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Optical Investigations of stacking faults in 4H-SiC epitaxial layers: comparison of 3C and 8H polytypes

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Abstract: We present an analysis of the electronic structure of in-grown 3C and 8H stacking faults (SFs) in a 4H-SiC matrix. First the concept of low temperature photoluminescence optical signature of SFs is discussed. Then, the results of type-II quantum well (QW) model calculations are displayed, taking into account the effect of valence band offset, internal polarization field and non homogeneity of the potential well. In this case, we show that a satisfactory description of 3C QWs signature can be reached. The situation is entirely different for 8H. Since a 8H unit cell is nothing but two 3C lamellae coupled by an hexagonal turn, we investigate in detail the effect of coupling more and more two 3C lamellae until a final 8H QW is found. In this way, we show that a reasonable agreement with experimental data can be reached.

1. Introduction

Silicon carbide (SiC) is an attractive material system for high power device applications. During the last 15 years the material quality has been very much improved and an increasing number of devices has been introduced on the market [1]. Unfortunately, still, the degradation of high voltage bipolar diodes under operating conditions limits the potential field of applications [2-4]. This comes from the uncontrolled formation and expansion of stacking faults (SFs) in p-i-n diodes under electrical stress [5].

SFs constitute a very important class of defects in SiC epitaxial layers, which can form in many different ways. When they appear spontaneously during the growth, they are called “in-grown” SFs. When they appear after some mechanical stress [6, 7] or during a later processing step like doping [8], annealing [9] or oxidation [10], they are called “process-induced” SFs. In this case, they are the source of electrical defects (the so-called “degradation-induced” SFs) that will reveal later in aging and electrically stressed bipolar diodes [3-5]. In most cases, the foreign polytype is 3C-SiC [4, 6-8, 10-12] but, in some cases, 8H-SiC has also been identified [13, 14].

Generally speaking, most SiC SFs result from the dissociation of a perfect dislocation in two partials (one leading and one threading) in the basal plane. This mechanism is better known in the literature as Shockley SF (SSF) formation mechanism. In most cases, it results in a 3C-SiC defective lamella expanding perpendicular to the C axis [4, 6-8, 10-12]. In this work, we review some of the optical investigation techniques that have been used to define the corresponding SF signature. We discuss the experimental results in the light of a type-II quantum well (QW) transfer matrix method, taking into account the valence band offset and the quantum confined Stark effect (QCSE). We show that the model works well for 3C but not for 8H. To solve the discrepancy we speculate that a 8H defect is nothing but a 4SSF(4,4) coming from the combination of two single SFs :

1SSF(3,1) and 1SSF(1,3) merging together. Upon merging two new (additional) SSFs are generated in between the two 3C lamellae, forming then a more stable (faulted) sequence. This is the final 8H lamella. To investigate in details this system, we focus on the effect of coupling two 3C QWs separated by a 4H barrier of variable thickness.

2. Optical SF signature

Given an active epitaxial layer, it is often necessary to determine (rapidly and non destructively) if different types of SFs exist (or not) and, when they exist, to evaluate the effective thickness of the different defects. To help answering this question, the concept of “optical SF signature” has been introduced [15, 16]. It comes from low temperature optical measurements and allows matching unambiguously one defect with one series of lines.

Two examples are shown in Fig.1. Consider, first, Fig.1-a. It is extracted from the work of Ref. [12] and concerns a 3C SF-QW in a 4H-SiC matrix. At low temperature (2K) the luminescence spectrum displays four large lines, noted LO, TO, LA and TA which are indicative of phonon-assisted radiative recombination processes. The corresponding excitonic energy gap (E_{gX}) is equal to 2.172 eV and, from TEM results (not shown) we know that this optical SF signature is associated with a 14 bilayers (BLs) thick 3C lamella coming from a triple combination of double SFs of the type 6SSFs(14,2). In Fig.1-b, there is a similar example but, now, extracted from the work of Ref.[13] for a 8H SF-QW, again in a 4H-SiC matrix. Notice that the optical SF signature remains almost the same, except for some increased broadening and drastic change in radiative recombination energy. From TEM measurements, we know that, in this case, the defect is associated with a 8 BLs thick (one unit cell) lamella of the 8H polytype. This is a totally different features which comes now from a double combination of double SFs of

the type 4SSFs(4,4) but, since no new (specific) feature reveals, we conclude that the SF signature is not (or very poorly) sensitive to the well polytype.

