Emprirical Pseudopotential Calculations of Two-dimensional Electronic States in 4H-SiC Inversion layers

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Abstract—**Two-dimensional electronic states in inversion layers of 4H-SiC metal-oxide-semiconductor field-effect transistor have been calculated by taking account of the realistic band structure based on empirical pseudopotential method. It is found that the in-plane effective mass for electrons significantly increases under the strong confinement conditions in the case of (0001) oriented substrate. This modulation is attributed to the strong nonparabolicity effect confirmed in the *E-k* relation of bulk 4H-SiC along M-L direction.**

Keywords-Silicon Carbide; bandstructure; empirical pseudopotential method; subband energy; effective mass

I. INTRODUCTION

4H-SiC MOSFETs have been attracting great attention for the use of high-voltage power device applications because of the large band gap (3.26 eV) and a large critical electric field (3 MV/cm). The SiC based metal-oxide-semiconductor field-effect transistor (MOSFET) is a unipolar device enabling operation at higher switching frequencies than the silicon IGBT. However, the inferior channel mobility at the MOS interface is one of the serious issues to improve the power efficiency. The origin has been attributed to the poor quality SiO_2-SiC interface, and thus not many theoretical works have been reported so far for the 2D electronic states in ideal 4H-SiC inversion layers. Pennington et al. has presented the detailed study on the inversion layer properties based on the parabolic band effective mass approximation (EMA) [1]. However, they have also pointed out the concern about the limitation of EMA particularly for the case of (0001) orientation, because of the large lattice constant (c = 9.928 A) along the confining direction. In this work, we investigate the 2D electronic states in 4H-SiC inversion layers based on empirical pseudopotential (EP) approach, and discuss the nonparabolicity effects on the quantum confinement.

II. CALCULATION METHOD AND RESULTS

Although there have been several reports on EP calculations for the bulk 4H-SiC [2, 3], we have created a new parameter set. The analytical form of EP given in [4] was assumed for Si and C atoms:

$$V_{atom}^{ps}(q) = \frac{a_1(q^2 - a_2)}{a_3 \exp(a_4 q^2 - 1)}$$

where q is the wave number and a_1, a_2, a_3, and a_4 are the fitting parameters determined to obtain the accurate *E-k* curves especially focusing on the lowest two conduction bands. The EPs for Si and C atoms are plotted in Fig. 1, which well reproduce the experimentally obtained energy transitions and effective masses for bulk 4H-SiC [5-9] as shown in TABLE I. We have also confirmed the good agreement between the *E-k* curves obtained with the EP method and *ab initio* calculation using CASTEP code [10] as shown in Fig. 2.

Figure 3 shows the contour plot of the bulk band structure on the cross-sections containing the conduction band minima at M point. In this study, we have calculated the 2D electronic states confined along M-L and M-K directions to investigate the subband structures in MOS inversion layers for (0001) and $(11\bar{2}0)$ oriented substrates, respectively. By using the bulk energy dispersion relationship and the pseudo wavefunctions, the subband structures confined in the triangular potential wells with various electric fields were calculated [11]. As schematically illustrated in Fig. 4, we have taken into account the confinement potential in addition to the Si and C pseudopotentials, and solved the Shrödinger equation

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V_{LP}(\mathbf{R}) + U(z)\right\}\Psi(\mathbf{R}) = E\Psi(\mathbf{R}),$$

where $\hbar$ is the Planck constant, m is the electron mass, $\mathbf{R}$ is the three-dimensional position vector, $V_{LP}(\mathbf{R})$ is the lattice potential calculated with the EPs. $U(z)$ is the one-dimensional confining potential normal to the 4H-SiC/SiO_2 interface. The periodic boundary condition was applied along z direction with period of 120 x (lattice constant). The wave function $\Psi(\mathbf{R})$ was expanded with the pseudowavefunctions for the

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bulk states

$$\Psi(\mathbf{R}) = \sum_{K,n} c^n_K \psi^n_K(\mathbf{R}),$$

where $\Psi^n_{\mathbf{K}}(\mathbf{R})$ is the pseudowavefunction with the band index n and wave vector $\mathbf{K}$, and $c^n_{\mathbf{K}}$ is the expansion coefficient. In the present calculation, we have considered the lowest energy two conduction bands for the summation with respect to n.

