3D Monte Carlo simulatisns of strained Si GAA nanowire FETs with different channel orientations

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GAA NW FETs are considered to be the most promising candidates for sub-10 nm digital technology suitable for future CMOS integration due to their superior electrostatics, immunity to short channel effects and large on-current [1]. Strain technology can enhance the drain current [2] but the effective- ness of strain can be reduced due to the pre-existing quantum confinement induced valley splitting [3].

In this work, we study the effects of uniaxial tensile strain in nanoscale Si GAA NW FETs affected by surface and channel orientation with our in-house 3D Finite Element (FE) Monte Carlo (MC) toolbox which uses the calibration-free Schrödinger Equation based Quantum Corrections (SEQC) [4–6] allowing to account for exact nanoscale geometry and thus confinement. The 3D FE mesh contains predefined 2D planes perpendicular to transport direction to solve 2D Schrödinger Eq. separately for the three/six Δ valleys:

$$-\frac{\hbar^2}{2}\nabla_\perp \cdot \left[(\mathbf{m}^*)^{-1} \cdot \nabla_\perp \psi(y,z)\right] + U(y,z)\psi(y,z) = E\psi(y,z),$$

where $(\mathbf{m}*)^{-1}$ is the inverse effective mass tensor listed in Ta- ble 1, $U(y,z) = -[qV(y,z) + \chi(y,z)]$ is the potential energy, $\chi(y,z)$ is the electron affinity, $\psi(y,z)$ is the wavefunction penetrating into oxide, and E is the energy [5].

Fig. 1 shows 6 Si Δ valleys within confinement cross-section along the transport direction. The strain is modeled by shifting the Si valley by ΔE_C according to the strain type and strength (Table 2) [8]. For the uniaxial ⟨110⟩ strain, the transverse effective masses in Δ3 valley split due to a band-structure warping resulting in a lighter $m_t^{transport}$ and a heavier $m_t^{perpendicular}$ [8].

The GAA NW FET has an elliptical cross-section (R=5.7/7.17 nm) and a gate length of 10 nm with EOT=0.8 nm (Fig. 2). We simulate ⟨100⟩ and ⟨110⟩ channel orientations and two types of tensile strain: uniaxial ⟨100⟩ and uniaxial ⟨100⟩ with strengths of 0.5%, 0.7% and 1.0%. To show the effect of confinement on strain, the 10 nm gate NW is compared to a big- ger device with an elliptical cross-section (R= 11.3/14.22 nm) and a gate length of 22 nm with EOT=1.5 nm [1]. The MC tool- box was verified against experimental data for the 22 nm GAA NW with excellent agreement [1, 7].

Fig. 3 shows ID-VG characteristics at V_D=0.7 V for the 10 nm gate length NW in the ⟨100⟩ channel orientation un- der three uniaxial ⟨100⟩ strengths of strain delivering increase in the drive-current by 6%, 6.9% and 7.3%, respectively. The sub-threshold slope exhibits a small deterioration under the increasing strain strength. Fig. 4 plots the 3 Δ valleys contributions to the current in the ⟨100⟩ device under uniaxial ⟨100⟩ strain with indicated strengths. In this case, Δ1 valley is shifted up reducing its contribution to the drain current because it has the largest effective transport mass (ml) (see Table 2). Δ2 and Δ3 valleys (Table 2) are shifted down increasing their contributions to the drain current because of a smaller effective transport mass (mt).

Since a larger confinement (perpendicular-to-transport) mass results in a lower bound state, the Δ3 with a larger confinement effective mass (ml) contributes more to the current than Δ2. The reduction in the strain effectiveness caused by the quantum confinement due to the pre-existing valley splitting is seen in the less confined 22 nm device (Fig. 5). The 0.5/0.7/1.0% uniaxial ⟨100⟩ strain increases the drive current (at

VDD=1.3 V) in the 22 nm gate length NW FET by 16.6⁄19.3⁄21.4% com- pared to only 6⁄6.9⁄7.3% for the 10 nm gate length device.