To summarize, moving from one SF to the next one and even changing the well polytype, not much varies. The only sensitive parameter is the change in energy position of the SF signature which, for a given polytype, should be a direct function of the QW thickness.

3. Model calculation and discussion

To take into account the effect of the valence band offset and built-in electric field [17], we used a transfer matrix method (TMM) already described in the works of Refs [15, 18]. In such a case, using the band structure parameters listed in Table 1, one can easily compute the change in optical SF signature as a function of the QW thickness for a 3C or a 8H lamella in between two 4H barriers. For 3C SF-QWs, an excellent agreement can be found when using a value of ~ 1.2 MV/cm for the electric field [18]. This is shown in Fig.2. Unfortunately, no similar agreement can be found for the 8H unit cell. While the optical SF signature is close to ~ 2.72 eV [13] (black circle in Fig.2) the computation predicts an energy which about ~ 150 meV higher.

To solve the problem, and since a 8H unit cell is nothing but two 3C QWs coupled by a hexagonal turn (a thin hexagonal barrier made of two BLs), we have investigated the effect of coupling more and more two (initially well separated) 3C QWs. We start from a type-II heterostructure of the type 4H/3C/4H/3C/4H in which the outer barriers are semi-infinite and the central barrier is of variable length. This is schematically drawn in Fig.3. From the TMM, we compute the radiative recombination energy for different thicknesses of the 4H barrier in between the two 3C QWs. We use again the parameters listed in Table 1 and consider two different situations. First, the limiting case in which

there is no internal electric field (total screening) and, second, the case in which there is an internal built-in electric field of about 1.2 MV/cm across the two 3C-QWs.

Results are shown in Fig.4. Consider, first, Fig.4-a. We show the radiative recombination energy computed for different thicknesses of the intermediate 4H barrier, without any built-in electric field. As long as the barrier thickness exceeds some critical value (hereafter noted L_0) which is of the order of 10 BLs, nothing happens. We are in the limiting case in which both 3C-QWs are completely independent and inter-well coupling is negligible. With respect to a single 4H/3C/4H structure, the same value of the fundamental energy transition is found (~ 2.81 eV) in both wells. It is simply two times (accidentally) degenerated.

Upon excitation, two different families of electrons localize inside the wells and their wave functions never overlap. The holes stay in the 4H barriers, either in the central or outside parts of the 3C QWs, with the same probability of presence. Simply, because of the electron-hole interaction, they localize close to the interfaces. The two (left and right) radiative transition probabilities remain identical.

When the thickness of the intermediate (coupling) 4H barrier decreases and becomes lower than 10 bilayers, inter-well coupling starts to manifest. This arises from the overlap of electronic wave functions and results in a splitting of the two energy states to give one fundamental and one excited state. This is shown in Fig 3-b. The electrons remain localised in both 3C QWs but, now, the fundamental energy state being lower than the one of a single isolated fault, this is the driving force to continue moving closer and closer. At the beginning of process, when the two faults are still far apart, the holes tend to localize in the thin (intermediate) 4H barrier. Unfortunately, this is not a viable situation. As soon as the thickness of the coupling barrier decreases the holes, which start experiencing a confinement energy, tunnel from the central to the outer barriers in order to lower energy (i.e. return to the maximum of the top valence band). In this way,

when the barrier thickness changes from 8 to 2 BLs, the radiative recombination energy decreases from ~ 2.81 to 2.72 eV. This is shown in Fig.4-a. Before taking into account the effect of the built-in electric field, it should be noticed that the transition energy ~ 2.72 eV found in this way is very close to the experimental one, reported from PL measurement by Izumi and al for a 8H SF-QW [13].

Let us now consider the same situation, but taking into account the built-in electric field. Results are shown in Fig.4-b. The new result is that three different radiative recombination energies appear, calculated for different thicknesses of the intermediate 4H barrier. When the barrier is thick (thicker than 7 BLs which corresponds to the new critical value L_F), there should be no difference between the right and left QW systems. In both cases, the holes localize at high energy (on the left sides of the well) and both radiative recombination energies have identical value. For details, see Fig.3-c. When the two SFs start to couple (i.e. below a 7 BLs thickness of the coupling barrier) two different energy states appear in both wells: At low energy is one state that originates from the well at the right side, at high energy is the state that originates from the state in the left well. At the same time, the holes begin to move from the coupling barrier to the left side of the left well, see in Fig. 3-d. The net consequence is that three series of recombination energies appear. Two of them, labelled E_{t_1} and E_{t_3} are separated by a constant energy ~ 90 meV, which come directly from the effect of the electrical field. Increasing again the inter-well coupling, the transition energies shift but the energy difference between E_{t_1} and E_{t_3} remains constant. Simply the holes tunnel more and more to the left do the electrons. The respective intensities of E_{t_1} and E_{t_2} decrease. The one of E_{t_3} increases. At the very end, for a 2BLs barrier (8H polytype) remains only the (low energy) E_{t_3} transition (see Fig.3-d). The final value is ~ 2.62 eV.

