Stacking fault band structure in 4H–SiC and its impact on electronic devices

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First principles calculations of the stacking fault (SF) in 4H–SiC indicate the occurrence of an interface band in the gap with maximum depth of 0.2–0.3 eV below the conduction band minimum at the $\bar{M}$ point. The energy of formation of SFs in 3C–, 4H–, and 6H–SiC on the other hand is found to be of order a few meV/pair. Thus, there is a thermodynamic driving force promoting growth of SF area in an *n*-type sample. Radiationless recombination of electrons trapped at the SF with holes is proposed to provide sufficient energy to overcome the partial dislocation motion barriers towards formation of additional SF area in a device under forward bias. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1427749]

Much progress has been made in developing SiC high-power devices based on hexagonal polytypes such as 4H and 6H–SiC.[1] Still numerous problems need to be overcome. Recently, studies of SiC diodes under long term operation revealed a deterioration in forward voltage $I-V$ curves, known as an ''electronic stress.'' [2,3] Significantly, this deterioration of the devices was found to be correlated with an increasing number of stacking faults (SF). At first sight, this is surprising because coherent twin boundaries and stacking faults, i.e., simply different stackings of the basal planes are expected to be rather benign defects. In fact, the polytypism itself can in some sense be viewed as being the result of alternative choices for the stacking of basal plane layers. Consequently, one does not expect these to introduce defect levels in the fundamental gap which could act as traps and thereby deteriorate the current in a device. A previous computational study by Käckel *et al.*[4] for stacking faults in 3C–SiC indeed revealed no interface states in the fundamental gap, although an interface band does appear in the projected band structure near the $\bar{K}$ point of the projected Brillouin zone (BZ).

In this letter, we show by means of first principles calculations that in 4H–SiC, an interface band does occur in the fundamental gap, with a maximum depth of 0.2–0.3 eV below the conduction band at the $\bar{M}$ point. This is due to the fact that the local configuration of a SF is closer related to that in 6H–SiC which has a lower gap. On the other hand, we will show that the creation energy of the SF is only of order 9 meV per surface unit cell. While this indicates a thermodynamic driving force favoring SF generation in *n*-type material, the barriers to overcome, related to partial dislocation motion are of order eV. We propose that in a device under forward bias, radiationless recombination of trapped electrons with holes may provide the necessary energy to overcome these barriers.

First, we need to discuss the definition of SFs. In the usual manner, we label the layers as *A, B, C*, respectively, depending on their horizontal position. Cubic stacking then corresponds to *ABC*, and hexagonal stacking to *AB*, each periodically repeated. Alternatively, we may label two consecutive cubically (hexagonally) stacked layers by an up ↑ or down ↓ spin. Even simpler, we may just record the width of the bands of parallel spins in the unit cell.[5] In these notations, 4*H* corresponds to *ABCB* or ↑↑↓↓ or ⟨22⟩. A coherent twin boundary corresponds to reverting all the spins at the right of some point in the otherwise perfect sequence of the starting polytype. A SF corresponds to two nearby twin boundaries. For example, in 3C–SiC, the intrinsic SF (ISF) corresponds to flipping of a single spin: ...↑↑↑↓↑↑↑... or ...*ABCACABC*... in which a *B* layer is missing. The extrinsic SF (ESF) in 3C corresponds to flipping two consecutive spins ...↑↑↑↓↓↑↑... or ...*ABCACBCAB*... corresponding to an added *C* layer. In 4H, the SF is characterized by locally having a stacking ...↑↑↑↓..., or *ABAC*, or ⟨13⟩ instead of ⟨22⟩. It corresponds to a single spin flip and is thus called ISF. Of course ⟨13⟩ is energetically equivalent to ⟨31⟩. In 6H–SiC, two possibilities occur: ⟨33⟩→⟨24⟩ or ⟨33⟩→⟨1113⟩, which we will refer to as SF1 and SF2, respectively.

