Effective masses of two-dimensional electron gases around cubic inclusions in hexagonal silicon carbide

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The main purpose of this article is to determine the two-dimensional effective mass tensors of electrons confined in thin $3C$ wells in hexagonal SiC, which is a first step in the understanding of in-plane electron motion in the novel quantum structures. We have performed *ab initio* band structure calculations, based on the density functional theory in the local density approximation, for single and multiple stacking faults leading to thin $3C$-like regions in $4H$- and $6H$-SiC and deduced electron effective masses for two-dimensional electron gases around the cubic inclusions. We have found that electrons confined in the thin $3C$-like layers have clearly heavier effective masses than in the perfect bulk $3C$-SiC single crystal.

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I. INTRODUCTION

Recently, some SiC-based unipolar devices have been commercialized. On the other hand, when examining the reliability of $4H$-SiC pin diodes in long-term operations, the electronic degradation problem in connection with the occurrence of structural defects was discovered; the diodes degraded gradually during operation,[1] and the timing of the degradation coincided with the expansion of stacking faults (SF's) in the basal planes.[2] Then we revealed that certain types of SF's in $4H$- and $6H$-SiC can give rise to electrically active states in the fundamental band gap, which are strongly localized around the SF's.[3–7] More or less simultaneously, Miao *et al.* also came to a similar conclusion about SF-related interface states in SiC.[8] We interpreted these SF-induced gap states as planar quantum wells (QW's), as illustrated in Fig. 1. Because of the large conduction band offsets between the cubic and hexagonal polytypes, $3C$-like sequences can introduce locally lower conduction bands in the host hexagonal crystals.[4–9] They can hence act as QW's for

