An Analytical Model of Electron Mobility for Strained-Si Channel nMOSFETs*

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Abstract: An analytical model of electron mobility for strained-silicon channel nMOSFETs is proposed in this paper. The model deals directly with the strain tensor, and thus is independent of the manufacturing process. It is suitable for $\langle 100 \rangle / \langle 110 \rangle$ channel nMOSFETs under biaxial or $\langle 100 \rangle / \langle 110 \rangle$ uniaxial stress and can be implemented in conventional device simulation tools.

Key words: Strained-Si; electron mobility; analytical model; nMOSFET; uniaxial stress/strain

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1 Introduction

Having crossed the 65nm node, technology to induce strain into a channel has become a necessary to enhance the electron mobility in a channel, which falls quickly as the critical size decreases.

The modeling of electron mobility in a strained channel nMOSFET has been studied for a long time [1~3], but most models are based on specific technologies like SiGe substrate [4~6]. Since the method to induce strain is still studied and continuously improved, we need a process-independent model to meet these situations.

Dhar and $Enzo^{[7]}$ have developed a mobility model that deals directly with strain tensor and thus, is independent of the manufacturing process and can be applied to $\langle 100 \rangle$ bulk Si materials. They give an improved model that is also suitable for $\langle 110 \rangle$ bulk Si materials^[8]. Two points of their model should be noted. First, the model can only be used to calculate the bulk Si mobility. Second, the treatment of the $\langle 110 \rangle$ direction is somewhat simple. In this paper, we suggest a new electron mobility model, based on the model of Dhar and $Enzo^{[7]}$, for a strained Si channel nMOSFET. In this model, we can calculate not only the mobility of bulk Si, but also that of the strained channel, and we improve the treatment of the $\langle 110 \rangle$ direction over^[8].

2 Modeling

2.1 Model structure

In this model, the total mobility can be obtained by taking the weighted average of mobility tensors of each valley, expressed as

$$\overset{\wedge}{\mu} = \sum_{i=1}^{3} p^{(i)} \cdot \overset{\wedge}{\mu_{n}}^{(i)} \tag{1}$$

Here $\stackrel{\wedge}{\mu}$ is the mobility tensor, $p^{(i)}$ is the population of the ith valley (considering the symmetry of Si conduction band, the six conduction band valley can be treated as three equivalent classes sorted by axis, and i is the class index), and $\stackrel{\wedge}{\mu}{}^{(i)}$ is the mobility tensor of the ith valley.

The mobility tensor of a single valley can be expressed as a product of scalar mobility and scaled inverse effective mass tensor^[7]

$$\hat{\mu}^{(i)} = \mu \, \hat{m}_{(i)}^{-1} \,, \quad i = x, y, z \tag{2}$$

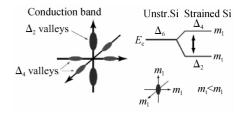


Fig. 1 Demonstration of the effects of stress on energy $\mathsf{band}^{\text{[10]}}$

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in which μ is the scalar mobility obtained by average effective mass and $\hat{m}_{(i)}^{-1}$, which will be discussed in section 2.3, is the effective mass correction tensor that represents the difference of effective mass for different directions.

The scalar mobility is

$$\frac{1}{\mu} = \frac{1}{\mu_{\text{equiv}}} + \frac{1}{\mu_{\text{nequiv}}} + \frac{1}{\mu_{\text{ni}}} + \frac{D}{\mu_{\text{ac}}} + \frac{D}{\mu_{\text{sr}}} + \frac{D}{\mu_{\text{cit}}}$$
(3)

Here μ_{equiv} , μ_{nequiv} , μ_{ni} , μ_{ac} , μ_{sr} and μ_{cit} denote intravalley scattering and intervalley scattering between the equivalent valley, intervalley scattering between the nonequivalent valley, impurity scattering, additional surface phonon scattering, surface roughness scattering, and interface coulomb scattering, respectively. These scattering terms are summed according to Mathiessen's rule, and D denotes the vanishing term as the channel depth from the Si-SiO₂ interface increases.