Ideally, one would like to model a single SF between two semi-infinite crystals. In order to use band-structure methods, however, we need to restore the periodicity. This will introduce SF–SF interactions. Obviously we want to space the SFs as far as possible compatible with computational feasibility and monitor the effect of the interactions by comparing different inter-SF distances. The SF in 4H induces a shift of the layers beyond the SF, say *A* moves to *B*, *B* to *C*, and *C* to *A*. The unit cell is then changed from *ABCB* to *BCAC*. If we insist on keeping the system periodic with a lattice vector perpendicular to the layers, i.e., if we want to maintain a hexagonal unit cell, we need to introduce another SF to return to the *ABCB* sequence. We call this second ISF an ''anti'' ISF, because one corresponds to rotation of the bonds by π the other by $-\pi$. On the other hand, we can also consider a rhombohedral cell that contains a lattice vector connecting the *A* layer to the *B* layer starting each of these sequences of four layers. To test the robustness of our results,

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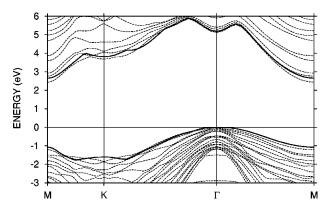[b]Electronic mail: wlambrecht@cwru.edu

FIG. 1. Valence band maximum and conduction band minimum of projected band structure of 4H–SiC, in full lines, and stacking fault model band structure in dashed lines.

we have used both approaches. First, we use a series of models that can be generally expressed as $(ABCB)(ABAC) \times (BCAC)_n$. The ISF is introduced in the unit $ABAC$. For convenience, we denote them as ISF-Rn, in which R stands for the rhombohedral cell and n is the number of the repeated $BCAC$ units. Calculations are performed for $n=0, 1, 2$ corresponding to systems with 8, 12, and 16 layers. The general formula for the hexagonal cells is $(ABCB)_m(ABAC) \times (BCAC)_n$. To keep the ISF and the "anti" ISF apart, one needs a larger repeat unit. The ISF is located in the $ABAC$ unit and the "anti" ISF occurs at the connection of the two repeated cells. We used both a full-potential (FP)[6] and an atomic sphere approximation (ASA) of the linear muffin-tin orbital method[7] to calculate the band structures. The basic underlying method is density functional theory in the local density approximation.[8]

We present the results of the ISF-$R0$ cell using the FP method. The band edges of 4H–SiC near the fundamental gap projected on the $\Gamma - M - K$ basal plane are shown in Fig. 1 as thick full lines. The dashed lines show the band structure results of the model containing the SFs. The highest occupied level of the defect model is aligned with the valence band maximum of 4H. The important feature is the appearance of an interface band with maximum depth of 0.21 eV below the conduction band at the $\bar{M}$ point. This feature is found for all the models as well as for both ASA and FP calculations. The ASA method gives a depth of 0.30 ± 0.01 eV for all the models investigated. The layer projected densities of states (LDOS) of the ISF-$R2$ model indicate a well separated peak just below the conduction band which is localized 31%, 20%, and 15% on the three cubically stacked layers just to the right of the ISF and 7% on the layer just to the left of the ISF, amounting to a total of 80%. This indicates that the interface state rapidly decays with distance away from the interface.

The origin of this interface state can simply be explained by the fact that locally the SF introduces a $\langle 31 \rangle$ unit, or three spins in a row whereas in 4H only bands of two consecutive spins occur. Since this local structure thus resembles a unit of 6H, which has a lower band gap somewhere along the ML line, the interface state emerges at the $\bar{M}$ point. It is well known that band gaps in SiC vary nearly linearly with hexagonality and that the conduction band minima lie at some point along the ML line corresponding to $\bar{M}$ in projection for

all polytypes studied except for 2H. Thus, we may expect that in 6H–SiC, the local four-parallel spin or $8H$ type unit in the stacking fault will also produce an interface state.

To model the total energy or energy of formation of the SFs, the axially next nearest neighbor Ising spin (ANNNI) model[9] with up to third nearest neighbor interactions

$$E = E_0 - \frac{1}{N} \sum_{i,n} J_n \sigma_i \sigma_{i+n} \tag{1}$$

can be used as described in Refs. 10 and 11. The ANNNI model parameters used are deduced from the total energy differences for the polytypes 3C, 2H, 4H, 6H, 9R, and 15R, using a least-square fit, and have the values

$$J_1 = 3.268, \quad J_2 = -2.23, \quad J_3 = -1.056 \text{ meV/pair}.$$

In terms of these parameters, the energies of formation of the ISF and ESF in 3C–SiC are given by:[4]

