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Impact of strain on ballistic current in Si n-i-n structures

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1 Introduction

The device dimensions of MOSFETs have been shrunk into sub-100 nm regime, where conventional device scaling concept is confronted with several limitations. To enhance CMOS performance, strained-Si technology has been widely introduced [1]. In our previous study, we investigated effect of a thin strained-Si layer ($\approx$ 1.1 nm) on transport characteristics in Si n-i-n structures and reported that the strained layer acts as a kind of defects and greatly enhances Zener interband current for both compressive and tensile strain [2]. In the present study, we consider Si n-i-n devices with uniform uniaxial strain in the whole region for investigating impact of the uniform strain on ballistic current. We adopt a nonequilibrium Green's function (NEGF) formalism [3] combining with tight-binding approximation (TBA) [4] for evaluating current in strained-Si n-i-n structures.

2 Simulation Method

We consider a $\langle 100 \rangle$-oriented n-i-n Si structure whose schematic diagram is given in Fig. 1. The device has a large cross-section in the y-z plane and current flows along the x-direction. The doping concentration in the n-regions, each of which is 7.5 nm long, is $N_D = 5 \times 10^{20}\,\mathrm{cm}^{-3}$. The central i-region is 5 nm long. We investigate two cases; one is uniaxial compressive strain ($-2\,\%$) along the x-axis and the other is uniaxial tensile strain ($2\,\%$) along the x-axis. For the y-z directions, we evaluate the lattice constants under the uniaxial strain using a macroscopic elastic theory [5]. For the x-direction, we use a discrete lattice of the atomic layer in real space. For the y-z directions, we assume periodic boundary conditions and use the eigenstate basis labeled by two-dimensional wavevectors of $\boldsymbol{k} = (k_y, k_z)$. We discretize the full two-dimensional $\boldsymbol{k}$-space into triangular meshes and evaluate spectral functions, $A(\boldsymbol{k}, E)$, and transmission functions, $T(\boldsymbol{k}, E)$, at each mesh point using the NEGF method. Carrier density and the total transmission are then calculated by summing those functions over $\boldsymbol{k}$- and energy-spaces. The full-band structure of strained-Si is included using an empirical $sp^3d^5s^*$ TBA [4].

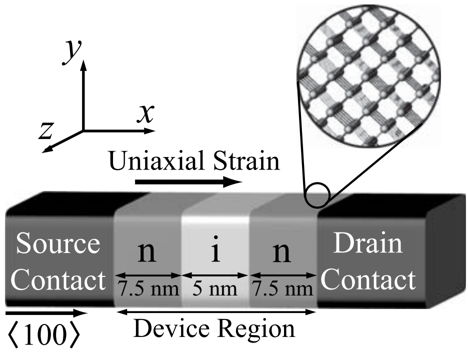

Figure 1: Schematic diagram of the device structure together with the coordinate axis.

3 Results and Discussion

Fig. 2 shows self-consistent solution of local density of states (LDOS) and current density spectrum, J, for a device without strain at applied voltage $V = 1.5$ V. Ballistic current component appears for $E \gtrsim 1.5$ eV and Zener tunneling current component appears at $E \approx 0$ eV. Figs. 3(a) and 3(b) show the LDOS for the compressive and the tensile strain, respectively. In Fig. 3, we used the same potential profile as in Fig. 2. The corresponding current density spectra are shown in Fig. 2, where we find that the compressive strain enhances the ballistic current, while the tensile strain reduces it. These features can be understood by considering a difference of the strain-induced energy shift between the transverse and longitudinal valleys (see Fig. 5). We also find that the compressive strain reduces the Zener tunneling current, while the tensile strain enhances it.

4 Conclusions

Atomistic transport simulation based on the NEGF method has been performed for Si n-i-n devices with uniform uniaxial strain. Simulation results show that the compressive strain enhances the ballistic current, while the tensile strain reduces it.

