Prediction of Urbach Tails and Band Gap Narrowing in Bulk and Confined III-V Devices with Atomistic Non-Equilibrium Green's Functions

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High-doping induced Urbach tails and band gap narrowing play a significant role in determining the performance of tunneling devices and optoelectronic devices such as tunnel field-effect transistors (TFETs) [1][2], Esaki diodes and light-emitting diodes [3][4]. In this work, Urbach tails and band gap narrowing values are calculated explicitly for four candidate bulk and confined III-V devices (GaAs, InAs, GaSb and GaN) with scattering self-energies using the non-equilibrium Green's function approach in a multi-band tight binding basis. The scattering self-energies and subsequent scattering rates (Fig. 1 and Fig 2.) are solved using the self-consistent Born approach. Dominant non-local scattering mechanisms such as polar optical phonons and charged impurity scattering are considered with Lindhard screening. Predicted Urbach tails (Fig. 3) and band gap narrowing (Fig. 4) results are shown to agree well with available experimental data for a range of temperature and doping regimes. Dependence with doping is observed to be strongly dependent on confinement and screening. Guideline values for Urbach tail and band gap narrowing will be presented for ultra-thin body and nanowire devices.

[1] E. Lind, E. Memisevic, A. W. Dey, and L.-E. Wernersson, J. Electron Devices Soc. 3, 96 (2015).
[2] U.E. Avci, D.H. Morris, and I.A. Young, IEEE J. Electron Devices Soc. 3, 88 (2015).
[3] J. Geng, P. Sarangapani, K.-C. Wang, E. Nelson, B. Browne, C. Wordelman, J. Charles, Y. Chu, T. Kubis, and G. Klimeck, physica status solidi (a)215, 1700662 (2018).
[4] A. Laubsch, M. Sabathil, J. Baur, M. Peter, and B. Hahn, Trans. Electron Devices 57, 79 (2010).
[5] S. Johnson and T. Tiedje, „Journal of App. Phys. 78, 5609(1995).
[6] H. Yao and A. Compaan, App. Phys. Lett. 57, 147 (1997).
[7] H. Luo, W. Shen, Y. Zhang, and H. Yang, Phys. Cond. Matt. 324, 379 (2002).
[8] E. Harmon, M. Melloch and M. Lundstrom, App. Phys. Lett. 64, 502 (1994).

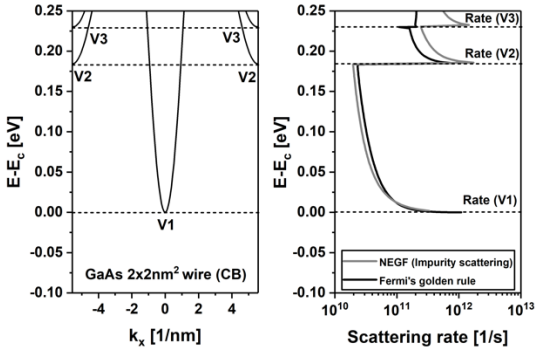

Fig.1: a) Conduction band profile of 2nmx2nm GaAs nanowire. b) Comparison of conduction band scattering rates obtained from NEGF against Fermi's golden rule for charged impurity scattering in 10-band sp3d5s* tight binding basis for a doping concentration of 2x10^{18} cm^{-3}. Screening length is set at 3 nm.

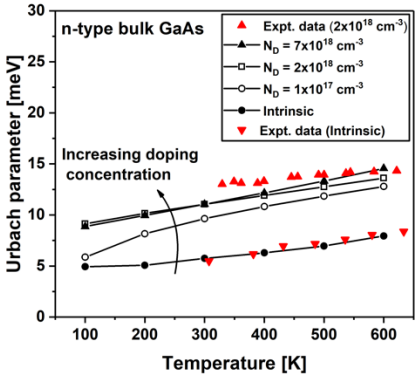

Fig.3: Variation of Urbach parameter as a function of temperature for n-type GaAs for different doping concentrations. Simulation results show good agreement with experimental data obtained from Ref. [5] for intrinsic case and for a doping concentration of 2x10^{18} cm^{-3}.

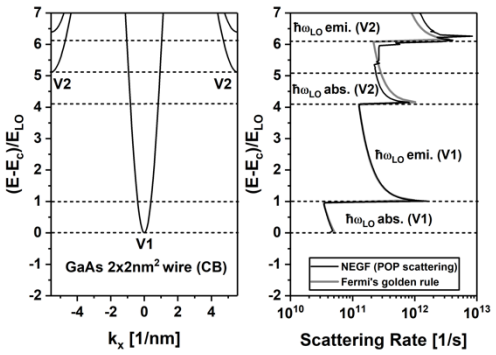

Fig.2: a) Conduction band profile of 2nmx2nm GaAs nanowire. b) Comparison of conduction band scattering rates obtained from NEGF against Fermi's golden rule for polar optical phonon scattering in 10-band sp3d5s* tight binding basis for a doping concentration of 2x10^{18} cm^{-3}. Screening length is set at 3 nm.

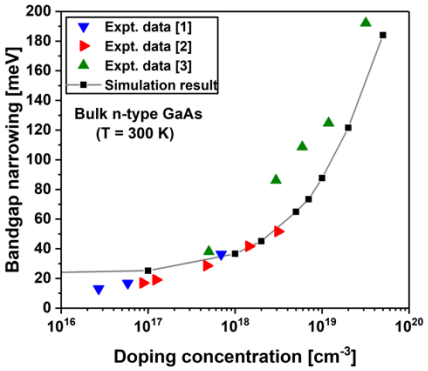

Fig.4: Variation of band gap narrowing of conduction band as a function of doping concentration for GaAs. Simulation results have been compared against a set of experimental results. Exp. data [1], Exp .data [2] and Exp. data [3]) obtained from Refs. [6], [7], and [8] respectively. Simulation results show very good agreement with available experimental data.