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Electron and Hole Mobilities in Orthorhombically Strained Silicon

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1. Introduction

Current successful realizations of novel devices comprise vertical MOSFETs [1, 2] as well as channels formed by strained Si for n-type and p-type planar MOSFETs [3, 4]. Recently, both concepts have been combined by a successful fabrication of a vertical NMOSFET with a channel consisting of orthorhombically strained Si [5], and enhanced electron mobility in orthorhombically strained Si was confirmed by Monte Carlo simulation [6]. The aim of this paper is to theoretically explore carrier mobility in orthorhombically strained Si and to extend the analysis both for electrons and holes to the ballistic regime. In Fig. 1, the schematic structure of a vertical MOSFET is shown to illustrate how a channel is formed under orthorhombic tensile strain. No relaxed SiGe buffer is necessary in above structure as compared to a conventional strained Si substrate with relaxed SiGe buffer layer. Instead, first a SiGe pillar is grown on an unstrained Si substrate which causes biaxial compressive strain in the SiGe pillar. In a second step, a Si layer is grown on the sidewall of the compressively strained SiGe pillar and on top of the unstrained Si substrate.

2. Band Structure and Mobility Model

Calculations of the full band structure are based on the framework of linear combination of atomic orbitals (LCAO) [7, 8] with spin-orbit splitting, strain. Since the lattice constant of Ge does not match with that of Si, there are strains in the Si layer grown on the sidewall of the compressively strained SiGe pillar and on top of the unstrained Si substrate. The lattice constant in *z* and *y* direction coincide with the values in strained SiGe and in unstrained Si, respectively,

$$\varepsilon_{zz} = \left(a_{sub2} - a_{Si}\right)/a_{Si}, \qquad \varepsilon_{yy} = \left(a_{sub1} - a_{Si}\right)/a_{Si}, \tag{1}$$

where a_{sub1} and a_{sub2} are lattice constants of Si substrate and compressively strained SiGe pillar,

$$a_{sub1} = a_{Si}, \qquad a_{sub2} = a_{SiGe}\cdot\left[1+\left(\frac{-2C_{12}}{C_{11}}\right)\cdot\left(\frac{a_{Si}-a_{SiGe}}{a_{SiGe}}\right)\right], \tag{2}$$

a_{SiGe} is linearly interpolated with virtual crystal approximation (VCA) and x is the Ge molar fraction,

$$a_{SiGe} = a_{Si}\left(1-x\right) + a_{SiGe}x, \tag{3}$$

whereas the lattice constant in *x* direaction relaxes according to elasticity theory

$$\varepsilon_{xx} = -\left(\frac{C_{12}}{C_{11}}\right)\cdot\left(\varepsilon_{zz}+\varepsilon_{yy}\right), \tag{4}$$

C_{11} and C_{12} are stiffness constants for Si.

Assuming uniform deformation of the diamond-like unit cell, the length of the vectors connecting nearest neighbour atoms is

$$d = \sqrt{\left(1+\varepsilon_{xx}\right)^2 + \left(1+\varepsilon_{yy}\right)^2 + \left(1+\varepsilon_{zz}\right)^2}. \tag{5}$$

Direction cosines between the vector and the *x*, *y*, and *z* axes are thus given by [8]

$$l_x = \left(1+\varepsilon_{xx}\right)/d, \quad l_y = \left(1+\varepsilon_{yy}\right)/d, \quad l_z = \left(1+\varepsilon_{zz}\right)/d, \tag{6}$$

For the off-diagonal TB parameters between atoms, Eqs. (6) are used to modify the nearest neighbor TB parameters. The change of the bond length dependence of the nearest and second-nearest neighbor modifies the off-diagonal TB parameters between different atoms V_{ij} according to the empirical scaling rule [8]

$$V_{ij} = V_{ij}^0\left(\frac{d_0}{d}\right)^{-n(ij)}, \tag{7}$$

where V_{ij} and V_{ij}^0 are the unstrained and strained TB parameters, respectively, for the interaction between state *i* and state *j*; d_0 and d are the unstrained and strained bond lengths, respectively, and $n(ij)$ is the scale index describing how TB parameters changes with distance and it is orbital dependent.

The major mechanisms included in the charged carrier mobility model are scattering by acoustic and optical phonons. The isotropic and elastic equipartition approximtions are taken for the intravalley phonon process [9, 10]. The Boltzmann transport equation (BTE) can be solved to linear order by a scalar microscopic relaxation time in the low-field regime, and the calculation of the drift mobility involves only a one-dimensional integration over energy. Intravalley and intervalley phonon scattering are underling mechanisms for velocity randomizing, and the inverse relaxation time is then identical with the scattering rate under nondegenerate conditions.

3. Results and Discussion

Strained causes a splitting of the Δ valleys in the conduction band as well as of the light-hole and the heavy-hole band at the Γ point. The light-hole band becomes the topmost valence band. The six-fold degenerate Δ valleys split into three two-fold degenerate valleys for orthorhombic strain with the lowest-lying pair of valleys being situated along the x axis in Fig. 1 and into one two-fold degenerate valley. The positions of the valence bands and the Δ valleys with respect to the conduction-band edge and the valence-band edge in unstrained Si are shown in Fig. 2 as a function of the Ge content. It can be seen from Fig. 2 that the reduction of the band gap is similar for biaxial strain, while the splitting of the first two lowest-lying bands/valleys is smaller for orthorhombic strain. The resulting strain dependence of the drift mobility is shown in Fig. 3 and Fig. 4, respectively. Here and in the following, the results always refer to the relevant transport direction in the corresponding MOSFET in Fig. 1, i.e., the <001> direction for orthorhombic strain.