Acknowledgment

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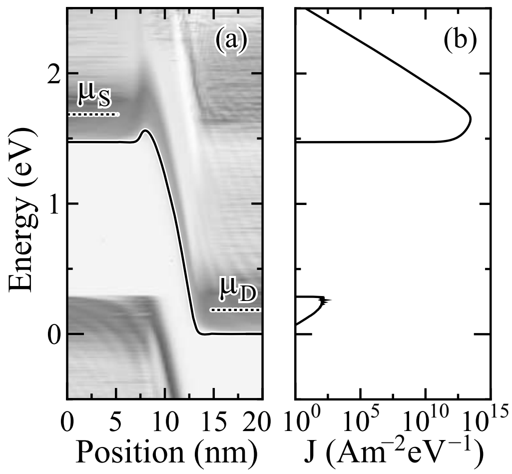

Figure 2: Calculated results for the device without strained at $V = 1.5$ V. (a) Local density of states. Solid line shows potential profile and dotted lines represent Fermi levels in the source (μ_S) and drain (μ_D) regions. (b) Current density spectrum.

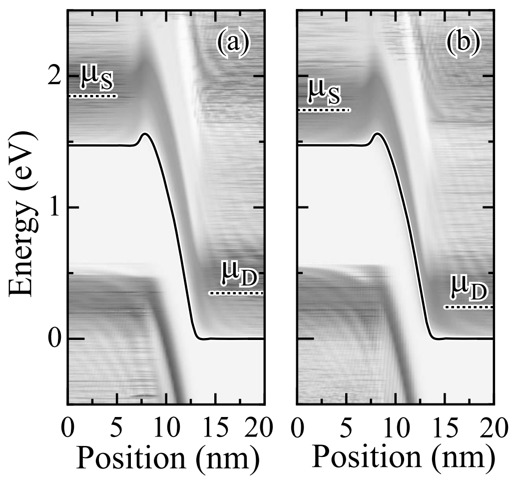

Figure 3: The same as Fig. 2(a) but for (a) −2 % compressive strain and (b) 2 % tensile strain.

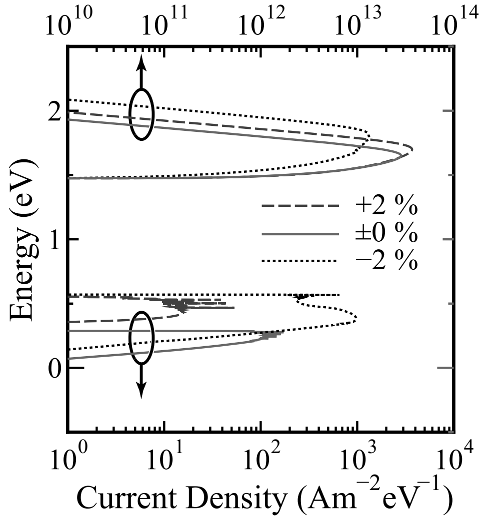

Figure 4: Ballistic and Zener tunneling current density spectra.

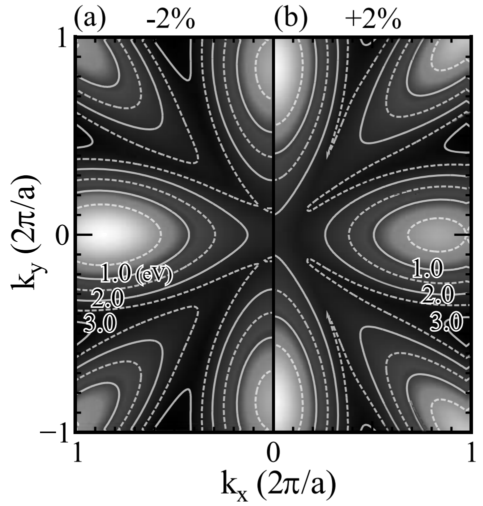

Figure 5: Conduction band structure at $\boldsymbol{k}_z = 0$ for (a) −2 % compressive strain and (b) 2 % tensile strain.

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