scheme of the device configuration with a length of the central MD region of 13 nm.

[1] T. Gunst, T. Markussen, K. Stokbro and M. Brandbyge, Phys. Rev. B 93, 035414 (2016)

[2] M. Brandbyge, J.-L. Mozos, P. Ordejon, J. Taylor, and K. Stokbro, Phys. Rev. B 65, 165401 (2002)

[3] M. Luisier, G. Klimeck, Phys. Rev. B 80, 155430 (2009)
[4] K. Stokbro, D. E. Pedersen, S. Smidstrup, A. Blom, M. Ipsen, and K. Kaasbjerg, Phys. Rev B 82 075420 (2010)
[5] T. Gunst, T. Markussen, K. Stokbro, and M. Brandbyge, Phys. Rev. B 93, 245415 (2016)
[6] T. Frederiksen, M. Paulsson, M. Brandbyge, and A.-P. Jauho, Phys. Rev. B 75, 205413 (2007)
[7] J. Schneider, J. Hamaekers, S. Smidstrup, J. Bulin, R. Thesen, A. Blom, and K.Stokbro, ArXiv:1701.02495
[8] Atomistix ToolKit, version 2016.3, QuantumWise A/S www.quantumwise.com
[9] T. Markussen, M. Paalsgard, D. Stradi, T. Gunst, M. Brandbyge, and K. Stokbro, ArXiv:1701.02883

Efficient quantum approach of electron-phonon scattering for nanoscale device simulations

Y Lee[1], M Lannoo[1], N Cavassilas[1], M Luisier[2] and M Bescond[1]

[1]Aix-Marseille University, France, [2] ETH Zürich, Switzerland

In recent decades various transport approaches have been proposed to describe quantum effects occurring in nano-devices [1], [2]. Among them, Nonequilibrium Green's function formalism (NEGF) has been proved very suitable at treating inelastic interactions [3]. However, within this formalism the description of inelastic scattering is usually based on the computationally expensive self-consistent Born approximation (SCBA). As an alternative method to SCBA, we have proposed an efficient technique, the so-called Lowest Order Approximation (LOA) coupled with Padé approximants [4], [5]. In this work, we apply this approach to the treatment of phonon scattering in two 1D systems where phonon scattering is known to be important: the atomic linear chain and the nanowire transistor. In NEGF the interacting Green's function is calculated by combining an electron-phonon self-energy ($\Sigma[G]$) with the Dyson equation [3]:

$$G = g0 + g0\Sigma[G]G, \quad (1)$$

where $g0$ is the non-interacting Green's function. Since Dyson's equation (1) is non-linear, solving Eq. (1) is typically based on the iterative SCBA scheme. Alternatively, we define LOA Green's functions at a given order N in interaction as follows:

$$gN = gN - 1 + g0 \sum_{n=0}^{N-1} \Sigma [\Delta gN - n - 1] \Delta g_n, \quad (2)$$

where $\Delta g_n = gn - \Delta g_{n-1}$ and $\Delta g0 = g0$. By using Eq: (2), we can calculate current series $I_N = I(gN)$ and carrier density series ρN = ρ (gN) to Nth order in interaction. According to the strength of the electron-phonon scattering, the LOA series can diverge. We then use Padé approximant technique to operate a convergent resummation. Note that the LOA series can be also coupled to Hyper geometric resummation technique [6].

We first apply our technique to the ideal 1D linear atomic chain (Fig. 1) where one optical phonon mode ($\hbar\omega$ = 60 meV) is coupled with electrons de- scribed by a two-band *k·p* Hamiltonian (inset of Fig. 1). Figure 2 shows current-voltage characteristics in the ballistic regime, SCBA and with our LOA- Padé technique when electron-phonon coupling *M* is large. It is clearly shown that 3*rd* order LOA currents combined with Padé 1/2 successfully reproduce the SCBA values. Figure 3 shows that electron density along the device can also be reconstructed with the LOA-Padé approach even though it needs up to 5*th order* LOA (i.e. Padé 2/3). Moreover, the series of LOA physical quantities can be derived from the SCBA algorithm [7]. The approach can then be applied to the n-type 3D nanowire transistor (Fig. 4 (a)) where a full- band atomistic treatment for electrons (Fig. 4 (b)) and phonons (Fig. 4 (c)) is considered [8]. Figure 5 compares Id-Vg curves of