Influence of Uniaxial [110] Stress on Silicon Band Structure and Electron Low-Field Mobility in Ultra-Thin Body SOIs

Viktor Sverdlov, Enzo Ungersboeck, and Hans Kosina

Institute for Microelectronic, TU Wien, Gusshausstrasse 27-29, Wien A-1040 sverdlov|ungers|kosina@iue.tuwien.ac.at

1. Abstract

Uniaxial [110] stress induced valley shifts and effective masses modifications are analyzed. Analytical expressions for both transversal and longitudinal masses are obtained for the first time. Analytical results are verified with pseudo-potential band structure calculations and excellent agreement is found. The low-field mobility enhancement in the direction of tensile [110] stress is due to the conductivity mass modification and is shown to exist in SOIs with arbitrary small body thickness.

2. Method and Results

Strain induced mobility enhancement is one of the ways to boost performance of modern CMOS devices. In biaxial stressed devices the mobility can be enhanced by 100%. Biaxial stress is naturally introduced by growing Si epitaxially on SiGe. This method requires a substantial modification of CMOS fabrication process and is not yet used in mass production. Instead industry is exploiting advantages of compatible with CMOS process uniaxial stress, which is created by local stressors and/or additional cap layers. Although already successfully used in mass production, the technology relevant stress along [110] has received little attention within the research community. Only recently a systematic experimental study of the mobility modification due to stress in [110] was performed [1]. It was shown that, contrary to [100] uniaxial stress, the electron mobility data under [110] stress condition is consistent with conductivity mass being a function of the stress value.

The [110] stress produces off-diagonal elements e_{xy} of the strain tensor, which lift the degeneracy between the two lowest conduction bands at the X points along [001] axis in the Brillouin zone [2]:

$$\Delta E_X = 2De_{xy}, \tag{1}$$

where D is interpreted as the deformation potential due to shear strain component. Since the conduction band minimum along [001] axis is located near the X point, it is affected by the strain e_{xy}. First, the conduction band minimum $k_{\min}$ moves closer to the X point:

$$k_{\min}/k_0 = \sqrt{1-\varepsilon^2}\ , \tag{2}$$

where k_0 is the position of the minimum with respect to the X point in unstrained Si, $\varepsilon = 2De_{xy}/\Delta$, and Δ is the conduction bands splitting at k_0. It is interesting to note that for $\varepsilon \geq 1$ the conduction band minimum stays exactly at the X point. Second, the minimum of each of the two [001] valleys moves down in energy with respect to the four remaining degenerate valleys. However, for $|\varepsilon| \leq 1$ it is proportional to the stress *square*:

$$\Delta E_{\min} = -\varepsilon^2 \Delta/4, \qquad |\varepsilon| \leq 1; \tag{3a}$$

while a linear dependence is recovered for $|\varepsilon| \geq 1$

$$\Delta E_{\min} = -(2|\varepsilon|-1)\Delta/4, \qquad |\varepsilon| \geq 1. \tag{3b}$$

Finally, the shear stress modifies the effective masses in [001] valleys. The transversal mass m_t acquires two different values along (+) and across (-) *tensile* [110] stress:

$$m_t(\varepsilon)/m_t = \left[1 \pm \varepsilon\, m_t/M\right]^{-1}, \qquad |\varepsilon| \leq 1; \tag{4a}$$

$$m_t(\varepsilon)/m_t = \left[1 \pm m_t/M\right]^{-1}, \qquad |\varepsilon| \geq 1. \tag{4b}$$

A closed expression for M is found within the *kp* perturbation theory. The longitudinal mass m_l is expressed

$$m_l(\varepsilon)/m_l = \left[1-\varepsilon^2\right]^{-1}, \qquad |\varepsilon| \leq 1; \tag{5a}$$

$$m_l(\varepsilon)/m_l = \left[1-|\varepsilon|^{-1}\right]^{-1}, \qquad |\varepsilon| \geq 1. \tag{5b}$$

In order to verify these expressions the band structure calculations with empirical pseudo-potentials method (EPM) [3] were performed. Results of comparison are reported in Figs 1-3 and display an excellent agreement. Comparisons with experimental data from [1] and [2] are shown in Fig.4 and Fig.5, correspondingly. Finally, an example of mobility calculations for UTB SOI is shown in Fig. 6. While the stress along [100] direction doesn't have an affect on the mobility, the mobility in a [110] stretched UTB SOI is enhanced along the stress.

3. Conclusion

Analytical expressions for the [110] stress induced valley splitting and effective masses variation are obtained and verified against band structure calculations. Results are used to demonstrate the mobility enhancement even in UTB stressed SOIs.

References

[1] K. Uchida *et al.*, IEDM 2005, p.135.

[2] J.C. Hensel *et al.*, *Phys.Rev.,* **138**, p.A225, 1965.

[3] M. Rieger and P. Vogl, *Phys.Rev.B,* **48**, p.14275, 1993.

