Full band Monte Carlo analysis of the uniaxial stress impact on 4H-SiC high energy transport

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Abstract **--- SiC is expected to be the next-generation semiconductor material especially for power devices, and some have been put into practical use. However, its stress response has not been completely elucidated, and there are concerns about performance degradation by mechanical stress in the wafer process and packaging. On the other hand, stress engineering may improve its performance.**

So, in this paper, we estimate the uniaxial stress impact on 4H-SiC by combination of first principal calculation and full-band Monte Carlo simulation. As a result, it was found that the stress dependence of the impact ionization coefficient of 4H-SiC is extremely small, and the risk of breakdown voltage degradation is low by small stress in manufacturing process. On the other hand, the electron mobility increases when tensile stress is applied, and it is expected that the device on-resistance will be reduced by stress engineering.

I. INTRODUCTION

In recent years, the demand for semiconductor devices capable of highly efficient power control has been increasing due to the electrification of automobiles and the increase in the amount of communication in data centers. However, conventional Si power devices have reached the limit of performance due to their physical characteristics, and it is difficult to dramatically improve their performance. So, next-generation power materials such as SiC, GaN and GaO are attracting attention because these materials have wide bandgap and higher dielectric breakdown electric field strength than Si and enhance the performance of power semiconductor device.

To predict characteristics of power devices in high electric field, conventional simulations that consider only the physical properties near the bandgap are not sufficient because electrons are transported to high energy bands Therefore, a full band Monte Carlo (FBMC) simulator have been used to discuss electron transport under high electric field [1].

Also, it is well known that stresses induced inside semiconductor devices during the wafer process or packaging affect silicon device performance [2], such as mobility. But there is not enough discussion in the next generation power device materials.

Therefore, in this paper, the impact of the stress on 4H-SiC is investigated by implementing the strained 4H-SiC band structure obtained by the first-principles calculation in the FBMC simulator. We also discuss the possibility of improving device characteristics by stress engineering.

II. METHOD

The band structure (Fig. 2) of 4H-SiC (Fig. 1) used in this paper is calculated by the first-principles calculation tool DMol3 based on the density functional theory (DFT) [3]. Since it is well-known that DFT tends to underestimate the bandgap, the bandgap and the curvature near

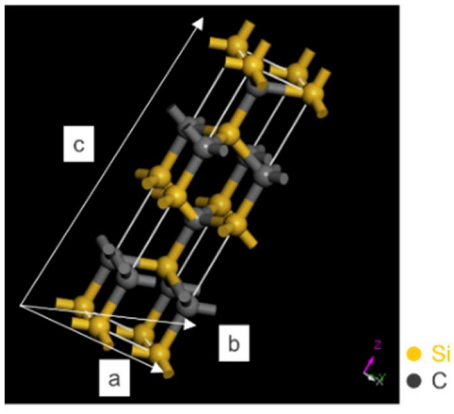

Fig. 1: Primitive cell of 4H-SiC.

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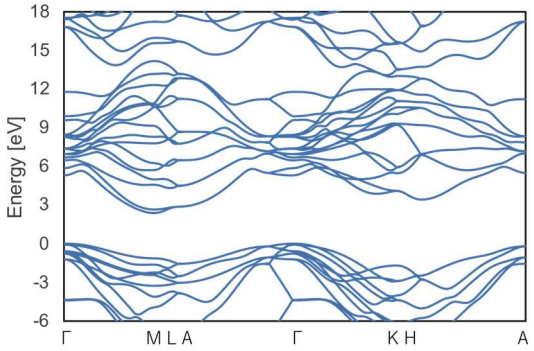

Fig.2 : Band structure of 4H-SiC.

the conduction band bottom are calibrated to match the calculation results of the high-precision first-principles calculation tool ecalj based on a quasiparticle self-consistent GW (QSGW) method [4]. After, calibration it is confirmed that the band structure is almost the same up to the high energy band of about 10 eV from conduction band bottom. This is a sufficient range to consider the electron transport under a high electric field. Then band calculation is performed on the assumption that uniaxial stress is applied in the c-axis direction. Lattice deformation was calculated according to Young's modulus and Poisson's ratio. Table 1 shows the parameters used for first-principles calculation and stress application.

The FBMC simulator used to derive the impact

Table I : Parameter of first-principles calculation.

