Electron Mobility Model for ⟨110⟩ Stressed Si Including Strain-Dependent Mass

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I. Abstract

Stress induced enhancement of electron mobility has primarily been attributed to the splitting of the conduction bands. However, experiments [1] have indicated that the mobility enhancement cannot solely be attributed to this effect, and a recent study has shown that a stress along the ⟨110⟩ direction leads to a change of the effective mass [2]. This work investigates the effect of the variation of the effective mass with stress along ⟨110⟩ direction on the electron mobility. An improved low-field mobility model incorporating the effective mass change is presented.

II. Introduction

The band structure (BS) of Si including the effect of stress/strain has been calculated using the empirical non-local pseudopotential method (EPM) [3]. For stress along ⟨110⟩, the effect of the internal displacement of the atoms [4] has been taken into account in the BS calculations. The effective masses for the two-fold degenerate Δ_2-valleys and the four-fold degenerate Δ_4-valleys were extracted from the BS data using curve fitting. Fig. 1 depicts the variation of the two transversal ($m_{t\|}$, $m_{t\perp}$) and the longitudinal (m_l) masses for the Δ_2-valleys as a function of the strain for different values of the internal displacement parameter, ξ. The variation of $m_{t\|}$, $m_{t\perp}$, and m_l has been fitted using a quadratic function of the stress. Fig. 1 shows that there is a significant change in Δm^* for increasing strain along ⟨110⟩ which translates into a mobility variation as shown in Fig. 2. Also shown in Fig. 3 is the splitting, $\Delta\varepsilon$ for biaxially/uniaxially strained Si. It is observed that biaxial tension is more effective in splitting the conduction bands than ⟨110⟩ uniaxial tension.

III. Modeling

The mobility tensor for a stress along ⟨110⟩ can be calculated analytically using an expression proposed in [5]. It includes the effect of strain-induced splitting of the conduction band valleys in Si, inter-valley scattering, doping dependence and temperature dependence. The model however assumes a constant m_t and m_l in Si. Band structure calculations show that for a uniaxial tensile stress along ⟨110⟩, the two-fold degenerate Δ_2-valleys, which are lowered in energy, experience a change in the effective masses. This results in a pronounced anisotropy of the mobility in the transport plane (see Fig. 4). For uniaxial compression, however, there is a negligible change in the effective masses of the lowered four fold degenerate Δ_4-valleys. We have therefore extended the model in [5] to account for the variation of the effective mass of the Δ_2-valleys with stress for uniaxial tensile stress. This in turn leads to a modification of the scaled inverse mass tensor $\widehat{m}_z^{-1}$ (Eq. (6) in [5]), which is obtained as shown below.

$$\widehat{m}_z^{-1} = m_c \begin{pmatrix} m_t^{-1} & m_\Delta^{-1} & 0 \\ m_\Delta^{-1} & m_t^{-1} & 0 \\ 0 & 0 & m_l^{-1} \end{pmatrix} \begin{array}{l} m_t^{-1} = (m_{t\|}^{-1} + m_{t\perp}^{-1})/2 \\ m_\Delta^{-1} = (m_{t\|}^{-1} - m_{t\perp}^{-1})/2 \end{array}$$

$$m_c^{-1} = (m_{t\|}^{-1} + m_{t\perp}^{-1} + m_L^{-1})/3$$

Here m_c and m_t denote the average conductivity and transversal mass respectively. The $m_{t\|}$ and $m_{t\perp}$ denote respectively the transversal masses along ⟨110⟩ and $\langle\bar{1}10\rangle$ of the Δ_2-valleys. The mobility tensor thus calculated using $\widehat{m}_z^{-1}$ becomes non-diagonal in the principal coordinate system. Fig. 5 and Fig. 6 show a comparison of the variation of the electron mobility components with increasing stress as obtained from Monte Carlo simulations and the analytical model. A good agreement is obtained.

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References

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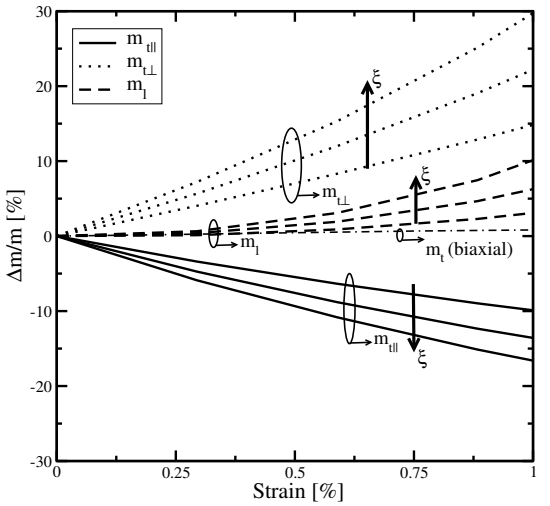

Fig. 1. Effect of the uniaxial ⟨110⟩ tensile strain on the transversal and longitudinal masses of the Δ_2-valleys (ξ = 0, 0.53, 1.0).