2, 2 Model details

(1) Phonon Scattering: The contribution of the phonon is evaluated by μ_{equiv} and μ_{nequiv} . According to Ref. [7], μ_{equiv} can be expressed as a constant. μ_{nequiv} is a function of stress,

$$\mu_{\text{nequiv}}^{(i)} = \mu_{\text{nequiv}}^{0} / h^{(i)}$$
 (4)

Here μ_{nequiv}^0 evaluates the effect of intervalley phonon scattering between a nonequivalent valley where no stress exists, and $h^{(i)}$ is the dimension factor of the ith valley under strain

$$h^{(i)} = \frac{g\left(\frac{\Delta_{ij}^{\text{emi}}}{k_{\text{B}}T}\right) + g\left(\frac{\Delta_{il}^{\text{emi}}}{k_{\text{B}}T}\right) + \exp\left(\frac{\hbar \omega_{\text{opt}}}{k_{\text{B}}T}\right) \left[g\left(\frac{\Delta_{ij}^{\text{abs}}}{k_{\text{B}}T}\right) + g\left(\frac{\Delta_{il}^{\text{abs}}}{k_{\text{B}}T}\right)\right]}{2\left[g\left(\frac{-\hbar \omega_{\text{opt}}}{k_{\text{B}}T}\right) + \Gamma\left(\frac{3}{2}\right)\right]}$$
(5)

in which g has the form

$$g(z) = \begin{cases} \exp(-z) \cdot \Gamma(3/2) & \forall z > 0 \\ \exp(-z) \cdot \Gamma(3/2) & \forall z < 0 \end{cases}$$
 (6)

Here $\Delta_{ij}^{\rm emi}(\Delta_{ij}^{\rm abs})$ is the phonon energy needed when an phonon is emitted (absorbed) from the j(i)th to i(j)th valley.

The effects of strain on μ_{nequiv} result from the strain induced valley splitting that change the energy needed for a phonon to be emitted or absorbed between nonequivalent valleys. Δ_{ij}^{emi} and Δ_{ij}^{abs} under strain can be expressed as

$$\Delta_{ii}^{\text{emi}} = \Delta E_{\text{C}}^{(j)} - \Delta E_{\text{C}}^{(i)} - \hbar \omega_{\text{opt}}$$

$$\Delta_{ii}^{\text{abs}} = \Delta E_{\text{C}}^{(j)} - \Delta E_{\text{C}}^{(i)} + \hbar \omega_{\text{opt}}$$
(7)

where $\hbar\omega_{\rm opt}$ is the phonon energy, and $\Delta E_{\rm C}^{(i)}$ ($\Delta E_{\rm C}^{(j)}$) denotes the strain induced splitting of the i(j) th valley

$$\Delta E_{\rm c}^{(i)} = \mathcal{E}_{\rm d}(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \mathcal{E}_{\rm u}\varepsilon_{ii} \tag{8}$$

Here, Ξ_d , Ξ_u are the dilatation and shear deformation

potential, and ε_{ii} is the *i*th diagnose component in the strain tensor.

(2) Impurity Scattering: We assume that the impurity scattering is independent of stress. Thus, the μ_{ni} in the unstrained mobility model is appropriate for our strained Si mobility model.

In this model, we employ the Masetti model [11] to evaluate the effect of impurity, which is the default mobility model to deal with impurity in Sentaurus $^{\bigcirc}$

$$\mu_{\text{ni}} = \mu_{\text{min}1} \exp\left(-\frac{P_{\text{c}}}{N_{\text{i}}}\right) + \frac{\mu_{\text{const}} - \mu_{\text{min}2}}{1 + \left(\frac{N_{\text{i}}}{C_{\text{r}}}\right)^{\alpha}} + \frac{\mu_{1}}{1 + \left(\frac{C_{\text{s}}}{N_{\text{i}}}\right)^{\beta}}$$
(9)

Here, $N_i = N_A + N_D$ denotes the total concentration of ionized impurities. μ_{const} is the intrinsic mobilities. μ_{min1} , μ_{min2} and μ_1 are reference mobilities. P_c , C_r , and C_s are reference doping concentrations. The remaining variables are fitting parameters whose values can be found in Ref. [11].

