Strain-Induced Valley Splitting in Slightly Misaligned Silicon Films

O. Baumgartner, V. Sverdlov, H. Kosina, and S. Selberherr

Institute for Microelectronics, TU Wien
Gußhausstraße 27–29, A–1040 Wien, Austria
E-mail: {baumgartner|sverdlov|kosina|selberherr}@iue.tuwien.ac.at

1. Abstract

The subband structure in thin silicon films is computed using the Hensel-Hasegawa-Nakayama model for the conduction band. It is demonstrated that unprimed subbands in (001) thin films are not equivalent. Application of tensile stress in [110] direction lifts the subband degeneracy. The value of splitting increases with decreasing film thickness. In films slightly misaligned from the (001) orientation, significant suppression of valley splitting in weak magnetic fields was predicted [1, 2]. We show that for stress values achieved by the semiconductor industry the large value for valley splitting is recovered.

2. The Model

We apply the following Hamiltonian [3, 4], which describes the dispersion of the [001] valleys relative to the X point

$$\mathbf{H} = \begin{bmatrix} \mathrm{H}_{-} & \mathrm{H}_{\mathrm{bc}} \\ \mathrm{H}_{\mathrm{bc}} & \mathrm{H}_{+} \end{bmatrix} \qquad \text{with} \tag{1}$$

$$\mathrm{H}_{\mp} = \mathcal{E}_{\mathrm{c}}(z) + \frac{\hbar^2 k_{\mathrm{z}}^2}{2m_{\mathrm{l}}} + \frac{\hbar^2 \left(k_{\mathrm{x}}^2 + k_{\mathrm{y}}^2\right)}{2m_{\mathrm{t}}} \mp \frac{\hbar^2 k_0 k_{\mathrm{z}}}{m_{\mathrm{l}}},$$

$$\mathrm{H}_{\mathrm{bc}} = D\epsilon_{\mathrm{xy}} - \frac{\hbar^2 k_{\mathrm{x}} k_{\mathrm{y}}}{M}.$$

Here $\mathcal{E}_{\mathrm{c}}$ is the conduction band edge, m_{l} and m_{t} are the electron masses, $\frac{1}{M} \approx \frac{1}{m_{\mathrm{t}}} - \frac{1}{m_{\mathrm{e}}}$, and $k_0 = 0.15\frac{2\pi}{a}$ is the distance from the valley minimum to the X point. The shear strain deformation potential $\mathrm{D} = 14\mathrm{eV}$ and the shear strain component $\varepsilon_{\mathrm{xy}}$ describe the effects of strain on the bandstructure. To find the structure of unprimed subbands in a (001) film, the substitution $k_{\mathrm{z}} \rightarrow -\mathrm{i}\,\partial_{\mathrm{z}}$ in (1) is performed. In order to obtain a numerical solution, a finite difference discretization scheme with symmetric operator ordering is implemented. For an arbitrary substrate orientation an appropriate rotation of (1) must be performed before substituting $k_{\mathrm{z}} \rightarrow -\mathrm{i}\,\partial_{\mathrm{z}}$.

3. Results and Conclusion

Unprimed subband dispersions along the [100] and [110] axes in an unstrained (001) film with a thickness of 1.6nm are shown in Fig. 1. The subbands are two-fold degenerate at the minimum and parabolic along the [100] direction. The degeneracy of the unprimed subbands along the [110] axis is lifted. The dispersion in [110] direction is non-parabolic and depends strongly on the subband index. The effective masses given by the subband curvature in [110] direction for the two ground subbands are shown on Fig. 2. Although these masses are different, the subband minima remain two-fold degenerate. This is a consequence of the purely parabolic band dispersion (1) in z-direction for $\mathrm{H}_{\mathrm{bc}} = 0$ (Fig. 3 for $\varepsilon_{\mathrm{xy}} = 0$).

Shear strain $\varepsilon_{\mathrm{xy}}$ due to [110] stress opens the gap between the conduction bands at the X point and makes the z dispersion non-parabolic (Fig. 3). Hence, the degeneracy of the unprimed subbands is lifted (Fig. 4). The band splitting of the two ground subbands as a function of thickness for $\varepsilon_{\mathrm{xy}} = 0.4\%$ is shown in Fig. 5. This strain level is achived by applying tensile [110] stress of 2GPa, a value routinely used in the semiconductor industry.