tion for orthorhombic strain. While the electron mobilities are similar for biaxial tensile strain, the enhancement of the hole mobility under orthorhombic strain, though significant, is considerably weaker than under biaxial tensile strain. In particular, the trend of an increase in mobility above a Ge content of 30% is much stronger for tensile strain. This can be seen in Fig. 4 where three diagonal components of the drift mobility tensor are shown as a function of the Ge-content in the SiGe pillar. The anisotropy is relatively small, although the mobility in the growth direction at higher Ge contents is larger than other components. As a general result, a strong mobility enhancement relative to unstrained Si is found, ranging from a factor of two at a Ge content of 20% up to a factor of about three at a Ge content of 40%. However, the increase in mobility above a Ge content of 20% is weaker than in the case of biaxially strained Si where e.g. a value of roughly 2000 $cm^2/(Vs)$ is reached at a Ge content of 30%.

4. Summary

Electron and hole mobilities in orthorhombically strained Si have been theoretically investigated. A strong mobility enhancement relative to unstrained Si has been observed. The absence of a relaxed SiGe substrate of conventional biaxial strained Si further makes this novel structure attractive for future applications.

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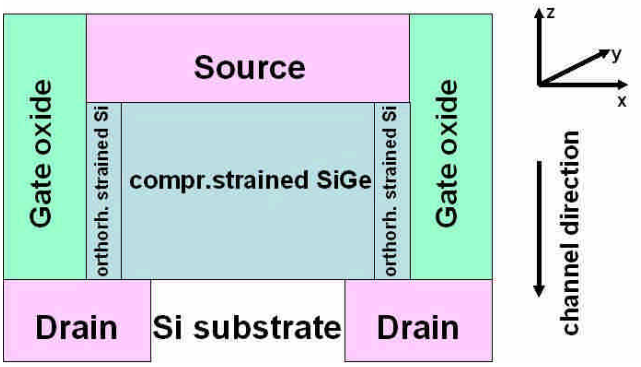

Fig. 1 Schematic structure of the vertical MOSFET. The lattice constants a_x and a_y of the compressively strained SiGe pillar assume the value of the unstrained Si substrate which leads to an increase in a_z . a_y and a_z of the orthorhombically strained Si layer (≡channel) coincide with the corresponding values in the Si substrate and the SiGe pillar, respectively, yielding a reduction of a_x .

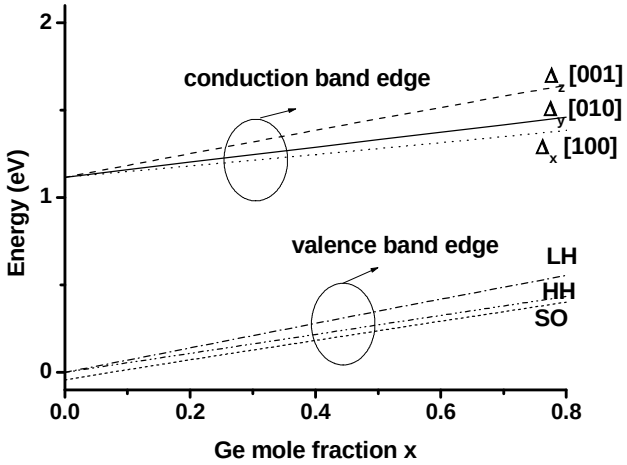

Fig. 2 Positions of the Δ valleys and valence bands in orthorhombically strained Si with respect to the conduction and valence band edge in unstrained Si.

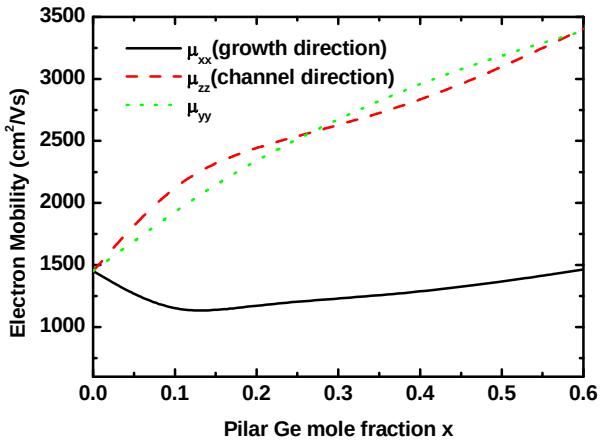

Fig. 3 Diagonal components of the Ohmic drift mobility tensor for electrons in orthorhombically strained Si as a function of the Ge content in the SiGe pillar.

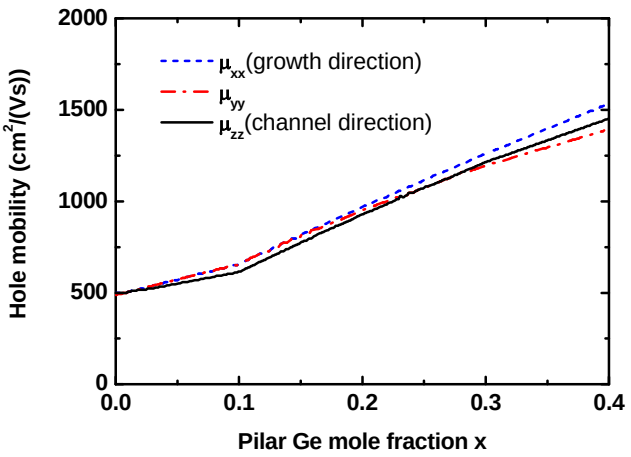

Fig. 4 Diagonal components of the Ohmic drift mobility tensor for holes in orthorhombically strained Si at 300 K as a function of the Ge content in the SiGe pillar.