Electronic States in 4H-SiC MOS Inversion Layers Considering Crystal Structure Using Empirical Pseudopotential Method

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4H-SiC MOSFETs have been attracting attention as a power switching device realizing high breakdown voltage and low on-resistance. A recent ab initio simulation revealed that the electronic states at the conduction band minimum (CBM) of SiC consist of the floating electron states [1], which distribute not near atomic sites, but in internal channel space. This feature is ignored in the effective-mass approximation. In this study, to analyze the electronic states in 4H-SiC MOS inversion layers taking account of this feature, we described the crystal structure of 4H-SiC including the internal channel space using the empirical pseudopotential method, and we calculated the electronic states in the triangular potential well.

We first obtained the empirical pseudopotential of bulk 4H-SiC. The pseudopotential of bulk 4H-SiC is described by the pseudopotentials of Si and C atoms arranged according to the crystal structure of 4H-SiC. Then, by arranging these pseudopotentials of each atom in a slab structure, we described the pseudopotential of a 4H-SiC slab. In the empirical pseudopotential method, the plane wave expansion is usually employed. In this study, however, we adopted real-space discretization for the thickness direction, while the plane wave expansion is used for the in-plane directions. To model the confinement of electrons at the MOS interface, we applied triangular potential determined by a uniform electric field to the 4H-SiC slab described above.

The empirical pseudopotential of bulk 4H-SiC and the calculated probability density distribution of the electronic states at the CBM are shown in Fig. 1. The feature of the floating electron states [1] is confirmed. Fig. 2 shows the model of the 4H-SiC slab adopted in this study. In the positive and negative directions of z-axis, there are surfaces terminated with C and Si atoms, respectively, with the latter set to $z = 0$. Fig. 3 shows the pseudopotential of 4H-SiC slab described using the above method. We applied a uniform electric field to the 4H-SiC slab to make the Si-terminated surface be the bottom of the potential. Fig. 4 shows the probability density distribution of the state at the CBM with a 0.8 MV/cm electric field. The feature of the floating electron states appeared also in this case, while the state is confined near the Si-terminated surface. Fig. 5 shows the dependence of effective-mass on applied electric field. As the electric field increases, $m_{\mathrm{M\Gamma}}$ increases, and m_{MK} decreases. These trends can be explained by the nonparabolicity of the band structure of bulk 4H-SiC. The results suggest that our methodology can describe the 4H-SiC MOS inversion layers taking account of the floating electron states and the band structure beyond the effective-mass approximation.

[1] Y.-I. Matsushita *et al.*, *PRL* **108**, 246404 (2012). [2] Y.-I. Matsushita *et al.*, *JPSJ* **86**, 054702 (2017).

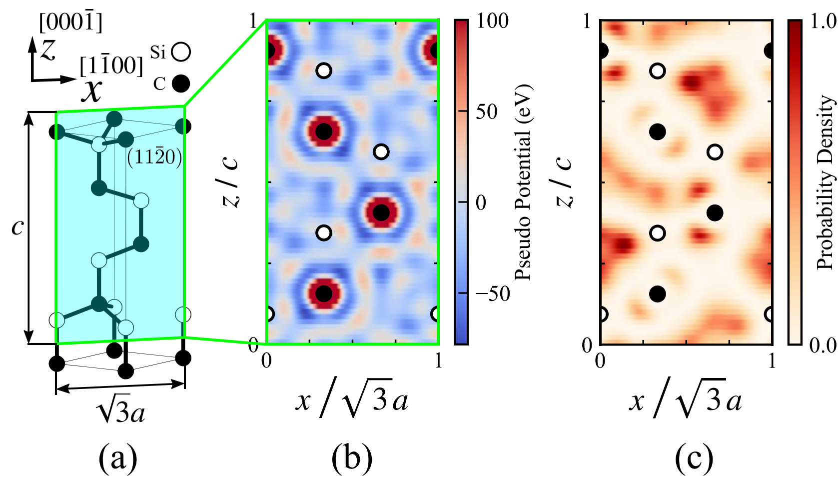

Fig. 1: (a) The primitive unit cell of 4H-SiC. c is the length of a unit cell in the [0001] direction. a is the distance between adjacent Si (or C) atoms. We set c = 1.008 nm and a = 0.3081 nm in this study. The blue plane is the $(11\bar{2}0)$ plane that is parallel to [0001] and $[1\bar{1}00]$ directions. On this plane, we defined x and z axes along the $[000\bar{1}]$ and $[1\bar{1}00]$ directions, respectively. (b) The pseudopotential distribution of bulk 4H-SiC on the $(11\bar{2}0)$ plane. (c) The probability density distribution of the state at the conduction band minimum of bulk 4H-SiC calculated with the empirical pseudopotential method.

