Effects of Shear Strain on the Conduction Band in Silicon: An Efficient Two-Band k·p Theory

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Abstract—We present an efficient two-band k·p theory which accurately describes the six lowest conduction band valleys in silicon. By comparing the model with full band pseudo-potential calculations we demonstrate that the model captures both the nonparabolicity effects and the stress-induced band structure modification for general stress conditions. It reproduces the stress dependence of the effective masses and the nonparabolicity parameter. Analytical expressions for the valley shifts and the transversal and longitudinal effective mass modifications induced by uniaxial [110] stress are obtained and analyzed. The low-field mobility enhancement in the direction of tensile [110] stress in {001} SOI FETs with arbitrary small body thickness is due to a modification of the conductivity mass and is shown to be partly hampered by an increase in nonparabolicity at high stress values.

I. INTRODUCTION

The k·p theory is a well established tool to describe the band structure analytically. After the pioneering work by Luttinger and Kohn [1] the six-band k·p method has become a standard approach to model the valence band in Si. However, the conduction band in Si is usually approximated by three pairs of equivalent minima located close to the X-points of the Brillouin zone. It is commonly assumed that close to the minima the electron dispersion is well described by the effective mass approximation. The nonparabolicity parameter $\alpha = 0.5 \text{ eV}^{-1}$ is introduced to describe deviations in the density of states from the purely parabolic expression, which become pronounced at higher electron energies. In ultra-thin body (UTB) FETs, however, the band nonparabolicity affects the subband quantization energies substantially, and it was recently indicated that anisotropic, direction-dependent nonparabolicity can explain the mobility behavior at high carrier concentrations in a FET with [110] UTB orientation [2]. Therefore, a more refined description of the conduction band minima beyond the usual nonparabolic approximation is needed. Another reason to challenge the standard description of the conduction band based on a single-band nonparabolic approximation is its inability to properly address the band structure modification under stress.

Stress-induced mobility enhancement in Si has become a key technique to increase performance of modern CMOS devices. In biaxially stressed devices the electron mobility can be nearly doubled. The reason for the mobility enhancement lies in the stress-induced band structure modification. The degeneracy between the six equivalent valleys is lifted due to stress-induced valley shifts. This reduces inter-valley scattering. In case of tensile biaxial stress applied in the {100} plane the four in-plane valleys move up in energy and become de-populated. The two populated out-of-plane valleys have favorable conductivity masses, which together with reduced inter-valley scattering results in the observed mobility increase [3]. Biaxial stress is naturally introduced by growing Si epitaxially on SiGe. This method, however, requires a substantial modification of the CMOS fabrication process and is not used in mass production. Instead, semiconductor industry is exploiting techniques compatible with existing CMOS process technology. Stress in the channel is created by local stressors and/or additional cap layers. Although already successfully used in mass production, the technologically relevant case of stress along [110] has received little attention within the research community. Only recently a systematic experimental study of the mobility modification due to [110] stress was performed [4]. It was shown that, contrary to [100] uniaxial stress, the electron mobility data for [110] stress suggest that the conductivity mass depends on stress. This conclusion was also supported by recent results of pseudo-potential band structure calculations [4], [5]. Any dependence of the effective masses on stress is neglected within the standard description of the conduction band and can only be introduced phenomenologically. In order to describe the dependence of the effective mass on stress a single-band description is not sufficient, and coupling to other bands has to be taken into account.

Recently, a 30 bands k·p theory was introduced [6]. Although universal, it cannot provide an explicit analytical solution for the energy dispersion. In this work we present an efficient two-band k·p theory. By comparing our results with predictions of the pseudo-potential band structure calculations we demonstrate that the theory accurately describes both the nonparabolicity effects and the stress induced band structure modification for general stress conditions. It accurately reproduces the stress dependence of the effective mass and of the nonparabolicity parameter. The analytical two-band k·p model allows one to study the influence of the conduction band structure on transport properties of stressed FETs for general UTB orientations.