Lattice constant of 4H-SiC	a=b=0.308nm, c=1.008nm
Young's modulus of 4H-SiC	400GPa
Poisson's ratio of 4H-SiC	0.16
Functional	GGA-PBE
Number of k point	30*30*10
Upper limit of calculation range*	27eV
Lower limit of calculation range*	-14eV

*valance band top is set to be 0eV

ionization coefficient includes scattering mechanisms such as acoustic phonon scattering, non-polar optical phonon scattering, and impact ionization. The impact ionization rate $P_{ii}(E)$ was also calculated through the QSGW method and implemented into the FBMC simulator as a function of the electron energy E by fitting to the Keldysh formula [1] [5]:

$$P_{ii}(E) = \alpha\left(\frac{E - E_{th}}{Eth}\right)^{\beta}\Theta(E - E_{th}) \qquad (1)$$

where Θ is the unit step function, α = 2.0×10^{11} s^{-1}, β = 3.4 and Eth = 3.26 eV.

Acoustic phonon scattering rate $P_{ac}(E)$, and non-polar optical phonon scattering rate $P_{op}(E)$ are given as a function of carrier energy E and bulk density of states $DOS(E)$. These formulae are given in [5] using the density of states calculated from the band structure [1]:

$$P_{op}(E) = \frac{D_{op}^2\hbar}{2\rho E_{op}\pi}\left[N(E_{op}) + \frac{1}{2} \mp \frac{1}{2}\right] * DOS(E \mp E_{op}) \qquad (2)$$

$$P_{ac}(E) = \frac{D_{ac}^2 k_B T}{\rho\hbar V_s^2\pi}DOS(E) \qquad (3)$$

D_{op} and D_{ac} are the acoustic and optical deformation potentials respectively, $\hbar$ is the Planck's constant, ρ is the crystal density, $N(E)$ is the Bose-Einstein distribution, $DOS(E)$ is the density of the states, k_B is the Boltzmann's constant, T is the lattice temperature, and v_s

Table II : Simulation parameters of FBMC.

α	2.0×10^{11} s^{-1}
β	3.4
E_{th}	3.26 eV
D_{op}	3.9×10^{10} eV/cm
D_{ac}	19 eV
E_{op}	85 meV
ρ	3.2 g/cm^3
v_s	1.4×10^6 cm/s
T	300 K

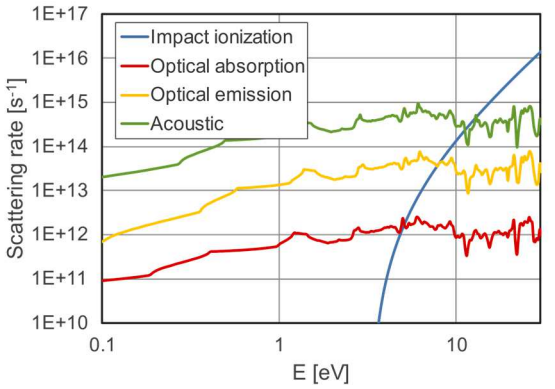

Fig.3: Energy dependence of scattering rate.

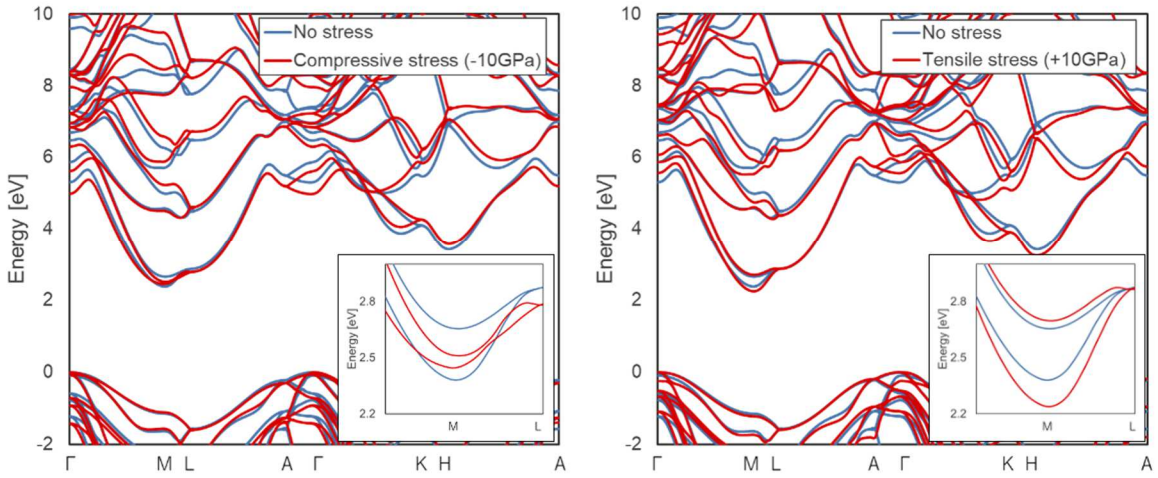

Fig.4: Band structure change by c-axis stress

is the sound velocity. Table 2 shows the parameters used in the FBMC simulation.