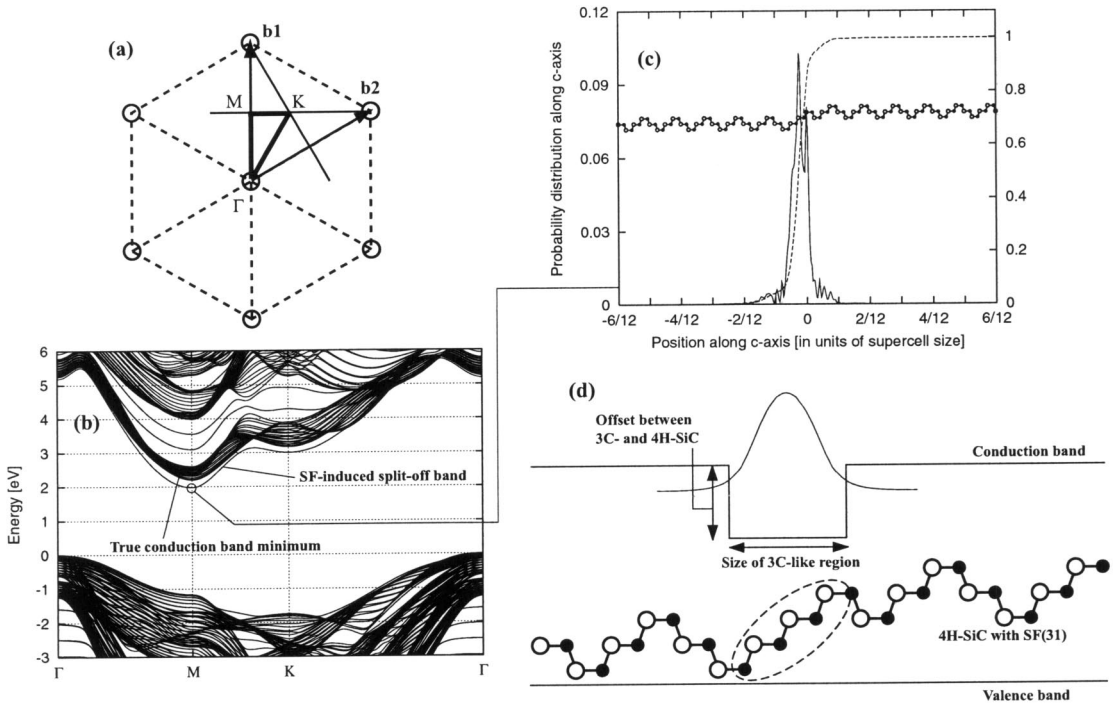

FIG. 1. Schematic illustrations of QW-like features. (a) The 2D irreducible first Brillouin zone and the locations of the Γ, *M*, and *K* points. (b) The 2D band structure of the 96-atom supercell for $4H$-SiC with SF(31). (c) The projected wave function along the *c* axis, $f(z)=\int\int|\psi(x,y,z)|^2 dx\,dy$, for the SF-induced split-off band at the *M* point. (d) A simple QW model for the SF structure. In the figure for the localized wave function, the normalization integral $I(z)=\int^z f(z')dz$ is also shown (right-hand scale), together with the corresponding stacking sequence.

the conduction-band electrons, preventing normal carrier transport in the devices.[1–8]

Such SF's in the pin diodes are expanded by the motion of partial dislocations in the basal planes (see Fig. 2).[1,2,10–15] If a partial, which is almost always from the glide set, propagates through the single crystal, the partial leaves behind an error in the stacking pattern. It is believed that a dominant energy source for the dislocation motion is the large electron-hole recombination energy, since in any of the SiC-based unipolar devices, the SF expansion has not yet been observed. Electron-hole plasmas are injected in bipolar devices, while there are no such plasmas in unipolar devices such as Schottky diodes. Another important material property to help the occurrence of SF's is its extremely small SF energy;[16] the polytypism of SiC is probably a natural consequence of the small SF energy. For example, according to our calculations,[6,7,16] the SF energy of 6*H*- and 4*H*-SiC is around 3 and 18 mJ/m^2, respectively, while that of Si and diamond is around 33 and 260 mJ/m^2, respectively. Our calculations are close to available experimental data.[17,18] Besides, it was suggested by Miao *et al.* that the QW nature of SF's in SiC can be a driving force for the SF expansion. The system can lower its energy by a transition of the conduction-band electrons into the QW state around SF's, and thus the expansion of SF's takes place through a capture of more conduction-band electrons into the locally lower conduction bands around 3*C*-like regions.[8] This model was evaluated by Kuhr *et al.*[19] and it was found that the QW action seems to be a plausible mechanism for the occurrence of double-SF structures in heavily doped *n*-type 4*H*-SiC, but the effect is expected to be too small to account for the SF expansion in the pin diodes in which the concentration of free electrons is not sufficiently high.[19,20] However, their arguments are based on the equilibrium property of the conduction-band electrons, and the situation in the pin diodes during high-current operations certainly deviates from the equilibrium state. The dynamic properties of the conduction band electrons inside the QW's may play an important role for understanding of the SF expansion mechanism under forward bias. The behavior of the two-dimensional (2D) electron gases around SF planes can be essentially characterized by their in-plane electron effective mass tensors.

Apart from the mechanism of dislocation glide to create 3*C*-like faulted regions, it is, of course, possible to have such SF's during crystal growth. Also, a few attempts to grow artificial QW's or superlattices composed of SiC only have been made, aiming at future nanotechnology application.[9,21–24] Fissel *et al.* have recently reported the controlled growth of SiC heteropolytypic structures such as 4*H*/3*C*/4*H*-SiC or 6*H*/3*C*/6*H*-SiC by solid-source molecular-beam epitaxy.[21,22,24] To understand the dynamical properties of these 3*C* QW's, a detailed knowledge of the *E*-*k* dispersion for the QW states is of importance.

In this work, we therefore calculate the effective masses of electrons confined in narrow 3*C* inclusions in 4*H*- and 6*H*-SiC (Ref. 25) based on the density functional theory in the local density approximation (DFT-LDA) and discuss some related phenomena. Our calculated in-plane effective mass tensors for the one-dimensionally localized electronic states around cubic inclusions are essential for the precise interpretations of electrical or optical measurements about these planar defects in SiC, investigations of 2D electron transport through these novel quantum structures,[26] etc.