Next, we use Dhar's method [7] to rewrite the expression,

$$\mu_{b}^{(i)} = \frac{1}{\mu_{\text{equiv}}} + \frac{1}{\mu_{\text{nequiv}}} + \frac{1}{\mu_{\text{ni}}}$$

$$= \frac{\beta \mu^{L}}{1 + (\beta - 1) h^{(i)} + \beta \left(\frac{\mu^{L}}{\mu_{\text{ni}}} - 1\right)}$$
(10)

where $h^{(i)}$ is the dimension factor for stress in Eq. (4), μ^L is the low field mobility in Si, and β can be evaluated as

$$\beta = f \times \frac{m_{\rm t}}{m_{\rm c}} \tag{11}$$

in which f is the ratio between the mobility of the high stressed channel and the low field mobility. f is not a constant and is decided by the environment, which will be discussed in section 2. 4. $m_{\rm t}$ and $m_{\rm c}$ denote the transverse normalized effective mass and average normalized effective mass, respectively. All normalized effective mass present in this paper are normalized to $m_{\rm 0}$.

(3) Surface Scattering. The effects of surface mainly result from the roughness of surface, surface charges, and other factors related to the environment. In this model, three types of surface effects are considered. They are additional surface phonon scattering (μ_{ac}) , surface roughness scattering (μ_{sr}) , and surface coulomb scattering (μ_{cit}) . We employ the Lombardi model [111] (the Lombardi model is the default model to deal with interface degradation of mobility in Sentaurus) for the former two types of scattering,

$$\mu_{\rm ac} = \frac{B}{F_{\perp}} + \frac{C(N_{\rm i}/N_{\rm 0})^{\lambda}}{F_{\perp}^{1/3} (T/T_{\rm 0})^{k}}$$
(12)

$$\mu_{\rm sr} = \left(\frac{F_{\perp}^3}{\eta} + \frac{(F_{\perp}/F_{\rm ref})^{A^*}}{\delta}\right)^{-1} \tag{13}$$

where F_{\perp} is the effective vertical electric field in units of V/cm, T is the temperature in units of K, N_i is the impurity density in units of cm⁻³, and $T_0 = 300$ K, $N_0 = 1$ cm⁻³, $F_{\rm ref} = 1$ V/cm. The remaining parameters are fitted with the values found in Ref. [11].

Surface coulomb scattering is caused by the trap charges and the mobile/fixed charges, which are mostly positive near the gate-channel interface. As the effective vertical electric field increases, the channel electrons increase, screen the surface charge, and finally weaken the effect of surface coulomb scattering. According to Ref. [12], surface coulomb scattering induced mobility $\mu_{\rm cit} \propto \sqrt{N_{\rm inv}}/N_{\rm it}$, where $N_{\rm it}$ is the surface charge density and $N_{\rm inv}$ is the charge density in the inversion layer. The effective vertical field and charge density in the inversion layer are related by [13]

$$F_{\perp} = \frac{Q_{\text{dep}} + \eta \, Q_{\text{inv}}}{\varepsilon_{\text{Si}}} \tag{14}$$

Here, $Q_{\rm dep}$ and $Q_{\rm inv}$ are the sheet charge density of the depletion layer and the inversion layer, respectively, $\varepsilon_{\rm Si}$ is the electric permittivity of Si, and η depends on the manufacturing process, usually 1/2 for electrons and 1/3 for holes.

Using these two relations, the surface coulomb scattering can be evaluated. However, the model obtained from the relationships above does not accord with the experimental results, and this disagreement can not be solved by simply adjusting parameters. Thus, to meet experimental results, we improve the relationship mathematically to

$$\mu_{\text{cit}} = \mu_0 \left(\frac{1}{\ln(N_i/N_0)} \times \frac{F_\perp}{N_{\text{it}}} \right)^{\alpha} \left(\frac{T}{T_0} \right)^{\beta}$$
 (15)

where μ_0 is the empirical mobility, and α , β , N_0 , T_0 are parameters extracted from available experimental data.

Generally, surface effects are strongly related to position (mainly the distance to the $Si\text{-}SiO_2$ interface). As the distance increases, the surface effect is weakened. Thus, a diminishing factor is necessary. We employ expression^[11]

$$D = \exp(-x/l_{crit}) \tag{16}$$

for the modification. Here x is the distance to the Si-SiO₂ interface in units of nm, $l_{\rm crit}$ is the average diminishing distance whose values can be found in Ref. [11]. This diminishing factor acts directly on the term of surface scattering by multiplication

$$\frac{1}{\mu_{\text{surface}}} = \frac{D}{\mu_{\text{ac}}} + \frac{D}{\mu_{\text{sr}}} + \frac{D}{\mu_{\text{cit}}}$$
 (17)

With the increase of distance, μ_{surface} will be enhanced swiftly and its contribution to the total mobility will

decline quickly.