Figures 5-6 shows the calculated results. Although the similar subband energies were obtained between EMA and EP method (see Fig. 5), the significant modulation of the E-k curve along M-Γ, i.e., the effective mass $m^*_{\text{M-}\Gamma}$, was found in EP results for (0001) orientation under the strong confinement conditions as shown in Figs. 6 and 7. Note that m^* perpendicular to the confining direction is not changed in parabolic EMA. This observation could be attributed to the nonparabolicity effect [12]; note that, in Fig. 2, the lowest conduction band along M-L exhibits narrow band width and strong nonparabolicity, which would originate from the relatively large lattice constant along c-axis. It has been experimentally observed that $(11\bar{2}0)$ shows better mobility than (0001) orientation, which was explained by the superior interface quality [13]. This work suggests that even if the ideal interface is obtained, (0001) orientation would have a disadvantage in terms of the conductivity effective mass.

III. Conclusion

The electronic states in the inversion layers of 4H-SiC MOSFETs have been calculated based on the empirical pseudopotential method. It has been found that the in-plane effective mass significantly increases under the strong confinement conditions in the case of (0001) orientation, while less change was confirmed for $(11\bar{2}0)$ oriented substrate. This modulation could be attributed to the strong nonparabolicity effect confirmed in E-k relation of bulk 4H-SiC along M-L direction. We believe that this might be one of the origins for the experimental observation indicating the inferior mobility of the (0001) substrate compared to the case of the $(11\bar{2}0)$ orientation.

Acknowledgement

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TABLE I. Energy Transitions at High Symmetry Points, and Effective Masses of 4H-SiC Calculated in This Work Compared to Experimental Data.

Energy Transitions (eV)

	E_g	ΔE	Γ	M	K	L
Expt.	3.26[5]	0.14[6]	6.18[7], 6.2[8]	4[8], 4.5[7]	7.8[8]	6.7[8]
This work	3.18	0.14	6.0	5.0	7.5	5.9

Effective masses (m_0)

	$m^*_{M\Gamma}$	m^*_{MK}	m^*_{ML}
Expt.	0.58[9]	0.29[9]	0.34[9]
This work	0.58	0.29	0.34

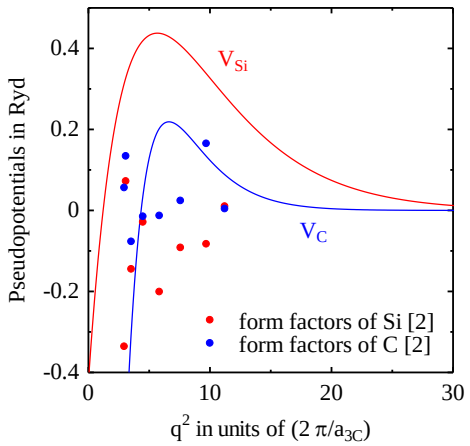

Figure 1. Atomic model potential of Si and C used in this study (lines). We have assumed the continuous analytical form of EP[4]. and 8 parameters for $V_{Si}(q)$ and $V_C(q)$ were determined through the fitting procedure. The form factors given in [3] are also plotted (dots).

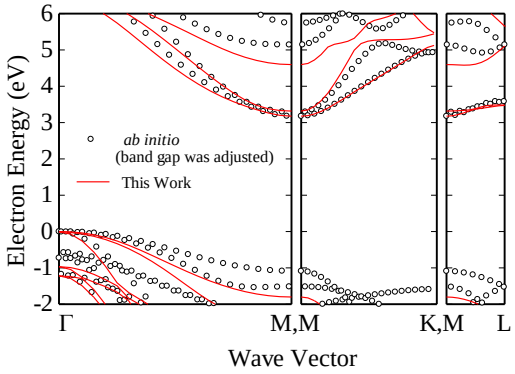

Figure 2. Energy bands of bulk 4H-SiC calculated with EP method and *ab initio* method (using CASTEP)

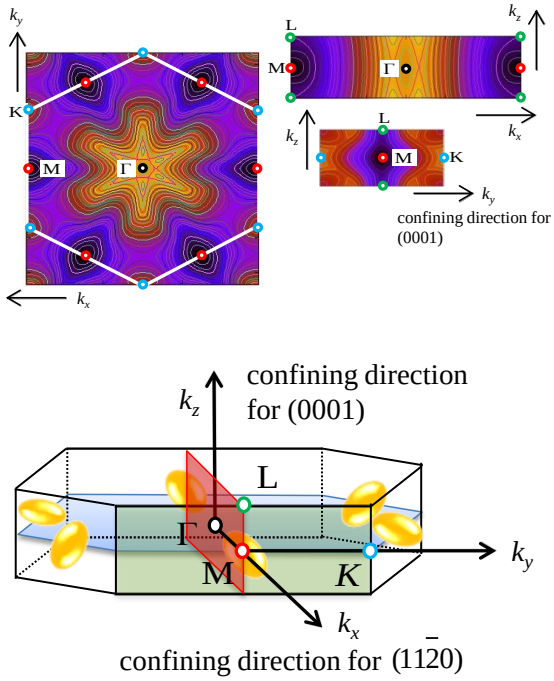

Figure 3. Schematic view of the 1st Brillouin zone of 4H-SiC and the location of the conduction band minima at M-point. The contour plots of the bulk energy dispersion relations calculated with EP method are also shown. In this study, the quantum confinement along M-L direction (for(0001) orientation) and M-K direction (for $(11\bar{2}0)$ direction) was considered.