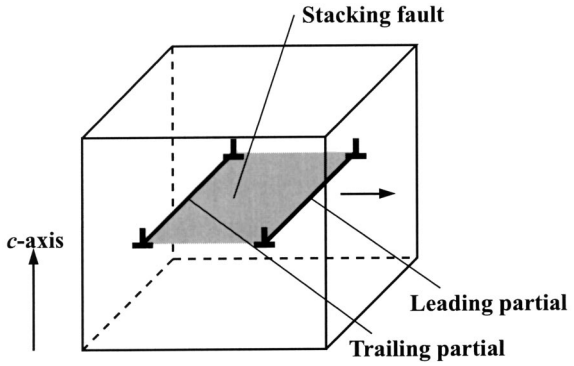

FIG. 2. Schematic illustration of a pair of dissociated partial dislocations in the basal plane. The leading partial leaves behind a SF and the trailing partial removes it when the extended dislocation propagates from left to right in the crystal.

II. COMPUTATIONAL METHOD AND STRUCTURAL MODEL

We model the properties of thin 3*C* QW's in 4*H*- and 6*H*-SiC single crystals using 96-atom supercells.[4–7,27,28] These supercells are expected to be sufficiently large to extract the essential information of such planar defects. A detailed description of the numerical method is given in Ref. 7.

We assume that the ideal SF's repeat after 48 bilayers along the *c* axis and spread infinitely perpendicular to the *c* axis, while in reality SF's are usually isolated and bounded by two Shockley partial dislocations as shown in Fig. 2. Our supercells give rise to a nearly 2D first Brillouin zone, in which the *E*-*k* dispersion along the *c* direction almost disappears while there still remains the complete dispersion parallel to the basal plane. One can thereby define 2D effective mass tensors along the (0001) basal plane—i.e., $m^*_{M\text{-}\Gamma}$ and $m^*_{M\text{-}K}$, as shown in Fig. 3. This is not merely a consequence of the use of periodic boundary conditions. In fact, most SF's in degraded diodes penetrate large portion of the devices, and thus the essence of such SF's can be reproduced. Also, the

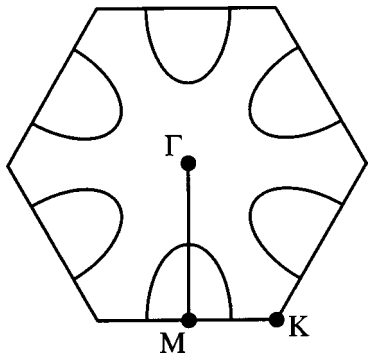

FIG. 3. Constant-energy surfaces in the first Brillouin zone for the 2D electron gas around a 3*C*-like region.

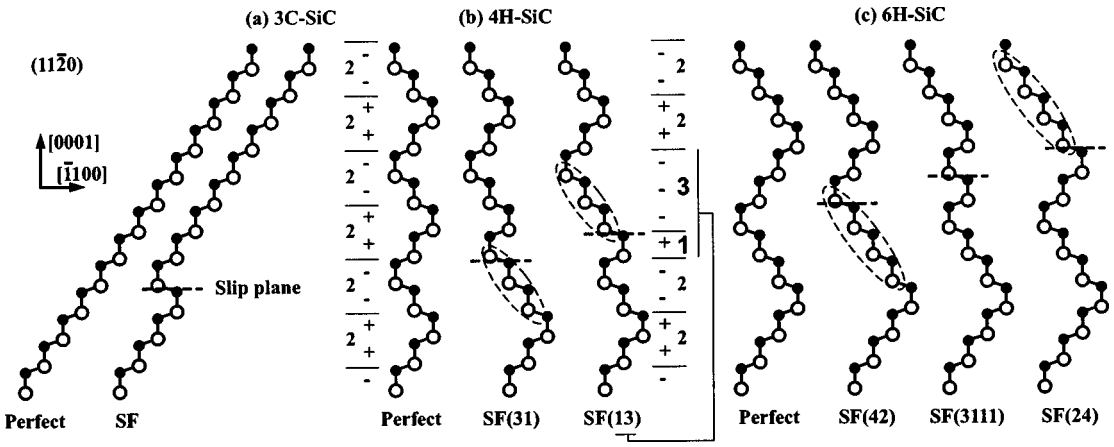

FIG. 4. Geometrically distinguishable SF's in 3*C*-, 4*H*-, and 6*H*-SiC. The 3*C*-like sequences indicated by the solid curves can act as planar QW's for the conduction-band electrons. The notation system is briefly described using perfect 4*H*-SiC and 4*H*-SiC with SF(13). A detailed description for the notation of these SF's is given in Ref. 7.

nature of the artificial SiC QW's based on heteropolytype structures[21–24] can be represented by our theoretical scheme.