(4) Relative Population: The relative population of the *i*th valley $p^{(i)}$ in Eq. (2) is approximated by

$$p^{(i)} \approx n_{\text{str}}^{(i)} / \sum_{i=1}^{3} n_{\text{str}}^{(i)}$$
 (18)

where $n_{\text{str}}^{(i)}$ is the electron density of the *i*th valley and $\sum_{i=1}^{3} n_{\text{str}}^{(i)}$ is the total electron density.

The valley splitting induced by strain causes divergence in the electron density of each valley. We have

$$n_{\rm str}^{(i)} = N_{\rm c}^{(i)} \exp[-(E_{\rm C} - E_{\rm F})/k_{\rm B}T] \exp[-\Delta E_{\rm c}^{(i)}/k_{\rm B}T]$$
(19)

where $N_c^{(i)}$ is the effective density of states for electrons in the *i*th valley, E_c is the conduction band edge of unstrained Si, E_F is the Fermi level, and $\Delta E_c^{(i)}$ is the splitting of the valley with the same form as Eq. (8).

For a $\langle 110 \rangle$ stress, the effective density of states $N_{\rm c}^{\rm (i)}$ will depend on strain, which will be discussed in the following section.

2.3 Channel direction

In this model, the default reference axis is parallel to $\langle 100 \rangle$, $\langle 010 \rangle$, and $\langle 001 \rangle$, and the default channel direction is $\langle 100 \rangle$. To calculate the mobility of other channel directions, like $\langle 110 \rangle$, going directly through the coordinate transformation of the results of the $\langle 100 \rangle$ channel will lead to a wrong answer. According to Ref. [9], electrons will have a higher mobility under $\langle 110 \rangle$ stress. The reason for this phenomenon is unclear, but there is a view that the influence of strain on effective mass of electron is anisotropic. The effective mass of the $\langle 100 \rangle$ direction of Δ_2 valleys is not sensitive to the strain, while that of the $\langle 110 \rangle$ direction is. With tensile strain, the effective mass of the $\langle 110 \rangle$ direction of Δ_2 valleys will decrease and the mobility will then rise.

The view above does have theoretical support. Energy band calculation has pointed out that under $\langle 110 \rangle$ stress, the shape of energy band in the $\langle 110 \rangle$ direction has a notable change that cannot be neglected [13,14]. Using nonlocal EPM, we calculated the modification of the z-valley effective mass correction tensor $\stackrel{\wedge}{m}_z^{-1}$ as

$$\stackrel{\wedge}{m}_{z}^{-1} = m_{c} \begin{pmatrix} m_{t}^{-1} & \Delta_{\epsilon_{xy}}/2 & 0 \\ \Delta_{\epsilon_{xy}}/2 & m_{t}^{-1} & 0 \\ 0 & 0 & m_{1}^{-1} \end{pmatrix}$$
(20)

Here $m_{\rm t}$ and $m_{\rm c}$ are the transverse normalized effective mass and average normalized effective mass in Eq. (11), $m_{\rm l}$ is the longitudinal normalized effective mass, and $\Delta_{\epsilon_{xy}}/2$ gives the effective mass correction under stress as

$$\Delta_{\epsilon_{xy}} = \frac{(\alpha + \beta \, \epsilon_{xy}^2) \, \epsilon_{xy}}{(\hbar^2 \, k^2 / 2 \, m_{\odot})} \tag{21}$$

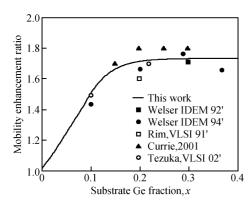


Fig. 2 Dependence of electron low field mobility on biaxial stress ($T=300\rm K$, $N_{\rm A}=10^{15}\rm \,cm^{-3}$, $E_{\perp}=0\rm MV/cm$, Ge fraction = $0{\sim}40\%$)

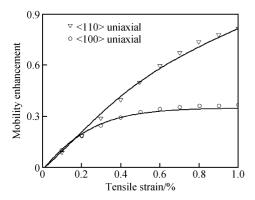


Fig. 3 Dependence of electron low field mobility on uniaxial stress (T=300K, $N_{\rm A}=1.5\times10^{10}\,{\rm cm}^{-3}$, $E_{\perp}=0{\rm MV/cm}$, Tensile strain = $0\sim1\%$)