II. THEORY

We consider the pair of equivalent conduction band valleys along the [001] direction. Other valleys can be analyzed...
The off-diagonal matrix elements of the Hamiltonian are also modified by strain [7]:

\[ H_{ij}(k) = H_{ij}^0 - D \delta_{ij}, \]

where \( D \geq 0 \) denotes the deformation potential for the off-diagonal strain component. When the off-diagonal components in the Hamiltonian are ignored, the influence of the shear stress component is completely lost. The off-diagonal elements of the

\[ \frac{1}{M} = \frac{2}{m_0} \sum_{\nu \neq \alpha, \beta} \frac{(p_\alpha)_\nu (p_\beta)_\nu}{E_k(X) - E_{\Delta \alpha}(X)}, \]

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strain tensor are, however, generated by [110] uniaxial stress. Since this is exactly the stress direction used to enhance the performance of modern MOSFETs, shear strain must be taken into consideration. The dispersion relation of the [001] valleys including the shear strain component for the conduction band now reads as:

\[
E(k) = \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 (k_y^2 + k_z^2)}{2m_1} + \delta E_c - \left( \frac{\hbar^2 k_y k_z}{m_1} \right)^2 + \left( D \varepsilon_{xy} - \frac{2 \hbar^2 k_y k_z}{M} \right) \frac{1}{2}, \tag{6}
\]

where the value of \( \varepsilon_{xy} \) is positive for tensile stress in [110] direction. In Fig. 2 the analytical band structure (6) is compared with the results of the EPM calculations for uniaxial [110] tensile stress of 3 GPa. Even for such large stress values the agreement between the analytical model and the numerical EPM results is excellent up to 200 meV. The band structure shown in Fig. 2 suggests a strong effective mass modification, which is analyzed in more details in the next section.

III. CONDUCTION BAND MODIFICATION DUE TO SHEAR STRAIN

The usually ignored off-diagonal strain component lifts the degeneracy between the two lowest conduction bands at the \( X \) points along the [001] axis in the Brillouin zone [7]. This lifting of degeneracy has a strong effect on the band structure. We investigate the shifts of the valley minima, changes in the effective masses and in the nonparabolicity parameter.

A. Valley shifts

Since the conduction band minimum along the [001] axis is located near the \( X \) point, the gap opening at the \( X \) point affects the position of the minimum. First, the conduction band minimum \( k_{min} \) moves closer to the \( X \) point. From (6) we obtain

\[
k_{min} = -k_0 \sqrt{1 - \eta^2}. \tag{7}
\]

Here, the dimensionless off-diagonal strain \( \eta = 2D \varepsilon_{xy}/\Delta \) is introduced. For \( \eta \geq 1 \) the conduction band minimum is located exactly at the \( X \) point.

The minima of the two [001] valleys move down in energy with respect to the remaining four fold degenerate valleys. For \( \eta \leq 1 \) the strain dependence is quadratic, while it is linear for \( \eta \geq 1 \):

\[
\Delta E_{\text{shear}} = \begin{cases} 
-\frac{3}{4} \eta^2, & |\eta| < 1 \\
-(2|\eta| - 1)\Delta/4, & |\eta| > 1
\end{cases} \tag{8}
\]

In Fig. 3 the shifts predicted by (8) are compared with results from EPM calculations. Excellent agreement is found.

B. Stress dependent effective masses

Shear strain modifies the effective masses in the [001] valleys. Evaluating the corresponding second derivatives of (6) at the band minimum (7), we obtain two different branches for the effective mass across \( (m_{11}) \) and along \( (m_{12}) \) the stress direction:
The strain dependence of the nonparabolicity parameter taken into account, are shown in Fig. 7. The stress dependence of the nonparabolicity parameter is obtained and analyzed. It is demonstrated that the enhancement of low-field mobility in uniaxially stressed UTB FETs is partly hampered by an increase in nonparabolicity at higher stress.

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REFERENCES