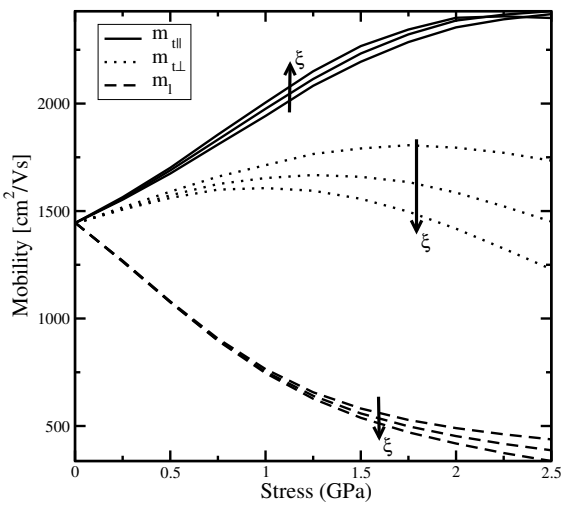

Fig. 2. Mobility as a function of tensile stress with internal displacement as a parameter (ξ = 0, 0.53, 1.0).

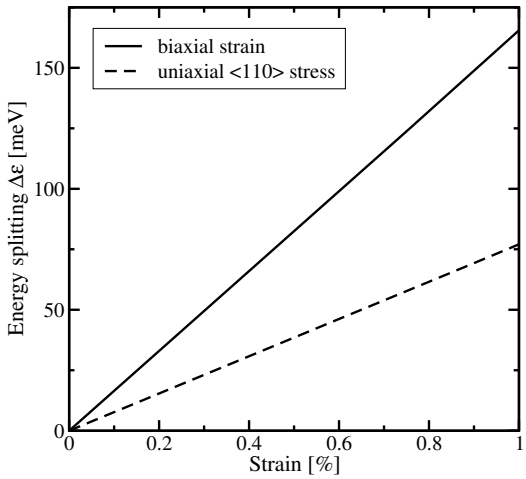

Fig. 3. Effect of biaxial tensile strain and uniaxial ⟨110⟩ tensile stress on valley splitting. Strain component in the stressed direction is plotted.

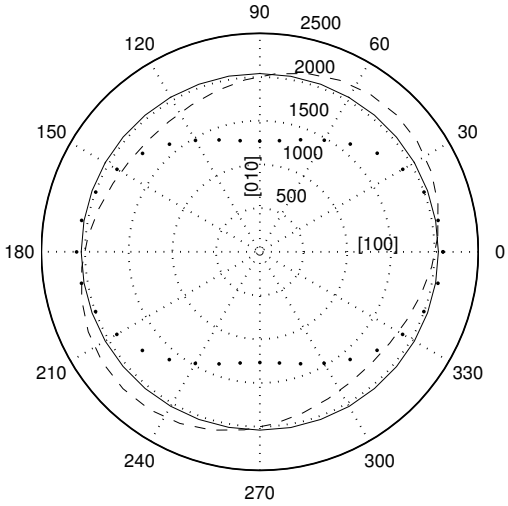

Fig. 4. Variation of the in-plane mobility with in-plane angle for uniaxial ⟨110⟩ and ⟨110⟩ tensile stress. solid: ⟨110⟩ without mass correction; dashed: ⟨110⟩ with mass correction; dotted: uniaxial ⟨100⟩ stress.

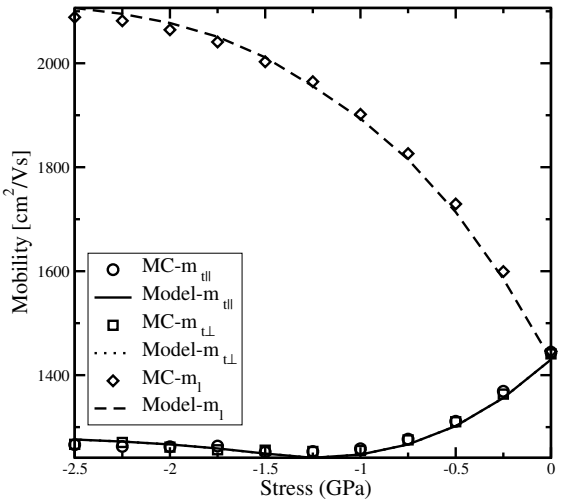

Fig. 5. Comparison of electron mobility components obtained from the MC simulations and the analytical model for uniaxial ⟨110⟩ compressively strained Si. Here $m_{t\|} = m_{t\perp}$

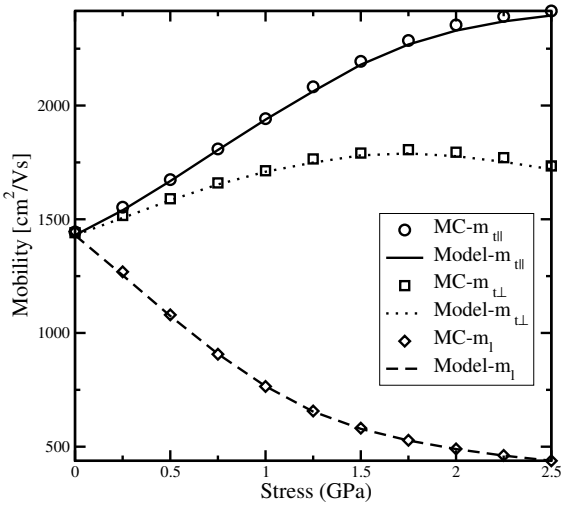

Fig. 6. Comparison of electron mobility components obtained from the MC simulations and the analytical model for uniaxial ⟨110⟩ tensile strained Si.