4. Conclusion

To summarise, after defining the concept of the optical SF signature by LTPL, we have used a transfer matrix method to model the thickness dependence of type-II quantum well (QW). We have taken into account the valence band offset and QCSE (Quantum Confined Stark Effect) to discuss the effect of the thickness of the coupling 4H barrier sandwiched in two 3C QWs of one 3BLs unit cell. We have shown that 8H is a particular case in which two 3C QWs (1SSF(3,1) and 1SSF(1,3)) merge to form a final 4SSF(4,4) defect. We have found two theoretical recombination energies of about 2.62 eV with a build-in electrical field of about 1.2 MV/cm and 2.72 eV without any electrical field. Comparing with the experimental result from Ref. 13 (at about 2.72 eV), we find that the build-in electrical field was completely screened. Unfortunately, no other data from 8H PL measurement has been published to compare with.

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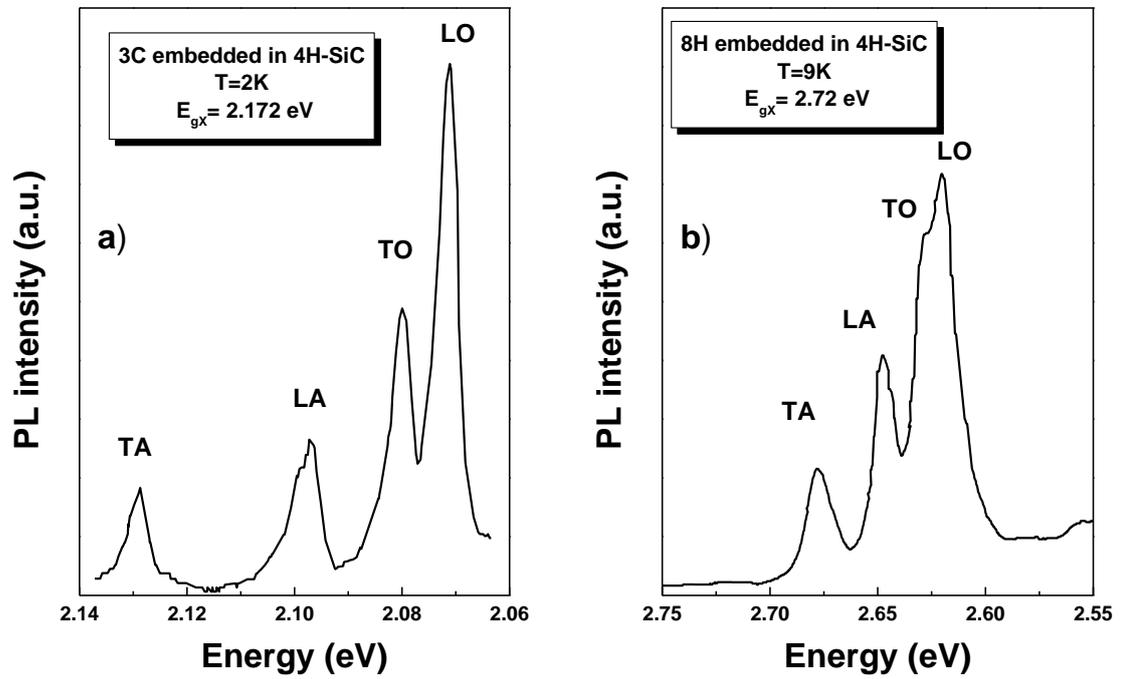


Figure 1: Low temperature photoluminescence spectra obtained for undoped 4H-SiC epitaxial layers with a) a 3C-SiC inclusion (14BLs thick) (after Ref.[12]) and b) a 8H-SiC one unit cell (8 BLs) (after Ref.[13]).