For a film slightly misaligned from the (001) direction the ground subband develops the two minima symmetrically situated around the point $\mathbf{k} = 0$ (Fig. 6). These two minima produce the two ladders of the Landau levels in the external magnetic field. Due to Zener tunneling between the two minima the difference between the cyclotron frequencies decreases exponentially with the inverse of the magnetic field. However, for stress values employed by the semiconductor industry there is only a single minimum (Fig. 6), and a large value for the valley splitting is recovered.

Acknowledgment: This work was supported by the Austrian Science Fund, the project P-19997-14 and the special research program IR-ON (F2509).

References

[1] T. Ando, Phys. Rev. B **19**, 3089 (1979).

[2] Mark Friesen *et al.*, Applied Physics Letters **89**, 202106 (2006).

[3] J. C. Hensel *et al.*, Phys. Rev. **138**, A225 (1965).

[4] E. Ungersböck *et al.*, IEEE T. Electron. Dev. **54**, 2183 (2007).

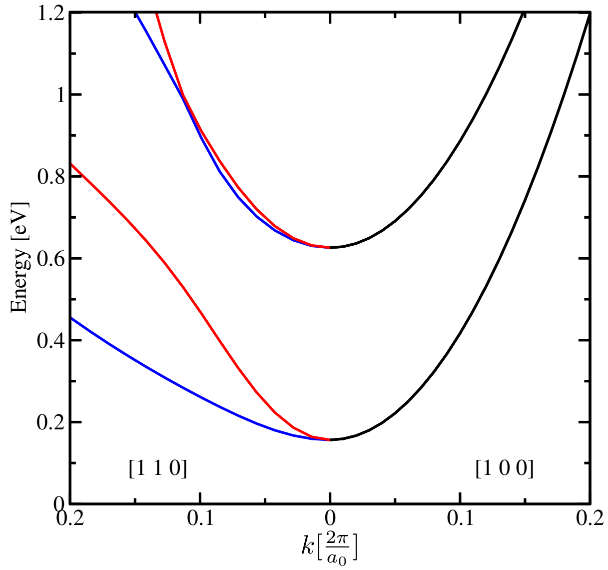

Fig. 1: *Dispersion of (001) Si with 1.6nm film thickness*

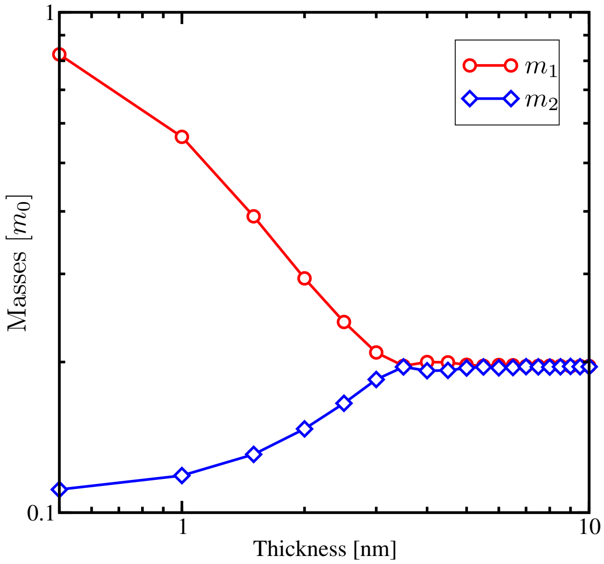

Fig. 2: *Electron masses in [110] of the two ground subbands of (001) Si as a function of film thickness*

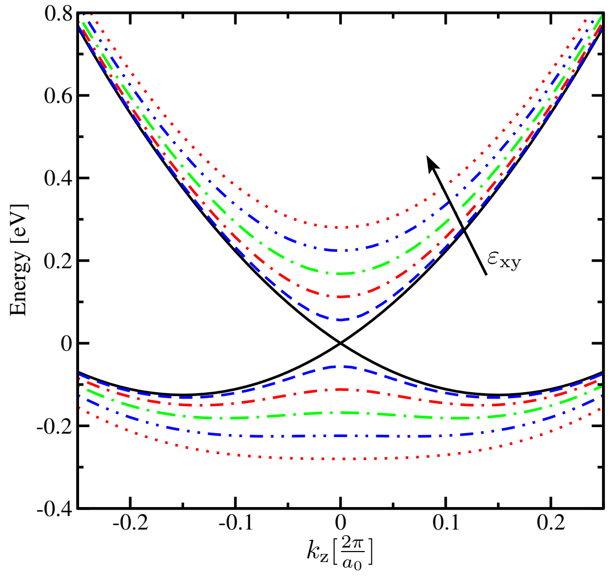

Fig. 3: *Silicon bulk dispersion of the two ground subbands in [001] for shear strain ε_{xy} ranging from 0 to 2%*

