Dependence of Matthiessen's Rule on Complex Phonon Self–Energies: A NEGF Study

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Matthiessen's rule is a useful tool to estimate mobilities, however at nanoscales it should be used with care. Previous work on the validity of the Matthiessen's rule [1], [2] using only the imaginary part of the phonon self–energies was carried out. Ref. [2] estimated a 13% breakdown of the rule. Refs. [3], [4] showed that when the real part of the self-energy is not taken into account the Density of States (DOS) is underestimated, and as a consequence, the drain current is lower when only the imaginary part of the self–energy is considered. In this work the impact of the full self–energy (real+imaginary) in the current voltage characteristics of a gate–all–around Si nanowire transistor has been studied at low drain bias. In addition, the deviation of the Matthiessen's rule considering the full self–energy has been calculated and the results have been compared with our previous work [2]. The simulated device has a 20 nm channel length and a 2.2×2.2 nm^2 cross–section with an oxide thickness of 0.8 nm. The source and drain regions are 15 nm long with doping concentration of 10^{20} cm^{-3}. The I_D–V_G characteristics at V_D=1 mV with different phonon mechanisms are shown in Fig. 1. The low drain bias has been chosen in order to evaluate the Matthiessen's rule under low field conditions. At low gate bias, the current for the case of full self–energy is larger than the case with only imaginary self–energies. At high gate bias the situation is reversed. The contribution of each scattering mechanism to the total phonon scattering process has also been calculated and compared with the ballistic case. Fig. 1 shows that the largest contribution to the scattering process corresponds to the acoustic phonons and the lowest one to the f phonons. Fig. 2 shows the first sub–band along the channel at low and high gate bias (V_G = 0.3 V and V_G = 0.7 V) for the case of full self–energy and for the case of the imaginary part only. The gate barrier height relative to the source is similar for both cases and gate bias. Fig. 3 shows that the spectral current density for the full self–energy and imaginary cases in the middle of the channel. The curve for the full self–energy case is shifted to the left relative to the imaginary case curve and it has a large area at low gate bias. This implies a larger current for the full self–energy case. Fig. 4 shows an smaller shift but the area of the curve for the full self–energy case is larger than the corresponding area of the other case. Finally, we have calculated the resistances as a function of the gate bias for the full and the imaginary self–energies cases in order to evaluate the deviation of Matthiessen's rule. Fig. 5 shows the extracted resistances as a function of gate bias, we observe the exponential dependence of the inversion charge. The resistance values of the full self–energy case is lower than the other case at low gate bias. The Matthiessen's rule deviation has been calculated using 100×(1-R_{Mat}/R_{NEGF}), where R_{Mat} is the total resistance, which is obtained by adding the resistances from the simulations with each individual scattering mechanism and R_{NEGF} is the resistance obtained from simulation considering all the scattering mechanisms. The Matthiessen's rule deviation has been calculated for the full self–energy and with only the imaginary part. Fig. 6 shows the Matthiessen's deviation as a function of the inversion charge. The deviation is larger for the case of only imaginary self–energy at very large inversion charges. At low inversion charge Matthiessen's rule over–estimates the resistance. In conclusion, the off-current for the full self–energy case is two times larger than the corresponding current of the imaginary case but at high bias the difference is only 7%.

References

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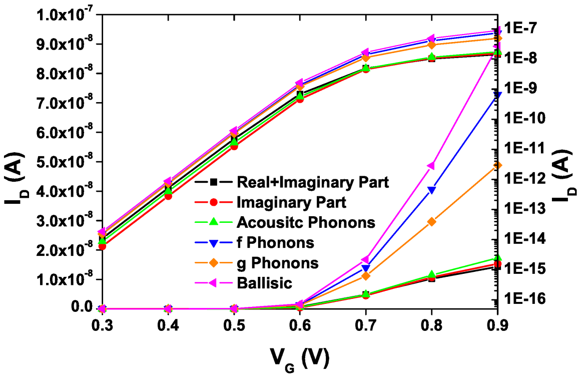

Fig. 1: I_D–V_G characteristics at V_D = 1 mV for the 20 nm gate length silicon nanowire transistor with different phonon mechanisms in operation for the full self–energy and its comparison with only the imaginary part of the self–energy when all the phonon mechanisms are active.

