

# Strain Effect on the Final State Density-of-State for Hole Scattering in Silicon

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## ABSTRACT

Strain-induced change of density-of-state for final state holes in phonon scattering is estimated by using a low field model. Analytical model for density-of-state effective masses of heavy and light holes in high temperature, which approximates the complicated constant energy surfaces of valence bands of strained Si to ellipsoids, is taken into account. Band splitting effects on the final state density-of-state in the phonon scattering are estimated at  $\Gamma$  point in  $k$ -space. It is shown that the band splitting enhances the mobility more effectively, while the effect from density-of-state effective mass depresses. The present model that predicts up to about 2.36 times enhancement for hole mobility in strained Si is shown to be useful for checking.

**Keywords:** density-of-state, hole scattering, final state, strain, silicon

## 1 INTRODUCTION

Since strained-Si on  $\text{Si}_{1-x}\text{Ge}_x$  substrate is expected to enhance the carrier mobility in MOSFETs, recent transport simulation technique such as full-band Monte Carlo simulation are applied to investigate their transport phenomena. In the full-band Monte Carlo simulation, pseudopotential method is usually used to determine the final state density-of-state (FSDOS) so that whole band structure of strained Si is taken into account.

The hole transport mechanism, however, has not been completely understood yet. Most important problem on this mechanism is the strain-induced change in FSDOS in hole scattering. Although the energy distribution of high energy holes can be taken into account in the full band Monte Carlo method [1], [2], low energy holes play an important role in strained-Si because strain shifts the band edge largely where most of holes are exist [3].

In the present study, hole transport model in strained-Si for low energy region is shown, so that physical understanding on the hole transport mechanism in strained-Si is possible quantitatively. The strain-induced effects on hole scattering are modeled in two forms, which are the effect on DOS effective mass due to the distortion of the

valence band, and the effect on the splitting of heavy hole and right hole bands.

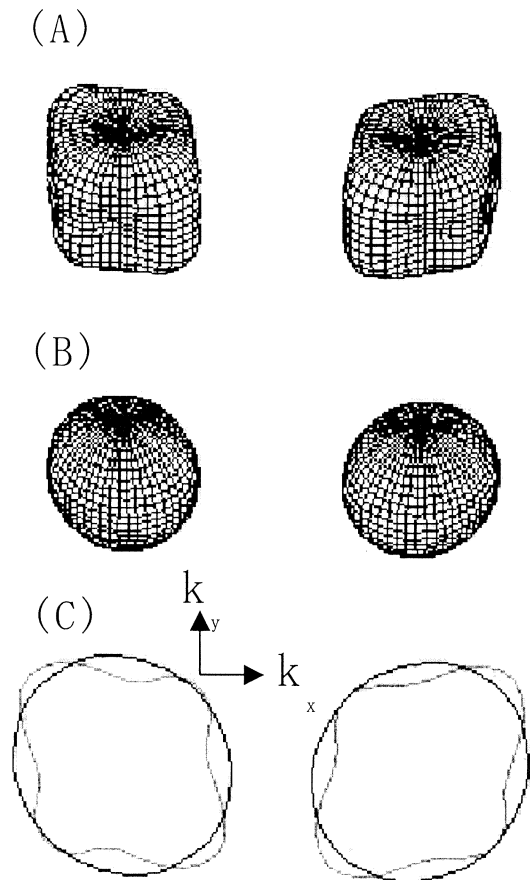


Figure 1: Constant energy surfaces of the heavy holes band: Stress is applied in  $\langle 110 \rangle$  by  $5 \cdot 10^8 \text{N/m}^2$  (left side) and  $-5 \cdot 10^8 \text{N/m}^2$  (right side). (A) Bir and Pikus model (B) High energy approximation (C) 2-D representation of the constant energy surfaces for (A) and (B).

