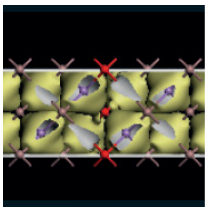

Non-equilibrium Green's function method: Band tail formation in non-local polar optical phonon scattering

P Sarangapani, Y Chu, J Charles, G Klimeck, and T Kubis

Purdue University, USA

Polar materials with their unique properties offer a wide variety of applications in electronics and optoelectronics. III-V materials such as InGaAs, GaSb and InAs are being considered as potential candidates to replace Si technology due to their low effective mass [1], [2]. Transition metal dichalcogenides (TMDCs) based 2D materials have found applications as FETs and TFETs and are promising candidates for future electronics [3],[4]. Polar optical phonon scattering (POP) is one of the dominant scattering mechanisms in these materials and is necessary for quantitative and qualitative prediction of device performance. Previous works on POP scattering within Non-equilibrium Green's function (NEGF) formalism are either confined to bulk systems [5], [6] or apply diagonal approximations [7] which is known to underestimate scattering.

In this work, a physically consistent model to treat POP scattering with full non-locality through selfenergies has been developed for bulk, ultra thin body (UTB) and nanowire devices. Through this approach, reliable scattering rates are computed and compared against FGR. Presence of band tails is demonstrated and the extracted Urbach parameter is shown to agree well with available experimental data. Local approximation of scattering is shown to underestimate both scattering rate and Urbach parameter.

NEGF is widely accepted formalism for nanoscale electronic, thermal and optoelectronic simulations [8], [9], [10]. Within the NEGF formalism, scattering is treated through the self-consistent Born approximation where the scattering self-energy is solved iteratively withthe Green's function until convergence. Scattering selfenergy formulas for POP have been derived assuming that the bulk phonons are in equilibirum. Fr¨ohlich coupling is used to model the electron-phonon interaction potential. Electrostatic screening is calculated through the Debye approximation. This method has been implemented within the multipurpose nanodevice simulation tool, NEMO5 [11]. All POP scattering mechanisms are available in all electronic models of NEMO5 (e.g. effective mass, tight binding, Wannier function representation etc.). The scattering self-energies are verified by comparing the scattering rates from NEGF against FGR. Fig. 1 shows comparison of scattering rates obtained for bulk and nanowire GaAs indicating the validity of self-energy expressions.

High doping in semiconductors is associated with band tails (known as Urbach tails) that drop exponentially below the band gap. At room temperature, the band gap narrowing is in the order of few kBT. This can strongly alter performance of devices such as TFET and LEDs where band gaps play an important role in device behaviour. Through POP scattering simulation, one can directly observe such Urbach tails and extract the Urbach parameter. Fig. 2 shows band tails observed for GaAs nanowire. Fig. 3 shows comparison of Urbach parameter for undoped GaAs with experimental data [12]. Simulation results show good agreement with experimental observation confirming the accuracy of the model.

POP scattering is inherently a non-local scattering process. This results in dense self-energy matrices which increase computational time considerably. Often, local approximations are made to speed up simulation. From Fig. 3, one can observe that local approximations severely underestimate the Urbach parameter of GaAs. Fig. 1a shows the scattering rate with and without local approximation where the rate is underestimated by a factor of 2. Therefore, to get meaningful results, nonlocality must be an essential component of the simulation and cannot be neglected.

POP scattering covering full non-locality within the NEGF formalism has been shown and is verified by comparing it against FGR. Presence of Urbach band tails is demonstrated and the extracted Urbach parameter is found to be in agreement with experimental results. Local approximation for such scattering is shown to underestimate physical quantities such as Urbach parameter and scattering rates requiring a non-local simulation approach.