Fig. 6 shows I_D-V_G characteristics for the 10 nm gate length NW FET with a ⟨100⟩ channel orientation at V_D=0.7 V under uniaxial ⟨100⟩ strain. In the ⟨100⟩ orientation, a transforma- tion of coordinates is performed since the ellipsoid principal axes are not aligned with the device coordinate system [4, 9]. Without applying any strain, the ⟨100⟩ channel device deliv- ers more current (20.4%) than the ⟨100⟩ channel device due to enhanced mobility (lighter effective transport mass). When ap- plying uniaxial ⟨100⟩ strain, the drive-current at V_{DD}=1.0 V in- creases by 4.2%, 4.8%, and 3.3% at increasing strain strengths, respectively. The drive-current drop at 1.0% strain is due to the swap of valley contributions to the current with increasing strain. Although Δ3 contributes more to the current than Δ1 and Δ2, it has smaller increment from 1.0% strain than 0.7% strain while the Δ1 and Δ2 valleys reduce the current more at the 1.0% strain (see Fig. 7). For the (110) side-walls, the Δ3 has a smaller confinement mass (0.19m0) than that of Δ1 and Δ2 (0.315m_0). However, the Δ1 and Δ2 have a larger confinement mass resulting in a confinement of carriers to appear closer to the interface charge. To see the effect of confinement, Fig. 8 shows a comparison for the less-confined 22 nm gate length NW in which the 0.5⁄0.7⁄1.0% uniaxial ⟨110⟩ strain increases the drive current (at V_{DD}=1.0 V) by 11.6⁄12.7⁄7.6% compared to only 4.2⁄4.8⁄3.3% in the 10 nm gate device.

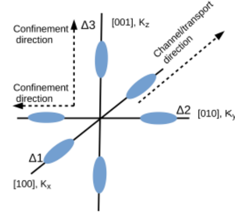

Fig. 1: Schematic of six Si valleys along a confinement plane. The transport direction is along the x-axis.

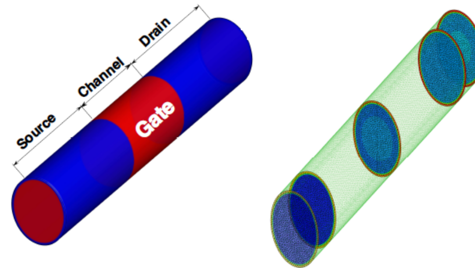

Fig. 2: Schematic of the investigated n-channel Si GAA nanowire FET (left) and the device mesh with sample of the 2D slices for the Schrödinger solver (right).

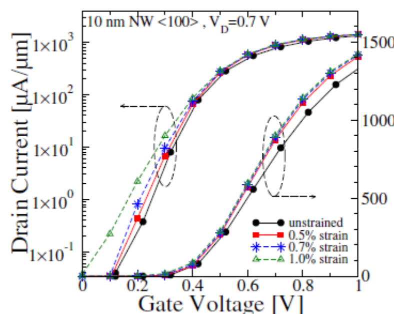

Fig. 3: I_D-V_G characteristics at V_D=0.7 V for the 10 nm gate length GAA-NW with ⟨100⟩ channel orientation under different uniaxial ⟨100⟩ strain strengths.

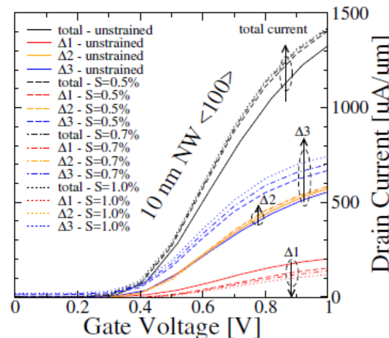

Fig. 4: Valley contributions to the current at V_D=0.7 V for the 10 nm gate length GAA-NW with ⟨100⟩ channel orientation under different uniaxial ⟨100⟩ strain strengths.