In the present study, we restrict the structures of narrow cubic-like sequences to the dislocation-induced type which can be introduced by the motion of a single or several partial dislocations in adjacent planes, but most concepts and conclusions should be equally applicable to the grown-in-type SF's or the artificially grown 3*C* QW's. As was already published by us,[4–7] there exist two and three geometrically distinguishable SF's of the glide type in 4*H*- and 6*H*-SiC, respectively (see Fig. 4). Both SF's in 4*H*-SiC and two types out of three in 6*H*-SiC result in QW's. Pirouz and Yang suggested that the propagations of partial dislocations with the same Burgers vector in neighboring basal planes lead to a local hexagonal→cubic solid phase transition.[29] We thereby employ this scheme and construct the cubic inclusions in 4*H*- and 6*H*-SiC corresponding to two, three, and four SF's in the neighboring basal planes—i.e., 2SF(62), 3SF(71), and 4SF(10,2) in 4*H*-SiC (Ref. 27) and 2SF(51), 3SF(93), and 4SF(10,2) in 6*H*-SiC (Ref. 28) (see Fig. 5).

Our infinite crystals for perfect and faulted structures are constructed from the positions of 96 atoms in each supercell and the translation vectors:

$$\mathbf{a}_1=(a,0,0),$$

$$\mathbf{a}_2=(-a/2,a\sqrt{3}/2,0),$$

$$\mathbf{a}_3=(x,y,c_s), \tag{1}$$

where a is the conventional lattice constant for hexagonal crystals and c_s is, in this case, 12 (8) times the corresponding lattice constant c for the primitive unit cell of 4*H*-SiC (6*H*-SiC). The coordinate (x, y) needs to be modified according to the faulted structures in order to avoid unnecessary SF's at the borders of the supercells—i.e., (x,y)

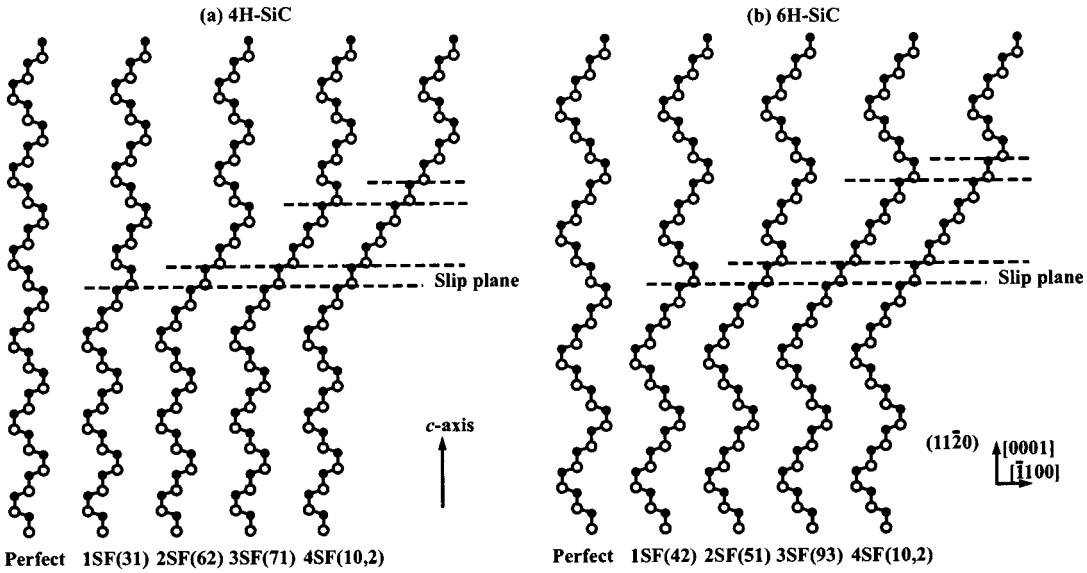

FIG. 5. Cubic inclusions introduced by the motion of partial dislocations in adjacent planes in the *c* direction: (a) 4*H*-SiC and (b) 6*H*-SiC. 1SF(31) [1SF(42)] is identical to SF(31) [SF(42)] in Fig. 4, but rotated by 180° around the *c* axis.

