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The effect of biaxial stress on the carrier-transport properties at SiO_2/4H-SiC interfaces

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Abstract

We investigate the biaxial stress effect on the electron transport properties at SiO_2/4H-SiC interfaces. The electron mobility is calculated based on the phonon scattering theory. The results indicate that the strain induced potential disturbances might act as scattering centers that affect electron mobility.

1. Introduction

In silicon-based metal-oxide-semiconductor field effect-transistors (MOSFETs), strain engineering has been widely employed to improve electron mobilities in highly scaled devices[1]. However, so far, in SiC-MOSFETs, strain engineering has not been able to effectively improve the electronic transmission performance. Therefore, a fundamental study of the carrier scattering mechanism is needed to understand the relationship between strain at the SiC surface and carrier transport properties in the inversion layer of SiC-MOSFETs.

It is known that strain-induced stress of lattice usually causes the modification of the effective mass and/or variations of the scattering rate, which affects the carrier transport[2]. However, the relationship between the biaxial stress at SiO_2/4H-SiC interface and the electron mobility is still unclear. In addition, due to the potential disturbances induced by the lattice vibration, the stress-induced electron transport is mainly limited by phonon scattering. Thus, in this work, the phonon limited electron mobility was calculated based on the acoustic and optical phonon scattering.

2. Theoretical background

2.1 phonon scattering probability

Using the Fermi golden rule, since the total electrons interact with acoustic phonon by the deformation potential coupling, the scattering probability for intravalley processes (ac) can be given as follows:

$$S_{ac}(k,k`) = \frac{2\pi E^2 k_B T}{V\hbar\rho c_L^2}\delta[\epsilon(k`) - \epsilon(k)] \quad (1)$$

Where E is the deformation-potential tensor, c_L is the longitudinal velocity, ρ is the mass density of the crystal, and V is the volume of the crystal.

For 4H-SiC, where the conduction band minimum occurs at a point either inside the Brillouin zone or at the edge, and there are several equivalent conduction band valleys. In these cases, electrons can be scattered from one valley to another via a large wave-vector phonon. And it has been found to play an important role in phonon-limited electron mobility[3]. The scattering probability for intervalley processes caused by optical phonons (op) is

$$S_{op}(k,k`) = \frac{Z_f \pi D_{if}^2}{V\hbar\omega_{if}}\left(n_{if}^{op} + \frac{1}{2} \mp \frac{1}{2}\right)\delta[\varepsilon_f(k`) - \varepsilon_i(k) \mp \hbar\omega_{if}] \quad (2)$$

Where D_{if} is the intervalley deformation potential (coupling constants), $\hbar\omega_{if}$ is the intervalley phonon energy.

2.2 Boltzmann transport equation in relaxation time approximation

For 4H-SiC, the band minima at the M points one contracts with three full ellipsoids. In an ellipsoidal energy band, both the effective mass and the relaxation time are anisotropic in principle. However, it seems that in the case of 4H–SiC, where the anisotropy of the band is not very conspicuous[4]. Thus, in our calculation, we use the isotropic relaxation time τ dependent on the energy into the scattering term in the Boltzmann transport equation. Therefore, we can relate the relaxation time to the scattering probability $S(k,k`)$, which calculated by using the Fermi golden rule. The relaxation time is given as follows[3]:

$$\frac{1}{\tau} = \int \frac{1-f_0`}{1-f_0} S(k,k`)(1 - \frac{\tau` v` F}{\tau v F})dk` \quad (3)$$

Here, f_0 is the Fermi-Dirac distribution. v is drift electron velocity, and F is electric field strength.

In general, this is a rather complex integral to solve. However, it becomes considerably simplified for certain simple cases. In the case of acoustic phonon scattering, which can be regarded as isotropic parabolic bands and elastic scattering. From Eqs. (1), (3) the relaxation time is represented as

$$\frac{1}{\tau} = \frac{\mathrm{E}^2 \mathrm{k_B T} m_d^{*\,3/2}(2\varepsilon)^{1/2}}{\pi\hbar^4 \rho \mathrm{c_L^2}}. \quad (4)$$

In the case of intervalley optical phonon scattering, from Eqs.

(2), (3) the relaxation time is represented by

$$\frac{1}{\tau}=\frac{Z_f {D_{if}}^2 {m_d}^{*3/2}\left(2\left(\varepsilon \pm \hbar\omega_{if}\right)\right)^{1/2}}{2\pi\hbar^3\rho\omega_{if}}\left(n_\omega+\frac{1}{2}\mp\frac{1}{2}\right) \quad (5)$$

Where $n_\omega = {1}/{exp^{(\hbar\omega/k_BT)}-1}$, ${m_d}^* = (m_1^* m_2^* m_3^*)^{1/3}$ is the density-of-states mass, ε is electron energy, and Z_f is the number of final valleys available for scattering, in our calculation, Z_f=4 for 4H-SiC crystal.