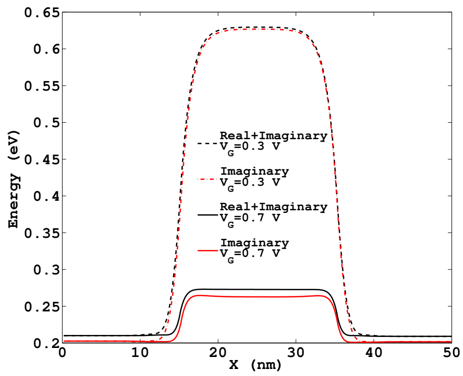

Fig. 2: First sub–band along the transport direction at low (V_G = 0.3 V) and high (V_G = 0.7 V) gate bias.

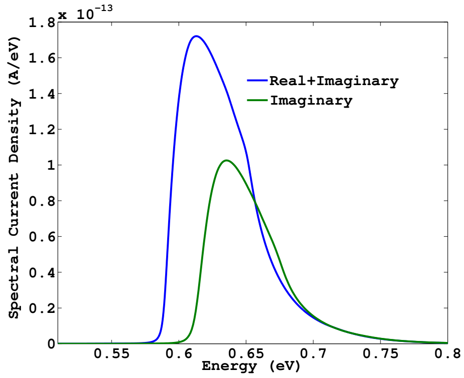

Fig. 3: Spectral current density in the middle of the channel for the the full self–energy and imaginary cases at low gate voltage (V_G = 0.3 V).

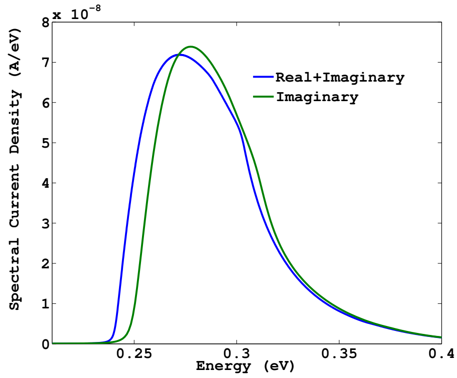

Fig. 4: Spectral current density in the middle of the channel for the the full self–energy and imaginary cases at high voltage (V_G = 0.7 V).

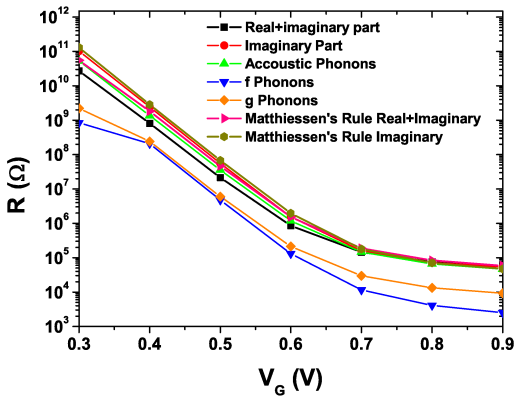

Fig. 5: Resistances of the silicon nanowire and comparison with Matthiessen's rule for both cases.

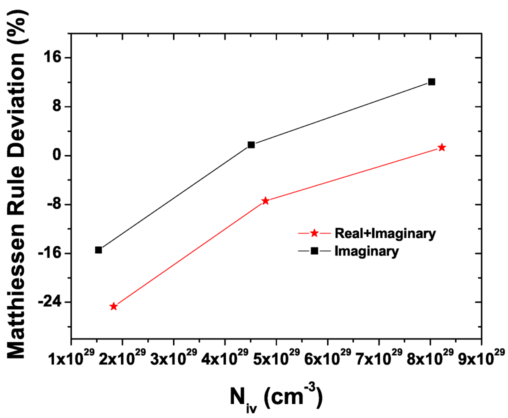

Fig. 6: Matthiessen's rule deviation as a function of the inversion charge for the cases of Fig. 5.