TABLE I. Electron effective masses for the perfect $3C$, $4H$, and $6H$ polytypes along Γ-M and M-K in the hexagonal reciprocal space (in units of free-electron mass m_0), from cyclotron resonance (CR), density functional theory (DFT), and Hall effect (HE).

		$3C$-SiC		$4H$-SiC		$6H$-SiC	
		M-Γ	M-K	M-Γ	M-K	M-Γ	M-K
CR	(Ref. 40)			0.58	0.31		
	(Refs. 38 and 39)			0.42[a]		0.42[a]	
DFT	(Ref. 31)	0.42	0.24				
	(Ref. 32)			0.58	0.28	0.77	0.24
	(Ref. 33)			0.57	0.28	0.75	0.24
HE	(Ref. 44)			0.58	0.30	0.75	0.24

[a]Average value $[m^*_{M\text{-}\Gamma} m^*_{M\text{-}K}]^{1/2}$.

$=(0,0)$ for $q=0,3,6,...$, $(x,y)=(-a/2,a\sqrt{3}/6)$ for $q=1,4,5,...$, and $(x,y)=(a/2,-a\sqrt{3}/6)$ for $q=2,5,8,...$, where q is the number of SF's in the 96-atom supercell ($q=0$ stands for the perfect structure). From the three translation vectors in Eq. (1), one can readily determine the reciprocal translation vectors $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$. In the present work, we calculate the Kohn-Sham eigenvalues along the closed path: $\mathbf{0}\rightarrow 1/2\mathbf{b}_1\rightarrow 1/3(\mathbf{b}_1+\mathbf{b}_2)\rightarrow\mathbf{0}$ corresponding to $\Gamma\rightarrow M\rightarrow K\rightarrow\Gamma$ in the hexagonal symmetry. Thereby, when $(x,y)\neq(0,0)$, the planes spanned by this path are slightly tilted, and consequently, the effective masses determined—i.e., the E-k dispersion for these planes—do not correspond exactly to the electrons running parallel to the real-space basal planes in the crystals, in a rigorous sense. However, if the lattice constant c_s is sufficiently large, such influence on the calculated effective masses becomes negligibly small. Indeed, the 96-atom supercell is very long along the c axis and we can therefore regard our computational scheme to be very close to the case where the tilt of the c axis can be neglected; the first Brillouin zone becomes a flat hexagon parallel to the real-space basal plane when $c_s\rightarrow\infty$.

Since we have found that the intrasupercell atomic relaxations have negligible influence on the Kohn-Sham band structures,[4–7] such relaxations have not been performed in the present work: i.e., no atom in the supercell is allowed to displace from its ideal position.

III. PREVIOUSLY DETERMINED IN-PLANE ELECTRON EFFECTIVE MASS TENSOR IN SiC

Electron effective masses are relatively well-established material parameters in SiC.[30] The electron effective mass tensors in $4H$- and $6H$-SiC have been calculated based on the DFT by several groups,[31–34] the calculated values being very similar to each other. Also, such calculations are in very good agreement with cyclotron resonance experiments.[35–43] However, the values of the electron effective mass in $6H$-SiC along the c axis seem to scatter widely depending on the theoretical methods or experimental conditions employed, perhaps because of the camel's back structure of the conduction band in $6H$-SiC along the c axis (M-L).[32–34,41] The in-plane effective mass components in $6H$-SiC, $m^*_{M\text{-}\Gamma}$ and $m^*_{M\text{-}K}$, have not yet been resolved by cyclotron resonance, but only the in-plane average value $[m^*_{M\text{-}\Gamma} m^*_{M\text{-}K}]^{1/2}$ has been obtained.[39] The scattered values of $m^*_{M\text{-}L}$ in $6H$-SiC, however, need not be considered, because in the present study we are interested in the in-plane masses only. About the unresolved in-plane mass in $6H$-SiC, only recently have the two in-plane components been resolved through the interpretation of a Hall effect measurement.[44–47] In Ref. 44, the average in-plane mass $[m^*_{M\text{-}\Gamma} m^*_{M\text{-}K}]^{1/2}$ determined by a cyclotron resonance experiment[39] was resolved into $m^*_{M\text{-}\Gamma}$ and $m^*_{M\text{-}K}$ by taking advantage of the anisotropy of the electron Hall mobility.[47] To summarize, the in-plane electron effective masses, $m^*_{M\text{-}\Gamma}$ and $m^*_{M\text{-}K}$, in $4H$- and $6H$-SiC have been determined by first-principles calculations, cyclotron resonance experiments, and Hall effect measurements, and they can be very well reconciled with each other.