The relaxation time will depend upon the energy of the electron. Thus, it is important to address the appropriate averaging procedure for τ to be used in macroscopic quantities such as mobility. The averaging relaxation time $\langle\tau\rangle$ is given as

$$\langle\tau\rangle=\frac{2}{3k_BT}\frac{\int \varepsilon^{3/2}\cdot\tau\cdot exp-(\frac{\varepsilon}{k_BT})\,d\varepsilon}{\int \varepsilon^{1/2}\cdot exp-(\frac{\varepsilon}{k_BT})\,d\varepsilon}. \quad (6)$$

3. Calculation and conclusions

Normally, electron mobility is calculated using $\mu = e\langle\tau\rangle/m^*$. However, for 4H-SiC, the constant-energy surfaces of 4H-SiC in k-space is an ellipsoid. By averaging all the ellipsoids, the conductivity mass was given as follows,

$$\frac{1}{m_c^*}=\frac{1}{3}\left(\frac{1}{m_x^*}+\frac{1}{m_y^*}+\frac{1}{m_z^*}\right) \quad (7)$$

which was used as the mobility effective mass in electron mobility calculation. In addition, as mentioned before, τ is the relaxation times for an electron having the kinetic energy due to phonon scattering. Thus, through the dependence of τ on m_d^*, the phonon-limited electron mobility in the stress relaxed 4H-SiC crystal is represented by Eqs.(4), (5), (6) and (7).

$$\mu=\frac{e\cdot\langle\tau(m_d^*)\rangle}{m_c^*} \quad (8)$$

Where the density of states mass defined as ${m_d}^* = (m_{M\Gamma}^* m_{MK}^* m_{ML}^*)^{1/3}$ for the directions ($M\rightarrow\Gamma$, $M\rightarrow K$ and $M\rightarrow L$). $m_c^* = 2(\frac{1}{m_{M\Gamma}^*}+\frac{1}{m_{MK}^*})^{-1}$ is the conduction-band effective mass of the in-plane ($M\rightarrow\Gamma$, $M\rightarrow K$).

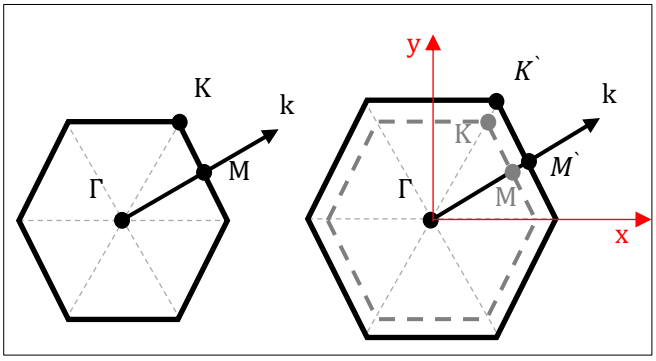

Fig. 1. First Brillouin zone and changes upon biaxial stress. Left: the equilibrium hexagonal first Brillouin zone and the special k-points Γ, M, K. Right: The first Brillouin zone after applying a biaxial stress of in-plane.

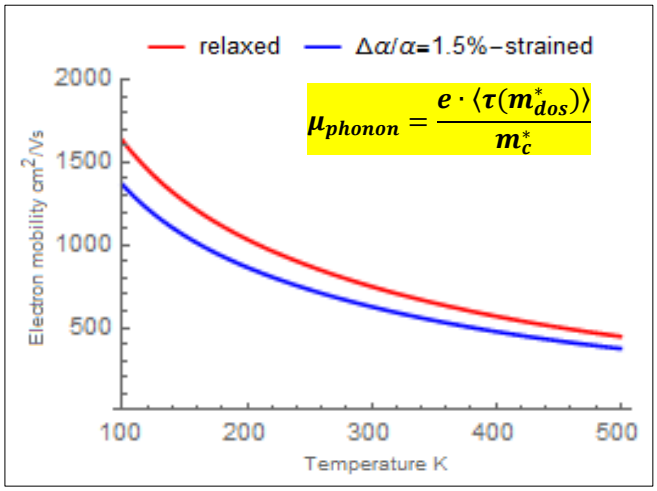

Fig 2 The phonon-limited electron mobility is stated as a function of the temperature of unstrained and strained.

Then, the electron mobility was calculated in the strained 4H-SiC using a strain value as ${\Delta a}/{a} = 1.5\%$ (Δa: the change in the lattice vector). Fig. 1 shows the Brillouin zone in the hexagonal plane for both relaxed case (Left) and strained case (Right). The conduction band minimum for 4H-SiC is located at point M of Brillouin zone. Although the biaxial stress is applied, the crystal symmetry does not change in the x-y plane when the surface is located at c plane. Consequently, the biaxial strain has no effect on lifting the band degeneracy, since the states are all on the x-y plane. However, the band-gap reduction for biaxially strained SiC has been reported as $\Delta E_{gap} = -0.04eV$ for ${\Delta a}/{a} = 1.5\%$.[5] Fig 2 displays the electron mobilities of relaxed and strained SiC as a function of temperature. A significant reduction in the electron mobility in strained SiC has been evident from the figure. Although the experimentally obtained strain value at the SiO_2/SiC interface is much smaller than 1.5%, yet the strain induced potential disturbances might act as scattering centers to affect the electron mobility in Fig. 2.

References

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