$$E_{ISF}^{3C} = 4J_1 + 4J_2 + 4J_3 \quad E_{ESF}^{3C} = 4J_1 + 8J_2 + 8J_3,$$

which give the numerical values: -0.072 and -13.216 meV/pair for the ISF and ESF, respectively. The corresponding interface energies, obtained by dividing by the unit cell area of $\sqrt{3}a_c^2/4$ in terms of the cubic lattice constant a_c, are $\gamma_{ISF}^{3C} = -0.14$ mJ/m^2 and $\gamma_{ESF}^{3C} = -25.8$ mJ/m^2. These turn out to be in excellent agreement with the directly calculated values by Käckel et al.,[4] which are -3.4 and -28 mJ/m^2. In particular, our ANNNI model parameters reproduce the fact that the ISF has a much lower energy than the ESF. For the 4H and 6H SFs we obtain:[11,12]

$$E_{ISF}^{4H} = -4J_2, \quad E_{SF}^{6H} = -4J_3, \quad E_{SF2}^{6H} = 4J_1 - 4J_2 - 4J_3,$$

or 9.8, 3.8, and 28.6 meV/pair, respectively, or 19.2, 7.4, and 55.9 mJ/m^2 for the corresponding γ values. Experimental values by Pirouz et al.[12] for the first two of these are 7.5 and 1.5 meV/pair. The SF2 stacking fault in 6H obviously is very unfavorable because of the occurrence of a local 2H type stacking. The main conclusion from this is that all these SF energies are of order of a few meV per pair of atoms.

In a purely intrinsic SiC material, the trap level would have no effect on the energetics because the defect level is unoccupied. In n-type material on the other hand, the SF trap states should be mostly filled and the energy gain by trapping an electron at a SF (0.2–0.3 eV/pair) exceeds the net energy cost (9 meV/pair) of forming an additional unit area of SF. This implies that n-type material favors the formation of SFs. Similarly, it has been argued in the past that n-type doping may favor 3C–SiC because of its lower band gap assuming the valence band edges are approximately aligned. The net thermodynamic driving force of 0.2–0.3 eV/pair of atoms per trapped electron may be viewed as a SF expanding force on the surrounding dislocation of about 0.4–0.6 N/m, or, dividing by the length of a Burger's vector, a stress of order 2–3 GPa per carrier trapped.

On the other hand, in order to increase the SF area, such that it can trap an electron and thus activate this force, the partial dislocation surrounding it must move. This happens by means of kink formation and migration which has an activation barrier of 1.7–2 eV for C-C core partial dislocations and 2.7–2.8 eV for Si-Si core partial dislocations.[13] Thus, although during growth, one may expect a somewhat

larger amount of SFs to be formed in *n*-type material, once the crystal is formed, the SF area is not expected to increase spontaneously by keeping on trapping the carriers and losing the doping, simply because the barrier towards this ultimately thermodynamically favored state is too large. In a device under operation, however, the situation is different. Under forward bias, holes are injected in the *n*-type region, and the trapped electrons may now recombine with the holes. In the *p*-type region, injected electrons may also become trapped and then recombine with the holes. In both cases, if this recombination happens radiationless, an energy of approximately the band gap is dumped into the phonon system per electron-hole pair recombining. Because this happens in the region of the SF itself, this "phonon kick" may be expected to lead to large local fluctuations which may promote the dislocation motion and thus ultimately the growth of the SF. Such an electronic defect generation mechanism is well known to lead to enhanced defect formation in semiconductor laser diodes.[14–18]

In summary, the SF in 4H–SiC exhibits an interface band with a maximum depth of 0.2–0.3 eV below the conduction band minimum at $\bar{M}$ because the local environment resembles that of the lower gap 6H polytype. A SF interface state is also expected in 6H–SiC. The SF costs only of order 9 meV/pair to form in 4H and 4 meV in 6H. This leads to a driving thermodynamic force towards increasing the SF area in *n*-type material. In a device under forward bias, the radiationless recombination of electron holes pairs at the trapping center may provide the necessary energy to overcome the barriers towards dislocation motion required to increase the SF area. This model explains the observed increase in SFs in SiC devices under long time forward bias operation and the deterioration of the devices by the adverse effects of trapping electrons on the transport.

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