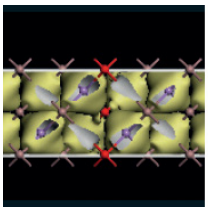

Physically based diagonal treatment of polar optical phonons in III-V p-type double-gate transistors: comparison of InAs *vs* Ge and Si

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III-V materials are considered to be a promising solution for the next generation of Complementary Metal Oxide Semiconductor (CMOS) technology [1]. It is then a central issue to predict the performances of III-V based devices through realistic quantum modeling [2]. Non- Equilibrium Green's Function (NEGF) is one of the most established technique to treat quantum transport in nano-devices. For numerical convenience carrier-phonon scattering is usually treated in NEGF within a local approximation through the concept of self-energy [3]. However III-V compound semiconductors are subject to long range polar optical (PO) interactions of the Fro¨hlich type [4]. The difficulty with these PO interactions is that the corresponding self-energy decays very slowly in real space, like a Coulomb potential. Furthermore they should be affected by the confinement. Previous studies have attempted to model them with diagonal self-energies multiplied by a scaling factor estimated to be of order 10 in some cases [5] but there is no general prescription. In this work we developped an original method to determine the scaling factor taking into account the confinement and the effective masses. We first use the electron-phonon PO coupling derived by Mori and Ando [6] for heterostructures. From this we determine the analytic form of the equilibrium self- energy which we average over the confined zone and compare it to its local approximation to get the scaling factor. This procedure is well defined and should at least be valid for small departures from equilibrium in the spirit of the quantum Boltzmann equation [7].

Based on a 8×8 k.p Hamiltonian, we then use this model for a performance benchmarking of Ge and Si with respect to the principal III-V materials (InAs, InSb, GaSb) considering 15 nm gate length (LG) double-gate pMOSFETs under uniaxial strain (Fig.1). Among the various strains and III-V material configurations which have been investigated, InAs $<110>$-compression presents the best ION *vs* IOFF ratio in the ballistic regime (Fig 2). Figure 2 also shows the impact of phonon scattering for three current coordinates in InAs, Ge and Si. We can see that ON-current decreases by 70% in InAs device. PO phonons represent the major contribution to this reduction since reduction with accoustic and non polar optical phonons is 26%. As a comparison the ON- current decrease in Ge and Si devices is equal to 30% and 50% respectively. The impact of phonon scattering in the different materials is illustrated *via* the spectral current in Figures 3, 4 and 5. The influence of phonon scattering is also shown in Fig. 6, which presents the broadening of DOS in the valence band. It has a gradual impact from Ge, Si and InAs. These results are in agreement with the trend in experimental bulk mobilities and effective masses shown in TABLE I. Indeed with the same values of effective masses, bulk InAs is found to have a very small mobility compared to Ge, pointing that phonon scattering is higher in InAs. When compared with Si (same hole mobilities but different effective masses), the InAs phonon scattering strength is also higher. This work then emphasizes the large impact of PO phonons on III-V double gate nanotransistor characteristics. This scattering must be correctly included to assess the real performances of such devices.

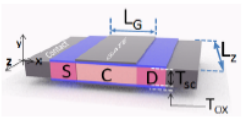

Fig. 1. Top view of the considered Double-Gate p-type MOSFETs. For all devices T_{SC}=2 nm, T_{OX}=1 nm, Source and Drain doping is 8.10^{19} cm^{-3}, L_G equal to 15 nm and V_{DS}= -0.6 V.

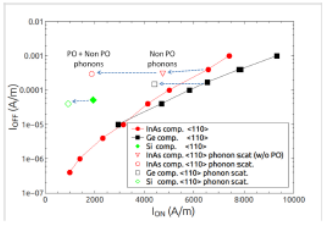

Fig. 2. I_{ON} *vs* I_{OFF} curves of $< 110 >$-compression III-V material based devices and Ge in the ballistic regime. Empty symbols represent current coordinates calculated with phonon scattering. Value of InAs with only acoustic non polar optical is also indicated (empty circle).

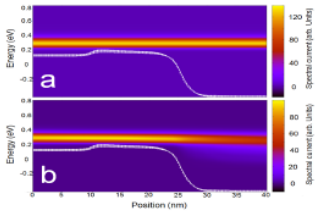

Fig. 3. Current spectrum (arb. units) of $< 110 >$-compressive Ge along the device (**a**) in the ballistic regime and (**b**) with phonon scattering calculated with the bulk deformation potentials. Phonon scattering is weaker than in Si (Fig. 4) and InAs (Fig. 5).

	Ge	InAs	Si
Hole mobility (cm^2/Vs)	1900	500	430
Hole Effective mass ($/m_0$) m_{HH} |m_{LH}	0.35|0.043	0.37|0.043	0.53|0.16

TABLE I
BULK HOLE MOBILITY AND EFFECTIVE MASS VALUES FOR Ge, InAs AND Si.

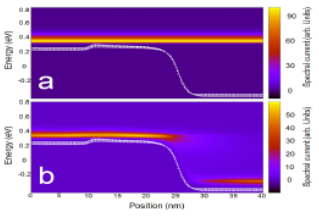

Fig. 4. Current spectrum (arb. units) of $< 110 >$-compressive Si along the device (**a**) in the ballistic regime and (**b**) with phonon scattering calculated with the bulk deformation potentials.

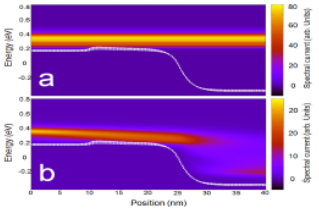

Fig. 5. Current spectrum (arb. units) of $< 110 >$-compressive InAs along the device (**a**) in the ballistic regime and (**b**) with phonon scattering. All phonon interations are included (accoustic, non polar optical and polar optical).

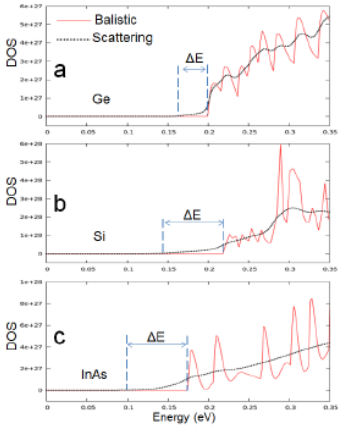

Fig. 6. Density of states (DOS) at the device source side for (**a**) Ge, (**b**) Si and (**c**) InAs, showing the broadening of states ΔE in the valence band due to phonon interactions. $\Delta E = 4$ meV for Ge $\Delta E = 8$ meV for InAs and $\Delta E = 9$ meV for Si.

[1] K. Kuhn *IEEE Trans. Electron Devices*, vol. 59, p. 1813, (2012).
[2] N. Cavassilas *et al. App. Phys. Lett.*, vol. 96, p. 102102, (2010).
[3] M. Luisier *et al. Phys. Rev. B.*, vol. 80, p. 155430, (2009).
[4] H. Fro¨hlich in *Proc. R. Soc. London, Ser. A*, p. 230, (1937).
[5] G. Klimeck *et al.*, "Numerical approximations for polar opti- cal phonon scattering in resonant tunneling diodes," in *Proc. Quantum Devices and Circuits. Imperial Press, London*, p. 154, (1996).
[6] N. Mori and T. Ando *Phys. Rev. B*, vol. 40, p. 6175, (1989). [7] M. Moussavou *et al. under preparation*, (2017).