## 2 MODEL

Various types of scattering rate are used in the carrier transport simulation. In general, the scattering rate

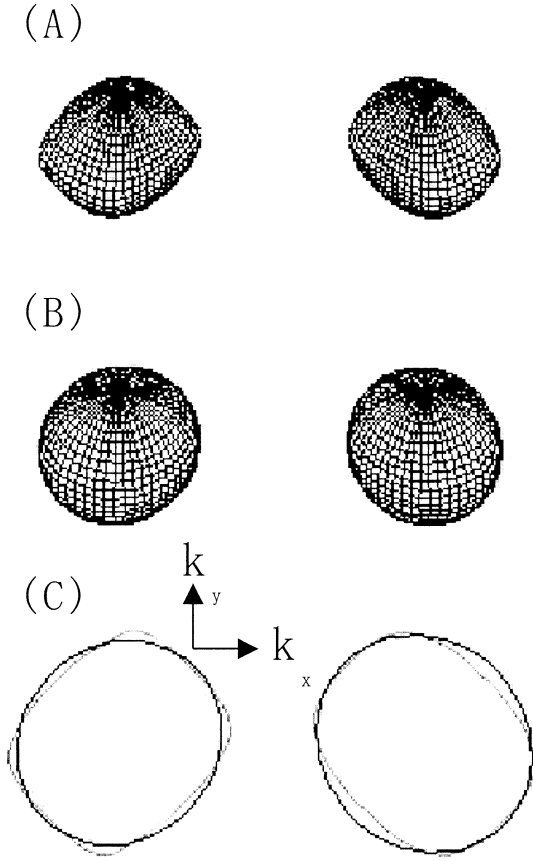


Figure 2: Constant energy surfaces of the light holes band: Stress is applied in (110) by  $5 \cdot 10^8 \text{N/m}^2$  (left side) and  $-5 \cdot 10^8 \text{N/m}^2$  (right side). (A) Bir and Pikus model (B) High energy approximation (C) 2-D representation of the constant energy surfaces for (A) and (B).

( $w$ ) includes FSDOS and can be written as follows,

$$w = \tau^{-1} = C \frac{(2m_d)^{3/2} D^2}{4\pi^2 \hbar^3} E^{1/2} \quad (1)$$

where  $C$  is the constant,  $m_d$  is the DOS effective mass and  $E = \epsilon - \epsilon_0$  is the carrier energy from the band edge.  $m_d$  and  $E$  are characterized in the post-scattering band, which are included in the FSDOS.

When strain is applied in bulk silicon the FSDOS changes in two ways. First, the DOS effective mass changes due to the distortion of the constant energy surfaces, although they are originally warped. Second, the band edge shifts due to the splitting of the degeneracy in bands.

## 2.1 Density-of-State Effective Mass

The strain changes holes band structures, i.e. light holes and heavy holes bands. Analytical expression for the band structure under strained condition has been

deduced near  $\Gamma$  point in  $k$ -space by the perturbation theory using the strain Hamiltonian [4]. This expression has a singular point where both  $k$  and strain are zero. Approximation for the expression is obtained by expanding either  $k$  (low energy approximation) or strain (high energy approximation). The latter is confronted with the analysis on the device under normal operation, so the average energy of hole is set to a certain energy,  $3KT/2 \simeq 40 \text{ meV}$ . The high energy approximation leads the expression of the hole energy to a quadratic form in  $k$ . The  $E(k)$  relation of valence bands in such approximation is given by [5], [1],

$$E_{l,h} = \frac{\hbar^2}{2} \cdot k \cdot M_{l,h}^{-1} \cdot k + \Delta E_{l,h} \quad (2)$$

where

$$\Delta E_{l,h} = \pm \frac{A \pm \sqrt{B^2 + C^2/5.82}}{3KT \sqrt{B^2 + C^2/5.82}} E_\epsilon \quad (3)$$

$A, B$  and  $C$  are the band parameters, and  $E_\epsilon$  is given with the deformation potentials ( $b, c, d$ ):

$$E_\epsilon = \frac{b^2}{2} [(\epsilon_{xx} - \epsilon_{yy})^2 + (\epsilon_{yy} - \epsilon_{zz})^2 + (\epsilon_{zz} - \epsilon_{xx})^2] + d^2 (\epsilon_{xy}^2 + \epsilon_{xz}^2 + \epsilon_{yz}^2) \quad (4)$$

$M_{l,h}^{-1}$  is the inverse effective mass tensor;

$$\begin{aligned} [M_{l,h}^{-1}]_{ii} &= 1 \pm \gamma_1 (3\epsilon_{ii} - \epsilon) / m_{v0} \\ [M_{l,h}^{-1}]_{ij} &= 1 \pm \gamma_2 \epsilon_{ij} / m_{v0} \quad (i \neq j) \end{aligned} \quad (5)$$

where

$$\begin{aligned} m_{v0} &= \frac{\hbar^2}{2(A \pm \sqrt{B^2 + C^2/5.82})} \\ \gamma_1 &= \frac{Bb}{3KT \sqrt{B^2 + C^2/5.82}} \\ \gamma_2 &= \frac{Dd}{3KT \sqrt{B^2 + C^2/5.82}} \\ \epsilon_{ij} &= \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz} \end{aligned}$$

and  $\epsilon_{ij}$  is the strain tensor. The plus sign corresponds to the light holes band and the minus sign to the heavy holes band.