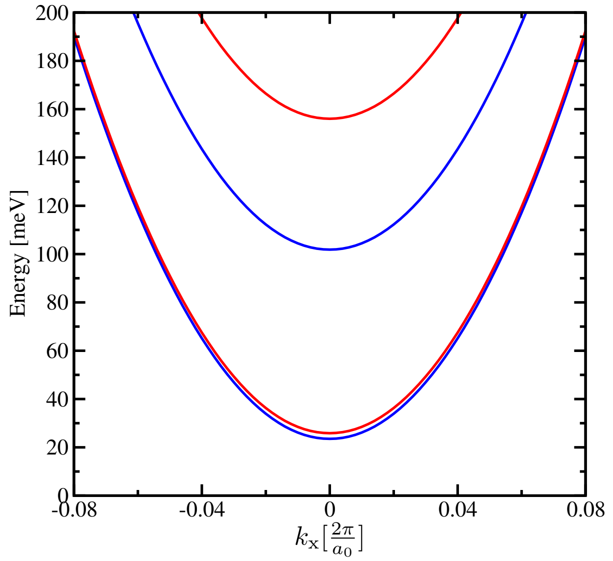

Fig. 4: *Dispersion in [100] of a (001) Si thin film with t=3.5nm and shear strain ε_{xy}=0.4%*

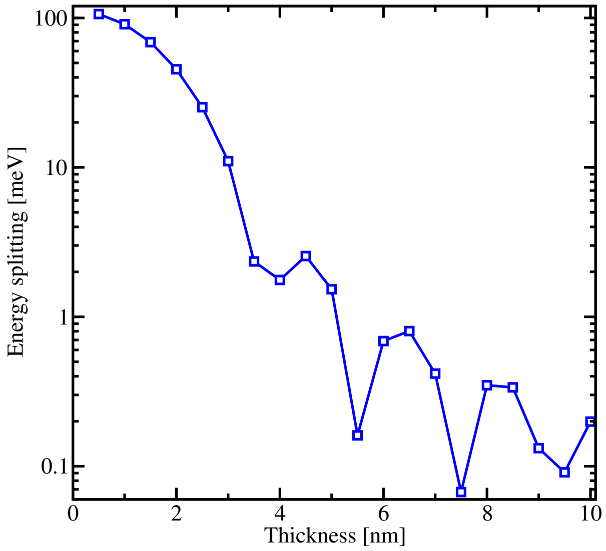

Fig. 5: *Splitting of the ground subbands of (001) Si with shear strain $\varepsilon_{xy} = 0.4\%$ as a function of film thickness*

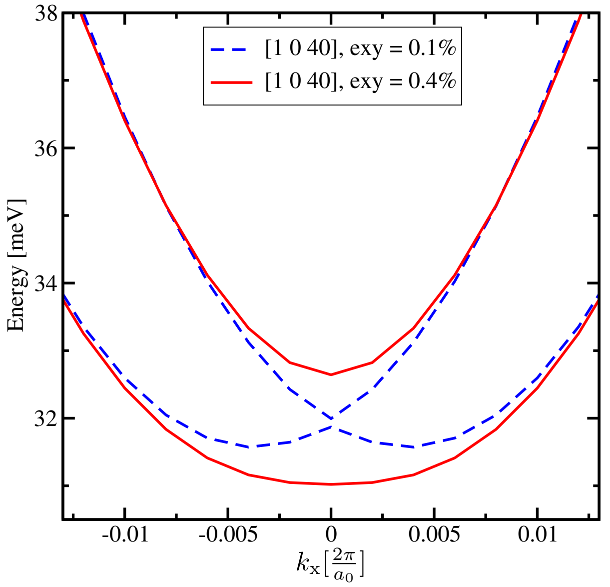

Fig. 6: *Dispersion of the ground subbands in [100] for a misaligned silicon film with $t = 3.5$nm*