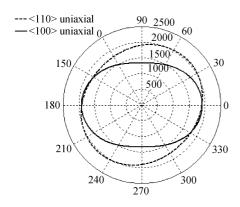


Fig. 4 Dependence of electron low field mobility (in cm²/(V · s)) on channel direction ($T = 300 \,\mathrm{K}$, $N_{\rm A} = 1.5 \times 10^{10} \,\mathrm{cm}^{-3}$, $E_{\perp} = 0 \,\mathrm{MV/cm}$, Tensile strain = 0.4%)

where m_0 is the static mass of electron in units of kg, ε_{xy} is the component of strain tensor of no units and α , β , k_{ε} are fitting parameters with values in Table 1. a_0 in Table 1 is the lattice constant.

Table 1 Parameters for mass modification under stress

Parameter	Unit	Value
α	eV	20
β	eV	- 3691. 1
<i>k</i> ε	$2\pi/a_0$	0.076

Using Eq. (20), we can write the normalized effective mass in the $\langle 110 \rangle / \langle 1\overline{10} \rangle$ direction

$$m_{110} = \frac{2m_{t}}{2 + \Delta_{\epsilon_{xy}}m_{t}}$$

$$m_{1\overline{1}0} = \frac{2m_{t}}{2 - \Delta_{\epsilon_{xy}}m_{t}}$$
(22)

Three points should be noted in our calculation. First, the results show changes of m_x^{-1} and m_y^{-1} are not significant and can be neglected. Second, changes of longitudinal effective mass m_1^{-1} in m_z^{-1} are also small enough to be neglected. Third, the modification of effective mass in z-valleys is only related to ε_{ry} .

The change of transverse effective mass not only influences the mass correction tensor m_i^{-1} in Eq. (2), but also alters the effective density of states N_c in Eq. (19) since $N_c \approx m_{\rm dn}^{3/2}$. The effective mass of density of states $m_{\rm dn}$ is

$$m_{\rm dn} = (S^2 m_1 m_{\rm t}^2)^{1/3}$$
 (23)

According to these relations, a corrected term to express the change of $N_{\rm c}$ is

$$N'_{\rm c} = N_{\rm c} \left(\frac{m'_{\rm dn}}{m_{\rm dn}}\right)^{3/2} \tag{24}$$

where $m'_{dn} = (S^2 m_1 m_t^{\parallel} m_t^{\perp})^{1/3}$.

2.4 Enhancement factor

The mobility enhancement factor f in Eq. (11) is an important parameter in this model. It is the ratio between the mobility of the high stressed channel and the low field mobility. According to Eq. [15], this factor is not constant but depends on the effective vertical electric field and the layer thickness of strained-silicon. Based on the data from Ref. [15], we modify f to $f = f(F_{\perp}, T_{\rm Si}) = p_1(F_{\perp}) T_{\rm Si}^2 + p_2(F_{\perp}) T_{\rm Si} + p_3(F_{\perp})$

in which $T_{\rm Si}$ is the thickness of the strained-silicon layer in units of nm, F_{\perp} is the effective vertical electric field intensity in units of V/cm, and p_1 , p_2 and p_3 are parameters related to F_{\perp} .

3 Results and discussion

Figures $2\sim4$ shows the influence of strain on low field mobility. Figure 2 represents the dependence of electron low field mobility on biaxial stress. Several results^[16] have been compared, and the trend of this model accords well with these data. Figure 3 gives the dependence of electron low field mobility on uniaxial stress and the data from Uchida's work^[9]. When the strain increases to about 0.4%, the mobility of the $\langle 100 \rangle$ channel stops increasing, but that of $\langle 110 \rangle$ channel continues to increase, although the rate of increase declines. Figure 4 shows the dependence of low

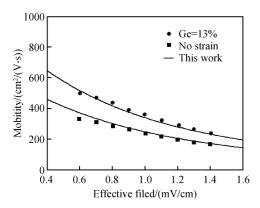


Fig. 5 Dependence of electron channel mobility on biaxial stress and effective electrical field ($T=300\,\mathrm{K}$, $N_\mathrm{A}=1.8\times10^{16}\,\mathrm{cm^{-3}}$, $E_\perp=0.4\sim1.7\,\mathrm{MV/cm}$, Ge fraction = 13%)