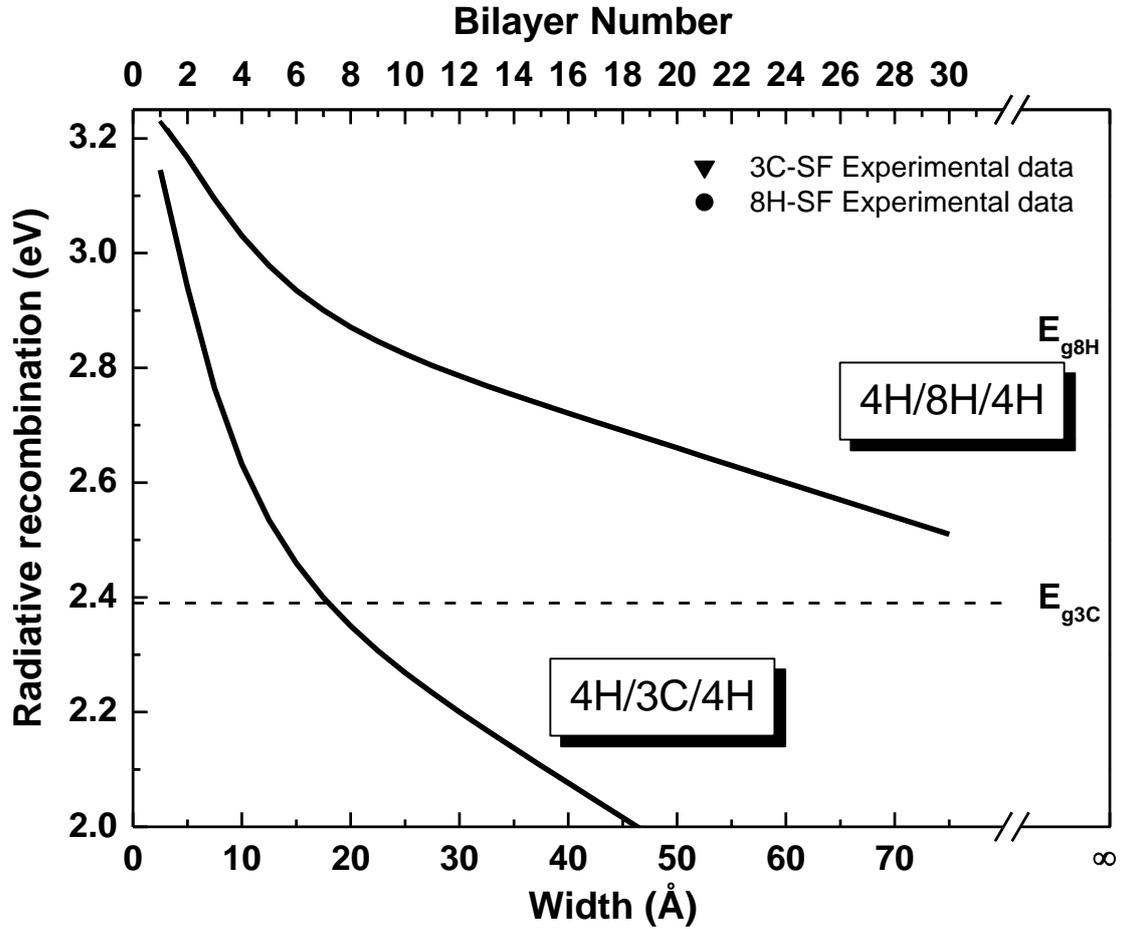


Figure 2: Recombination energies computed, respectively, for a 3C and a 8H-SiC lamella in a 4H-SiC matrix. In both cases we used a simple type-II QW model and a transfer matrix method to take into account the effect of the built-in electric field. The black triangles represent experimental data from Refs.[9, 12, 19] in which the SF thickness is independently determined from TEM data. The black circle represents the experimental signature obtained for a 8H unit cell in the work of Ref.[13].