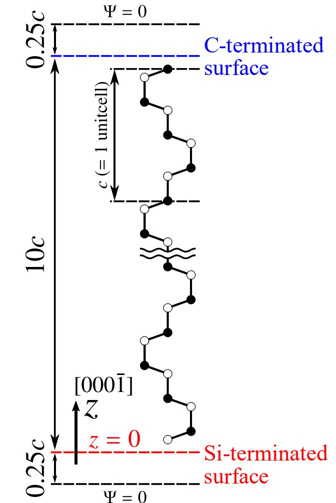

Fig. 2: The structure and dimensions of the 4H-SiC slab. The thickness direction is along the $[000\bar{1}]$ direction. The structure includes a $10c$-thick 4H-SiC slab and $0.25c$-thick vacuum regions terminated by the boundary conditions with the wavefunction Ψ set to zero.

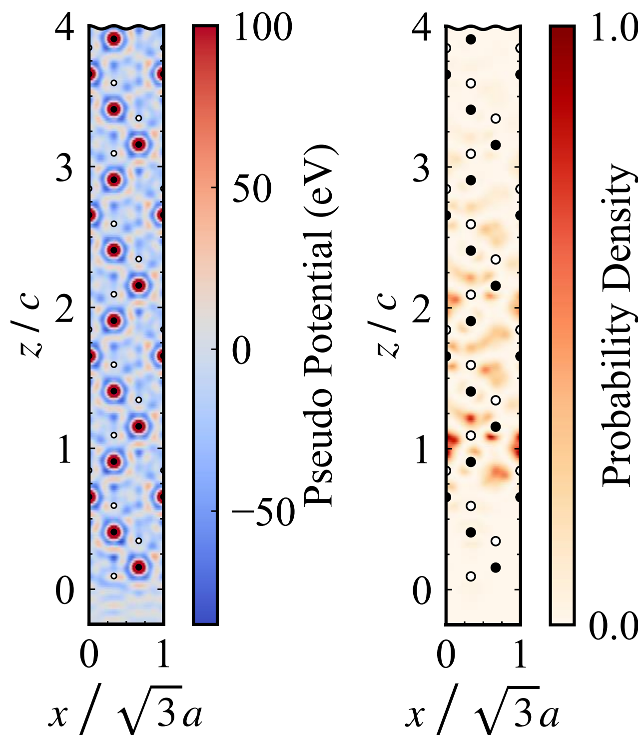

Fig. 3 (left): The pseudopotential distribution of the 4H-SiC slab on the $(11\bar{2}0)$ plane. Only the area near the Si-terminated surface is shown. The pseudopotential of atoms extends into the vacuum region.

Fig. 4 (right): The probability density distribution of the state at the conduction band minimum of the 4H-SiC slab with an electric field of 0.8 MV/cm .

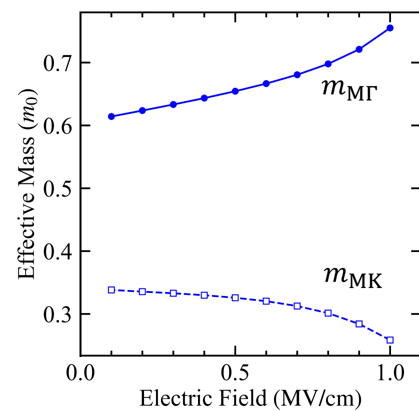

Fig. 5: The dependence of effective-masses at the conduction band minimum of the 4H-SiC slab on the applied electric field. $m_{\mathrm{M\Gamma}}$ and m_{MK} are the effective masses along the MΓ and MK directions, respectively. As the electric field increases, $m_{\mathrm{M\Gamma}}$ increases, and m_{MK} decreases. These trends are consistent with the change in effective mass with increasing wavenumber in the z direction in the E-k dispersion of bulk 4H-SiC.

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