Phonon scattering influence in single dopant nanowire transistors

H. Carrillo-Nuñez, M. Bescond, N. Cavassilas, E. Dib, and M. Lannoo

IM2NP, UMR CNRS 7334, Bât. IRPHE, Technopôle de Château-Gombert, 13384 Marseille, cedex 13, France e-mail: hacarrillo@gmail.com, marc.bescond@im2np.fr

Technological achievements have made possible to set the position of dopants in a deterministic way [1], which might indicate an original direction for controlled single dopant devices [2]. In this work we investigate the influence of phonon scattering through a single dopant in a silicon nanowire transistor (Fig. 1). Quantum transport simulations are performed via a 3D real-space non-equilibrium Green's function (NEGF) approach in which electron-phonon interactions are tackled within the self-consistent Born approximation (SCBA) [3].

Figure 2 shows the $I_D - V_G$ current characteristics in four transport regimes: i) ballistic, ii) SCBA with both acoustic and optical phonons, iii) SCBA with only optical phonons, and iv) SCBA with only acoustic phonons. We first note that ballistic current depicts a hysteresis from $V_G \simeq 0.32$ V to $V_G \simeq 0.42$ V, confirming the bistability reported by Mil'nikov et al. [4]. Figs. 3(a-c) show ballistic electron density and current spectra for the upper branch of the current characteristic at $V_G = 0.375$ V (represented by vertical dashed line in Fig. 2). In this configuration, the dopant level (ϵ_r) is above the source subband energy (ϵ_s) and impurity is mainly screened by electrons of the source. Figs.3(b-d) show the same physical parameters for the lower branch where ϵ_r is now below ϵ_s . The donor is then populated by electrons injected from the drain, leading to a different screening with a strong reduction of broadening of the impurity level.

Interestingly, incorporation all phonon interactions remove the current hysteresis (solid line in Fig. 2). As shown by Figs. 4(a-b) the broadening of the resonant site does not depend anymore on its position with respect to ϵ_s . It results a smooth transition of the current when ϵ_r goes below ϵ_s at $V_G=0.4$ V (Figs. 4(c-d)). Figure 2 shows also that current hysteresis remains when only optical phonon interactions are included while it disappears with only acoustic scattering. Indeed, the strong coupling with acoustic phonons in nanowires makes the broadening of the impurity level independent of V_G ($\Gamma_{ac} \simeq 20$ meV). The donor level is then progressively populated by electrons from the drain when it goes below ϵ_s without any abrupt variation of the impurity potential. On the other hand, the weaker coupling with optical phonons in nanowires induces less modifications of the electron density but it makes electrons relaxed into the donor state at high V_G . It results a phonon-assisted resonant tunneling (Figs. 5) which can significantly increase current in the on-regime. This effect can even induce a ballisticity [5] I_D^{scatt}/I_D^{ball} larger than 1 as shown in Fig. 6.

To summarize, acoustic phonon scattering reduces current at low V_G and suppresses the hysteresis, while optical phonons increase the current in the on-regime. However we expect the bi-stability of the system to be recovered at low temperature where acoustic-phonon interactions are significantly reduced.

This work is supported by Quasanova contract funded by the French National Research Agency.

REFERENCES

- T. Shinada, S. Okamoto, T. Kobayashi, and I. Ohdomar, , Nature 437, 1128 (2005).
- [2] M. Bescond, M. Lannoo, L. Raymond, and F. Michelini, J. Appl. Phys. **107**, 093703 (2010).
- [3] M. Bescond, C. Li, H. Mera, N. Cavassilas, and F. Michelini, J. Appl. Phys. **114**, 153712 (2013).
- [4] G. Mil'nikov, N. Mori, Y. Kamakura, and T. Ezaki , Phys. Rev. Lett. **102**, 036801 (2009).
- [5] M. Luisier, and G. Klimeck , Phys. Rev. B 80, 155430 (2009).



Fig. 1. Schematic representation of the considered silicon nanowire MOSFET with dopant located at the center of the channel. The silicon cross-section is $2 \times 2 \text{ nm}^2$ and L_{CH} =8 nm. In all the study V_{DS} =0.1 V, source/drain doping is N_D =10²⁰ cm⁻³, transport direction < 100 > and T=300 K.



Fig. 2. $I_D - V_G$ characteristics of the nanowire MOSFET of Fig. 1. Four transport regimes are considered: i) ballistic (squares), ii) SCBA with both acoustic and optical phonons (solid line), iii) SCBA with only optical-phonons (dotted line) and iv) SCBA with only acoustic phonons (dashed line with crosses).



Fig. 3. Ballistic electron density (top) and current (bottom) spectra for the two current points at $V_G = 0.375$ V in Fig 2 (defined by the vertical dashed line). Left column represents the higher branch of the current while right column represents its lower counterpart. The white line is the first subband energy profile along the transport direction.



Fig. 4. SCBA electron density (top) and current (bottom) spectra with both acoustic and optical phonons at $V_G = 0.40$ V (a-c) and $V_G = 0.45$ V (b-d)). In each sub-figure, the white line is the first subband energy profile along the transport direction.



Fig. 5. SCBA current spectrum with only optical phonon interactions at V_G =0.425 V. The component resulting from phonon-assisted resonant tunneling is clearly visible.



Fig. 6. Ballisticity of the nanowire transistor with i) only the optical phonons (triangles), and ii) including all the phonon interactions (circles).