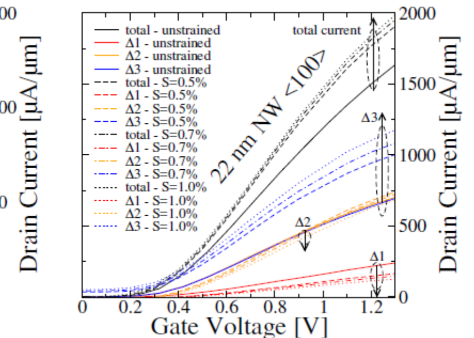

Fig. 5: Valley contributions to the current at V_D=1.0 V for the 22 nm gate length GAA-NW with ⟨100⟩ channel orientation under different uniaxial ⟨100⟩ strain strengths.

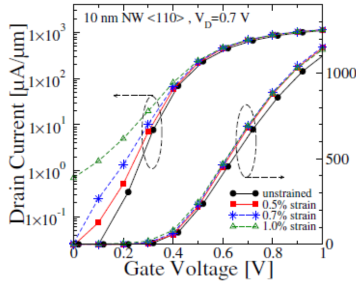

Fig. 6: I_D-V_G characteristics at V_D=0.7 V for the 10 nm gate length GAA-NW with ⟨110⟩ channel orientation under different uniaxial ⟨110⟩ strain strengths.

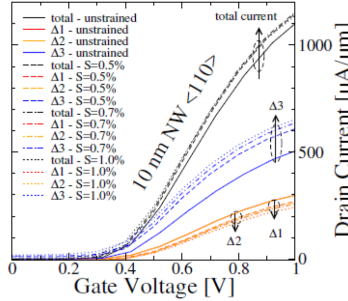

Fig. 7: Valley contributions to the current at V_D=0.7 V for the 10 nm gate length GAA-NW with ⟨110⟩ channel orientation under different uniaxial ⟨110⟩ strain strengths.

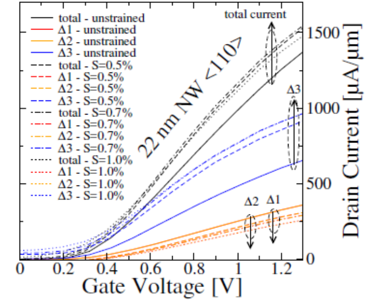

Fig. 8: Valley contributions to the current at V_D=1.0 V for the 22 nm gate length GAA-NW with ⟨110⟩ channel orientation under different uniaxial ⟨110⟩ strain strengths.

Orientation	Valley	$1/m^*_{yy}$	$1/m^*_{zz}$	m^*_{Tr}
⟨100⟩	Δ1	$1/m_t$	$1/m_t$	m_l
⟨100⟩	Δ2	$1/m_l$	$1/m_t$	m_t
⟨100⟩	Δ3	$1/m_t$	$1/m_l$	m_t
⟨110⟩	Δ1	$(m_t+m_l)/(2m_tm_l)$	$1/m_t$	$(m_t+m_l)/2$
⟨110⟩	Δ2	$(m_t+m_l)/(2m_tm_l)$	$1/m_t$	$(m_t+m_l)/2$
⟨110⟩	Δ3	$1/m_t$	$1/m_l$	m_t

Table 1: Effective-mass tensor and effective transport mass of Δ valleys for ⟨100⟩ and ⟨110⟩ channel orientations where $1/m^*_{yz}=0$ and degeneracy = 2.

Strain type	Uniaxial ⟨100⟩ strain			Uniaxial ⟨110⟩ strain		
strain strength	0.5%	0.7%	1.0%	0.5%	0.7%	1.0%
Δ1	+0.03eV	+0.042eV	+0.06eV	-0.01eV	-0.014eV	-0.02eV
Δ2	-0.045eV	-0.063eV	-0.09eV	-0.01eV	-0.014eV	-0.02eV
Δ3	-0.045eV	-0.063eV	-0.09eV	-0.065eV	-0.091eV	-0.13eV

Table 2: Valley-edge shifts for each valley with different types and strengths of tensile strain [8].

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