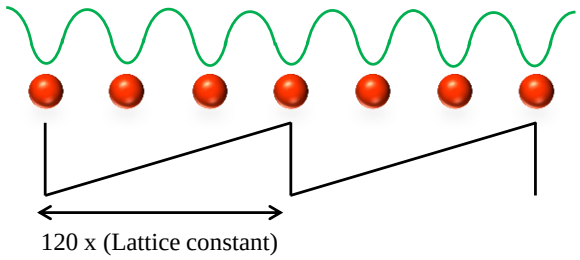

Figure 4. Calculation method of the quantized electron states based on EP method [5]. The Schroedinger equation taking account of the periodic potential of the lattice $V_{LP}(\mathbf{R})$ and the external confining potential $U(z)$ was solved by expanding with the pseudo wave functions. In this study, we assumed the periodic triangular potential well for $U(z)$.

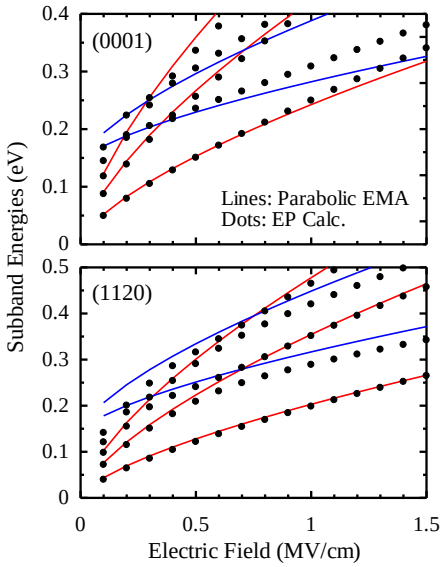

Figure 5. Subband Energies for (0001) and $(11\bar{2}0)$ orientations as a function of the confining electric field. The lowerst 5 subbands are shown. For comparison, the results of parabolic EMA are also plotted (red lines: originated from the lowert conduction band, blue lines: originated from the second lowest conduction band).

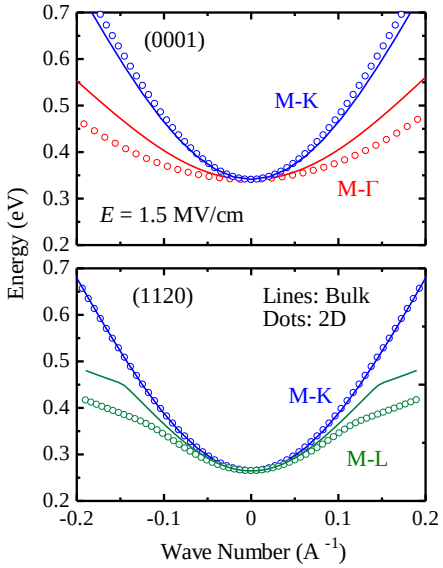

Figure 6. *E-k* curves of the lowest energy band around the bottom of M valley. The results of 2D electronic states for (0001) and $(11\bar{2}0)$ orientations are compared with the bulk dispersion curves along the two principal axes. The confining electric field is 1.5 MV/cm.

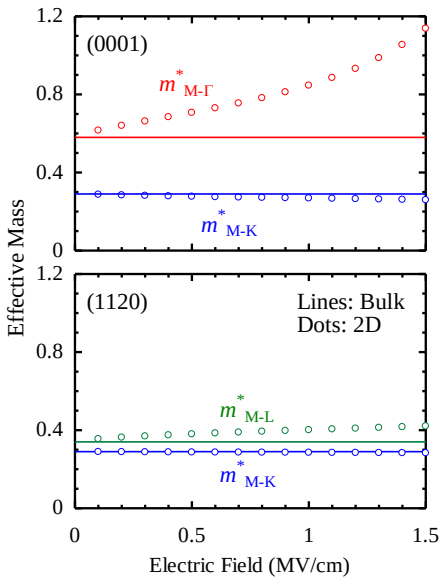

Figure 7. Effective masses of the lowest energy band at the bottom of M valley plotted as a function of the confining electric field. The results of 2D electronic states for (0001) and $(11\bar{2}0)$ orientations are compared with the bulk effective masses.

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