Since the inverse effective masses tensor is a Hermitian, the constant energy surface becomes an ellipsoid with a longitudinal mass  $m_l$  and transverse mass  $m_t$  by an appropriate unitary transformation. Therefore the inverse of DOS effective mass,  $m_d = m_d (m_l m_t^2)^{1/3}$ , is estimated from the product of three eigen values for this tensor, which can be easily obtained by its secular equation. The DOS effective mass affects the phonon scattering rate as  $w \propto (m_d)^{3/2}$ .

Constant energy surfaces for the heavy holes band and the light holes band in this approximation are shown in Fig.1 and Fig.2, respectively.

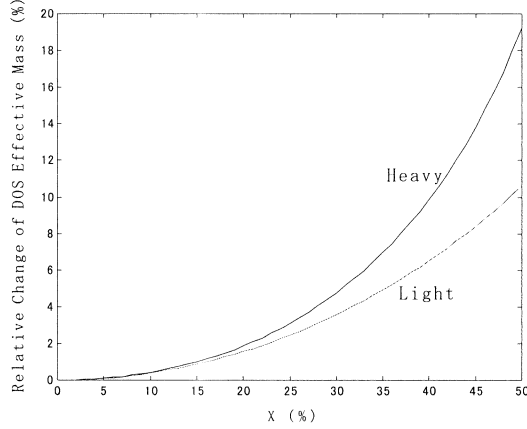


Figure 3: Relative change of DOS effective masses as a function of mole fraction  $x$  in  $\text{Si}_{1-x}\text{Ge}_x$  for heavy and light holes bands. Each of the valence bands is normalized at zero strain in Si.

## 2.2 Band Splitting Effects

The strain also resolves the degenerated valence bands at  $\Gamma$  point in  $k$  space into heavy and light holes bands and causes band splitting. The band splitting affects on the FSDOS, because holes shift their energy after their transfer to the other band by the band splitting energy  $2E_\varepsilon^{1/2}$  [see Eq.(4)], as well as gain or lose their energy by phonon energy [4], [5]. The band splitting effects appear in the optical phonon scattering rate as,

$$w'_{\text{op}} \propto \sqrt{E - 2E_\varepsilon^{1/2} + \hbar\omega_0} + e^{\theta/T} \sqrt{E - 2E_\varepsilon^{1/2} - \hbar\omega_0} \quad (6)$$

where  $\hbar\omega_0$  is the optical phonon energy whose equivalent temperature is  $\theta = 735$  K.

## 3 RESULTS AND DISCUSSIONS

Since phonon scattering is dominant in high temperature, we discuss with the acoustic phonon scattering and the optical phonon scattering. The total scattering rate  $w_{\text{tot}}$  is comprised of several scattering mechanisms, which are listed as follows,

1. Intraband scattering.
  - (a) Heavy hole band ( $w_{\text{ac}}^h$ )
  - (b) Light hole band ( $w_{\text{ac}}^l$ )
2. Interband scattering.
  - (a) Heavy hole band  $\rightarrow$  Light hole band ( $w_{\text{op}}^h$ )
  - (b) Light hole band  $\rightarrow$  Heavy hole band ( $w_{\text{op}}^l$ )

Optical phonon scattering for the intraband scattering is forbidden in silicon by the crystallographic symmetry, while it is dominant in the interband scattering.

Magnitude of the scattering rates under zero strain are proportional to the DOS effective mass ( $m_d$ ) and the coupling constant ( $W$ ). Their relative magnitude are shown in Table 1. As shown in the table, the intraband scattering in heavy holes band and the interband scattering from light holes band to heavy holes band are dominant, because of large DOS effective mass in the heavy holes band.

Table 1: Relative magnitude of scattering from the initial bands to the final bands by the DOS effective masses ( $m_{h,l}$ ) and the coupling constant ( $W$ ).