III. RESULTS AND DISCUSSION

Figures 4 shows the c-axis stress dependence of the band structure of 4H-SiC by first-principles calculations. The curvature of the conduction band bottom (M-point) decreases under compressive stress and increase under tensile stress. This indicates that the electron mobility of 4H-SiC under a low electric field improves with tensile stress. The bandgap shows a monotonous decrease in the range of -6GPa to +10GPa, but decreases slightly for compressive stresses exceeding -6GPa (Fig. 5).

Next, we performed FBMC simulations to analyze electron transport using the band structure under c-axis stress. The FBMC calculation results of the impact ionization

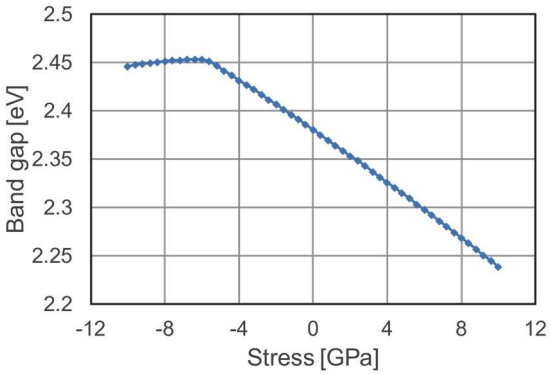

Fig.5: Stress dependence of bandgap.

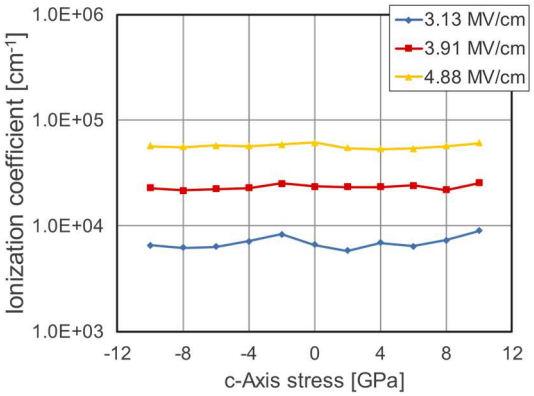

Fig.6: Stress dependence of ionization coefficient at each electric field.

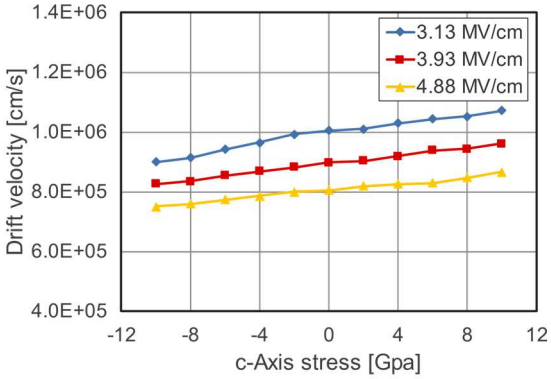

Fig.7: Stress dependence of drift velocity at each electric field.

coefficient under no stress are confirmed to be in good agreement with measured data in the past paper [1].

Figure 6 shows the applied c-axis stress dependence under uniform electric field. Both the electric field and the stress are applied in the c-axis direction. It shows that the stress dependence of the ionization coefficient is extremely small in the range of -10 GPa to 10 GPa. This suggests that the induced stress in a general wafer process and packaging has a negligible effect on the breakdown voltage of SiC device.

Next, the stress dependence of electron drift velocity is shown Fig. 7. The mobility increases in proportion to tensile stress. This can be explained by the change in curvature at the bottom of the conduction band. As shown in the inset in Fig.4, applying stress in the tensile direction increases the curvature and then mobility. This result suggests the possibility of the specific on-resistance reduction of SiC devices with keeping considerable breakdown voltage by c-axis stress engineering

IV. CONCLUSION

FBMC simulation has shown that the impact ionization coefficient of 4H-SiC has quite small stress dependence, so the breakdown voltage of the SiC power device is quite robust against the stress induced during the wafer process or the packaging. It is also found from the first principles calculation and the FBMC calculation that when tensile stress is applied in the c-axis direction of 4H-SiC, the curvature of the band increases, and therefore the electron mobility increases. So specific on-resistance can be reduced by appropriate device design with stress engineering.

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