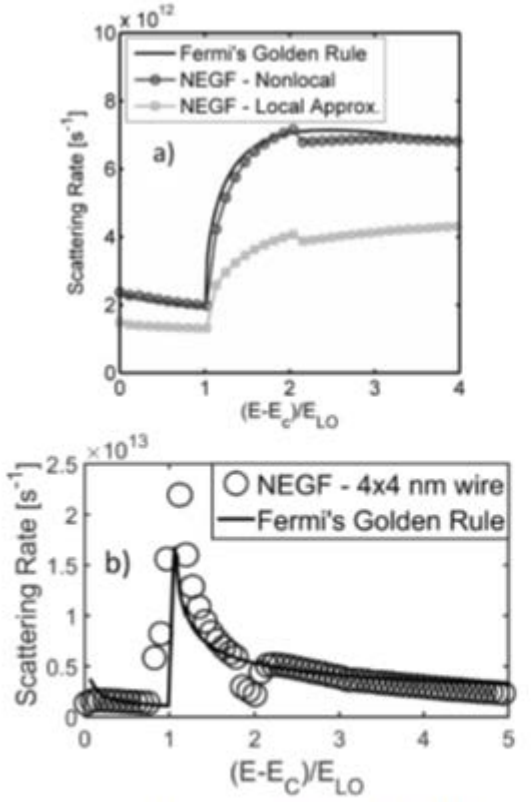

Fig. 1: a) Scattering rate comparison with FGR for bulk GaAs with and without local approximation. b) Scattering rate comparison with FGR for GaAs nanowire.

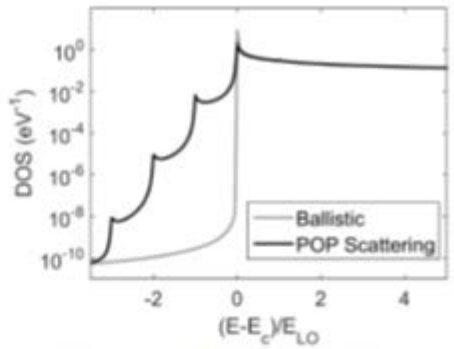

Fig. 2: Presence of band tails with POP scattering for GaAs nanowire. Peaks correspond to LO phonon side-bands.

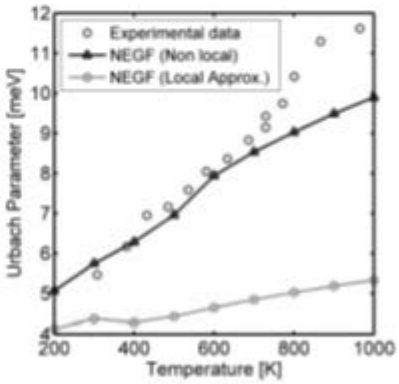

Fig. 3: Comparison of variation of Urbach parameter with temperature for undoped GaAs with experimental data [12]. Local approximation of scattering severely underestimates the Urbach parameter.

[1] P. Ye et al., Applied Physics Letters, vol. 84, no. 3, pp. 434–436, 2004.
[2] B. M. Borg et al., Nano letters, vol. 10, no. 10, pp. 4080–4085, 2010.
[3] B. Radisavljevic et al., Nature nanotechnology, vol. 6, no. 3, pp. 147–150, 2011.
[4] S. Das et al., Nano letters, vol. 13, no. 1, pp. 100–105, 2012.
[5] R. Lake et al., Journal of Applied Physics, vol. 81, no. 12, pp. 7845–7869, 1997.
[6] T. Kubis et al., physica status solidi (c), vol. 5, no. 1, pp. 232–235, 2008.
[7] M. Luisier et al., Journal of Applied Physics, vol. 107, no. 8, p. 084507, 2010.
[8] S. Datta, Superlattices and microstructures, vol. 28, no. 4, pp. 253–278, 2000.
[9] J. Taylor et al., Physical Review B, vol. 63, no. 24, p. 245407, 2001.
[10] S. Sadasivam et al., Ann. Rev. Heat Transfer, vol. 17, pp. 89–145, 2014.
[11] S. Steiger et al., "Nemo5: A parallel multiscale nanoelectronics modeling tool," 2011.
[12] M. Beaudoin et al., Applied physics letters, vol. 70, no. 26, pp. 3540–3542, 1997.