For comparison, we also have to know the in-plane electron effective mass tensor of $3H$-SiC, if regarded as having hexagonal symmetry with six atoms in the primitive unit cell. Such a 2D mass tensor was calculated by Käckell *et al.*[31] and the calculated values, after a proper transformation, were almost identical to the values from cyclotron resonance measurements of $3C$-SiC.[35–37]

The situation is summarized in Table I. These already established values are vital to judge and justify the accuracy of the present calculation, since, as is well known, the DFT-LDA method is a ground-state theory, hence offering no guarantee at all about any aspects of excited states, like electron or hole effective masses.

IV. RESULTS AND DISCUSSIONS

As was already reported by us,[4–7,25–28] SF(13) and SF(31) in $4H$-SiC and SF(24) and SF(42) in $6H$-SiC introduce split-off bands below their conduction bands due to the QW confinement effect. The cubic inclusions with two SF's in $4H$- and $6H$-SiC also lead to split-off bands corresponding to the ground state in the QW's (principal quantum number $n=1$), but the $3C$-like layers created by three and four SF's in both $4H$- and $6H$-SiC in adjacent planes as shown in Fig. 5 result in two split-off bands ($n=1$ and $n=2$).[27,28] The positions of these localized split-off bands are listed in Table II. Our theoretically determined values seem to be consistent

TABLE II. Positions of the localized split-off bands (in eV) below the conduction-band minima at the *M* point in the first Brillouin zone. In the case of three and four SF's in neighboring planes in both 4*H*- and 6*H*-SiC, the second bound states ($n=2$) are also seen.

	Type of SF	$n=1$	$n=2$
4*H*-SiC	SF(31)	0.22	
	SF(13)	0.18	
	2SF(62)	0.60	
	3SF(71)	0.71	0.11
	4SF(10,2)	0.75	0.35
6*H*-SiC	SF(42)	0.19	
	SF(24)	0.17	
	2SF(51)	0.35	
	3SF(93)	0.49	0.06
	4SF(10,2)	0.55	0.17

with recently available experiments.[48–54] Some of the free electrons in the conduction bands are trapped in these QW's, but free to move parallel to the 3*C* inclusions. Therefore 2D electron gases are formed around these SF's.

From the curvatures of the split-off bands below the conduction-band minima along *M*-Γ and *M*-*K* in reciprocal space, we have derived the electron effective masses for the QW-like localized gap states. We have also deduced the effective masses for the conduction-band minima of the perfect 4*H*- and 6*H*-SiC crystals both in the perfect and in the faulted 96-atom supercells. The calculated effective masses are listed in Table III.

It is seen that our calculated in-plane effective mass tensors for perfect 3*C*-, 4*H*-, and 6*H*-SiC are in good agreement with the available experiments and calculations given in Table I. However, the calculated effective masses for the conduction-band minima in the faulted supercells tend to slightly deviate from the values obtained from the perfect supercells, as the number of SF's inserted increases. This is most likely due to the artificial defect-defect interactions. Since the size of the supercell is fixed to be 96 atom, the percentage of a faulted portion increases as the planar defect becomes thicker. Bearing in mind the expected accuracy of the DFT-LDA supercell method, we think that the deduced effective masses for the conduction band minima in both the perfect and faulted supercells are in acceptable agreement.