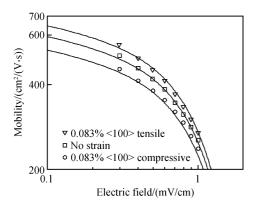


Fig. 6 Dependence of electron channel mobility on $\langle 100 \rangle$ uniaxial stress and effective electrical field ($T=300\mathrm{K}$, $N_\mathrm{A}=1.8\times10^{17}\,\mathrm{cm}^{-3}$, $E_\perp=0\sim2\mathrm{MV/cm}$, Tensile strain = -0.083%, 0, 0.083%)

field mobility on channel direction under stress of different directions.

Figures $5 \sim 7$ show the channel electron mobility under the influence of both stress and vertical electric field. The comparison data comes from the work of $Rim^{[17]}$ and $Uchida^{[18]}$, respectively.

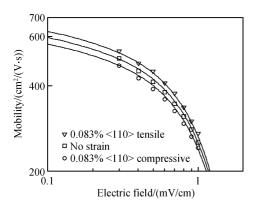


Fig. 7 Dependence of electron channel mobility on $\langle 110 \rangle$ uniaxial stress and effective electrical field ($T=300 \, \mathrm{K}$, $N_{\mathrm{A}}=1.8 \times 10^{17} \, \mathrm{cm}^{-3}$, $E_{\perp}=0 \sim 2 \, \mathrm{MV/cm}$, Tensile strain = $-0.083 \, \%$, 0, 0.083%)

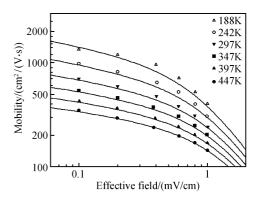


Fig. 8 Dependence of electron channel mobility on temperature and effective vertical electric field (T=188,242,297,347,397,447K, $N_A=3.9\times10^{15}\,\mathrm{cm}^{-3}$, $E_\perp=0{\sim}2\mathrm{MV/cm}$)

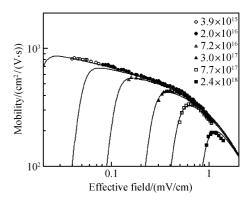


Fig. 9 Dependence of electron channel mobility on doping concentration and effective electric field ($T = 300 \, \text{K}$, $N_{\rm A} = 3.9 \times 10^{15}$, 2.0×10^{16} , 7.2×10^{16} , 3.0×10^{17} , 7.7×10^{17} , 2.4×10^{18} cm⁻³, $E_{\perp} = 0 \sim 2 \, \text{MV/cm}$)

Figures 8 and 9 show the dependence of channel electron mobility on temperature and doping concentration, respectively. The comparison data comes from the work of Takagi^[19].

Figure 10 gives the dependence of the f factor on layer thickness of strain-silicon and effective vertical electric field. The comparison data comes from the work of Mizuno $^{[15]}$.

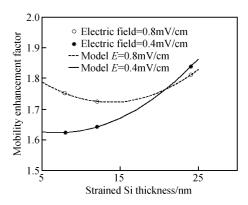


Fig. 10 Dependence of f factor on thickness of strain-Si layer and effective vertical electric field ($T=300\,\mathrm{K}$, $N_\mathrm{A}=1.5\times10^{10}\,\mathrm{cm}^{-3}$, $E_\perp=0.4$, $0.8\,\mathrm{MV/cm}$)

4 Conclusion

An analytical model of electron mobility for strained-silicon channel nMOSFETs is proposed in this paper. The model is independent of the manufacturing process because it deals directly with the strain tensor. It can be applied to both $\langle\,100\,\rangle$ and $\langle\,110\,\rangle$ channel nMOSFETs. The model accords well with experimental results.

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应变硅电子迁移率解析模型*

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摘要:提出了一个应变硅沟道电子迁移率解析模型.模型以应变张量为对象研究应变硅沟道电子迁移率,因此与工艺相独立;适用于施加双轴应力及 $\langle 100 \rangle / \langle 110 \rangle$ 方向单轴应力,沟道方向为 $\langle 100 \rangle / \langle 110 \rangle$ 的器件;易于嵌入常用仿真工具中.

关键词: 应变硅; 电子迁移率; 解析模型; n型场效应管; 单轴应力/应变

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