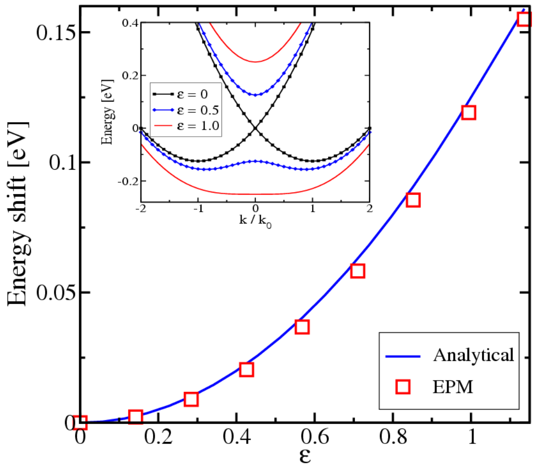

Fig.1: *Relative [001] alley shift as a function of shear off-diagonal component of [110] stress. Quadratic dependence on stress predicted by (2) is clearly visible for |ε|<1. Analytic expression (2) is in excellent agreement with EPM calculations. Inset: schematic conduction band profile along [001] direction for different stress values.*

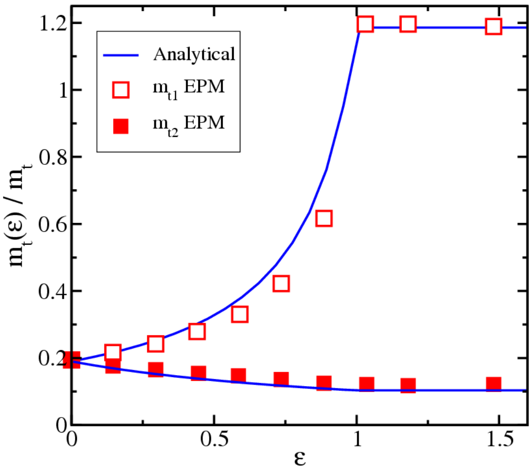

Fig.2: *Transversal masses dependences (3) in [001] valleys as a function of off-diagonal component of [110] tensile stress. m_{t2} is the mass along the tensile stress direction. For |ε|>1 transversal masses cease to depend on stress.*

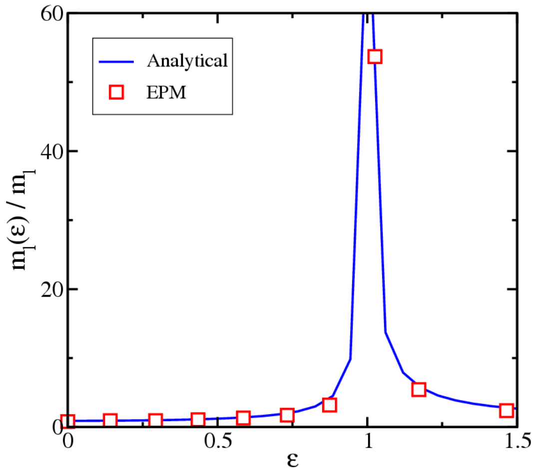

Fig.3: *Longitudinal mass (5) as a function of ε manifests divergence at the point when the valley minimum touches the X point.*

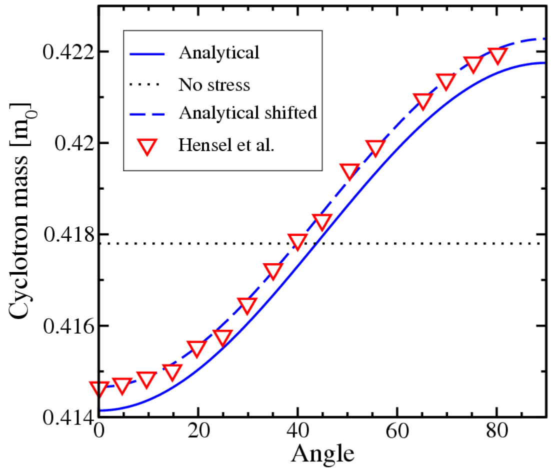

Fig.4: *Cyclotron mass as function of field direction obtained with (4) and (5). Parameters are the same as in [2]. While angular dependence described by (4) is accurate, an additional to (5) increase in m_l is introduced to reproduce the data [2].*

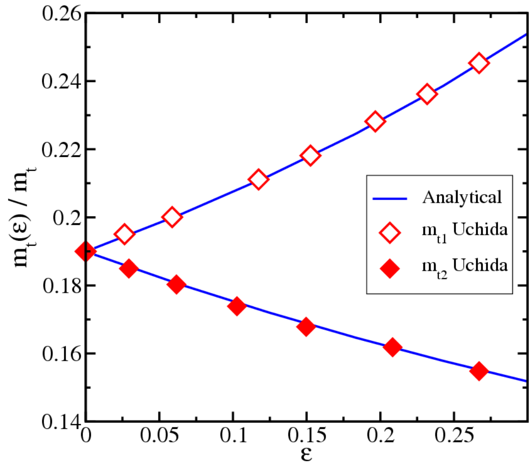

Fig.5: *Comparison of (4) with transversal masses dependenceson strain extracted from mobility measurements. Excellent agreement is found with the same parameters as in Fig. 4*

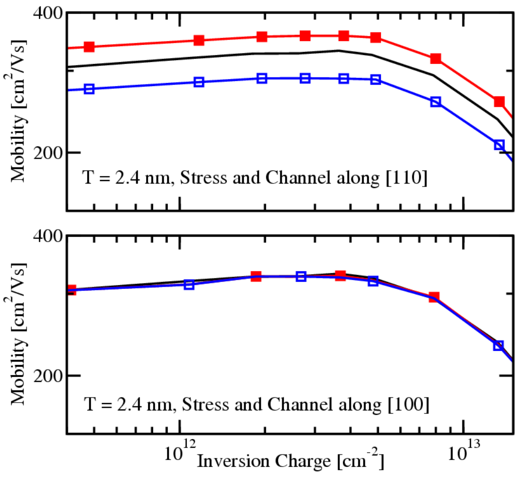

Fig.6: *Low-field mobility calculations in SOIs with body thickness of 2.4 nm. Clear mobility enhancement due to conductivity mass m_{t2} decrease in tensile [110] stress direction is observed. No mobility change is visible for [100] stress (lower panel).*