It is found that the effective mass components $m^*_{M\text{-}\Gamma}$ of electrons captured in the QW's are clearly heavier than those of perfect 3*C*-SiC, while $m^*_{M\text{-}K}$ is almost the same as that of perfect 3*C*-SiC. The effective masses of the 2D electron gases created by SF(31) and SF(13) in 4*H*-SiC, which introduce two of the thinnest QW's, are clearly larger than the others. But as the thickness of the cubic layer increases, the effective masses become closer to those of perfect 3*C*-SiC. In all the masses determined, $m^*_{M\text{-}\Gamma}$ is larger than $m^*_{M\text{-}K}$.

The detailed QW pictures associated with narrow 3*C*-like regions in the hexagonal host crystals raise a couple of insights and consequences. First, it is implied that the thinner the 3*C* QW, the heavier the effective mass of the 2D electron gas. Second, it is found that in heterocrystalline structures such as 4*H*/3*C*/4*H*, the narrow (at least up to ten straight bilayers) 3*C* regions cannot offer the light effective mass of perfect 3*C*-SiC. Third, we would like to indicate that it is quite interesting to fabricate bipolar devices on the {11-20} planes or the {1-100} planes, or any plane parallel to the *c* axis, since SF's parallel to the current flow direction are not expected to hinder electron transport, at least from the viewpoint of the electron scattering due to the QW-like perturbation potentials for the conduction-band electrons.

In the end, we point out one possibility in connection with the SF expansion in the pin diodes. The 2D electron gas formed around a SF can lead to so-called quantum mechanical pressure, which is applied to the surrounding partial dis-

TABLE III. Electron effective masses for the first split-off band ($n=1$), second split-off band ($n=2$), and conduction-band minima (CBM) along *M*-Γ and *M*-*K* in the hexagonal reciprocal space (in units of the free-electron mass m_0). The effective masses for the conduction-band minima of 4*H*- and 6*H*-SiC have also been calculated from the supercells containing single or multiple SF's.

		$n=1$		$n=2$		CBM	
96-atom supercells		*M*-Γ	*M*-*K*	*M*-Γ	*M*-*K*	*M*-Γ	*M*-*K*
3*C*-SiC	Perfect					0.42	0.23
4*H*-SiC	Perfect					0.59	0.29
	SF(31)	0.74	0.22			0.60	0.28
	SF(13)	0.72	0.22			0.60	0.28
	2SF(62)	0.60	0.22			0.63	0.28
	3SF(71)	0.60	0.22	0.59	0.21	0.62	0.28
	4SF(10,2)	0.56	0.23	0.65	0.21	0.65	0.28
6*H*-SiC	Perfect					0.76	0.26
	SF(42)	0.65	0.22			0.76	0.26
	SF(24)	0.66	0.22			0.76	0.26
	2SF(51)	0.63	0.22			0.76	0.26
	3SF(93)	0.57	0.23	0.69	0.22	0.74	0.24
	4SF(10,2)	0.56	0.23	0.66	0.21	0.75	0.25

locations as shown in Fig. 2. The origin of the pressure is of course the in-plane motion of the free electrons inside the $3C$ well: i.e., electrons reflected in the dislocation walls can give some impulses to the borders. Only in equilibrium have the effects of these trapped electrons been considered so far.[8,19,20] This pressure can, however, increase in magnitude when forward bias is applied. It is interesting to investigate whether this driving force can be strong enough to push and move partial dislocations—i.e., to estimate the quantum mechanical pressure as a function of the current flow applied.

V. CONCLUSIONS

We determined the in-plane effective mass tensors corresponding to the QW states of SF(31), SF(13), 2SF(62), 3SF(71), and 4SF(10,2) in $4H$-SiC and SF(42), SF(24), 2SF(51), 3SF(93), and 4SF(10,2) in $6H$-SiC, as well as those for the perfect $3C$, $4H$, and $6H$ polytypes. Our calculated electron effective masses for the perfect structures are in very good agreement with available data. It was found that the 2D electron gases inside the thin cubic regions have clearly heavier effective masses than in the perfect bulk $3C$-SiC single crystal.

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