Initial	Final Heavy holes band	Light holes band
Heavy holes band	$m_h^{3/2}$ 0.33	$Wm_l^{3/2}$ 0.13
Light holes band	$Wm_h^{3/2}$ 0.67	$m_l^{3/2}$ 0.062

Relevant scattering rates under strained condition are those of the interband scattering, as the final state DOS changes by the band splitting.

$$\frac{\Delta w_{\text{tot}}}{w_{\text{tot}}} = \frac{w'_{\text{op}} - w_{\text{op}}}{w_{\text{ac}} + w_{\text{op}}} = \frac{w'_{\text{op}}/w_{\text{op}} - 1}{1 + W^{-1}} \quad (7)$$

where  $W$  is the coupling constant between acoustic phonon scattering and optical phonon scattering, which is given by using acoustic deformation potential  $D_{\text{ac}}$ , optical deformation potential  $D_{\text{op}}$  and sound velocity  $v_s$ :

$$W = \frac{w_{\text{op}}}{w_{\text{ac}}} = \frac{D_{\text{op}}^2}{D_{\text{ac}}^2} \cdot \frac{v_s^2}{\omega_0^2} \sim 2 \quad (8)$$

Calculation results of the DOS effective mass for two bands are shown in Fig.3 as a function of mole fraction  $x$  of Ge to SiGe,  $\text{Si}_{1-x}\text{Ge}_x$ . As shown in the figure, the DOS effective mass increases with  $x$  and its absolute value is larger for the heavy holes band, although the DOS effective mass of heavy holes band at zero strain is about 3 times larger than that for the light holes band. The relative change of DOS effective mass is 10% around  $x = 40\%$  for the heavy holes band.

The band splitting effect is estimated by Eq.(6). Fig.4 shows the results for relative change of phonon scattering rate ( $w'_{\text{op}}/w_{\text{op}}$ ) as a function of  $x$  for some hole energies (25, 40, 60 meV). The band splitting due to tensile strain makes the phonon scattering rate decrease remarkably. The phonon scattering rate even vanishes in higher  $x$  region. Then the fractional scattering rate given in Eq.(7) decreases to about 1/3, which leads saturation in relaxation time  $\langle\tau\rangle$ .

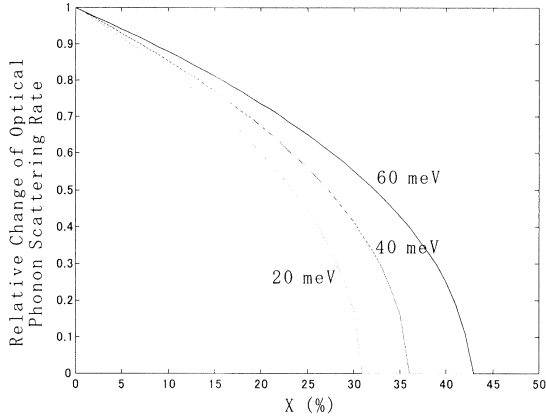


Figure 4: Relative change of phonon scattering rate ( $w_{op}/w_{op}$ ) as a function of mole fraction  $x$  in  $\text{Si}_{1-x}\text{Ge}_x$  for some hole energies (25, 40, 60 meV). Phonon scattering rate is normalized at zero strain in Si.

Since mobility ( $\mu = e\langle\tau\rangle/m_c$ ) is inversely proportional to the scattering rate through the relaxation time, the mobility increases with  $x$ . It is worth noticing that the mass appeared in this expression is the conductivity effective mass, which should be distinguished from the DOS effective mass. The conductivity effective mass is also affected by strain. However it can be assumed that the amount of change in the conductivity effective mass is similar to that in the DOS effective mass.

Relative change of the mobility behaves as,

$$\frac{\mu'}{\mu} \propto \left(\frac{m'_d}{m_d}\right)^{-5/2} \left(\frac{w'_{tot}}{w_{tot}}\right)^{-1} \quad (9)$$

where the pre factor comes from the change in DOS effective masses and the last factor from the change in optical scattering rate [see Eq.(7)]. It is estimated from this equation that the mobility enhances by about 2.36 in higher  $x$  region.

The results presented in this paper gives compatible with those of the recent works [7], [8], so our model can be useful for checking the hole mobility in the strained MOSFETs.

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