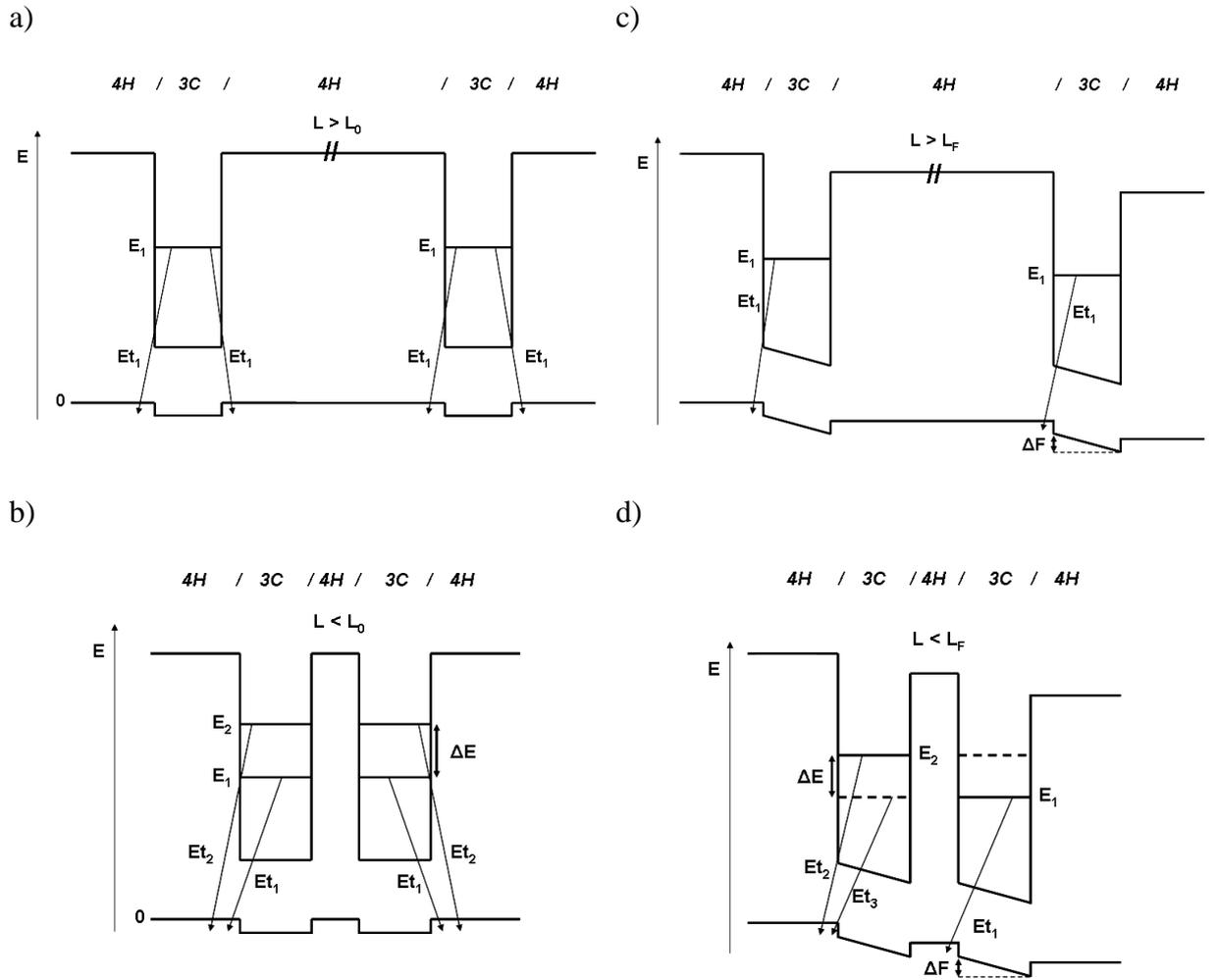


Figure 3: Schematic model of the 4H/3C/4H/3C/4H heterostructure considered in this work. The potential origin is taken at the top of the valence band in the left barrier. In panels a) and b) E_{t1} represents the radiative transition energy from the fundamental state (E_1) to the topmost valence band in the 4H barriers. E_{t2} appears upon coupling and represents the radiative transition energy from the excited state (E_2) to the top valence band in the 4H-SiC barriers. In panels c) and d) we assume that the holes thermalize on the left side of the well. In such a case, before coupling, only one transition manifests. See panel c). Upon coupling, three transitions manifest. E_{t1} and E_{t2} represent again the radiative transition energies from the fundamental state (E_1) and the excited state (E_2) to the top valence band on the left side of the left and right 3C QWs respectively. E_{t3} is a new feature that appears because of the interwell coupling. In both cases, L_0 and L_F indicate a critical value of the intermediate 4H barrier thickness.

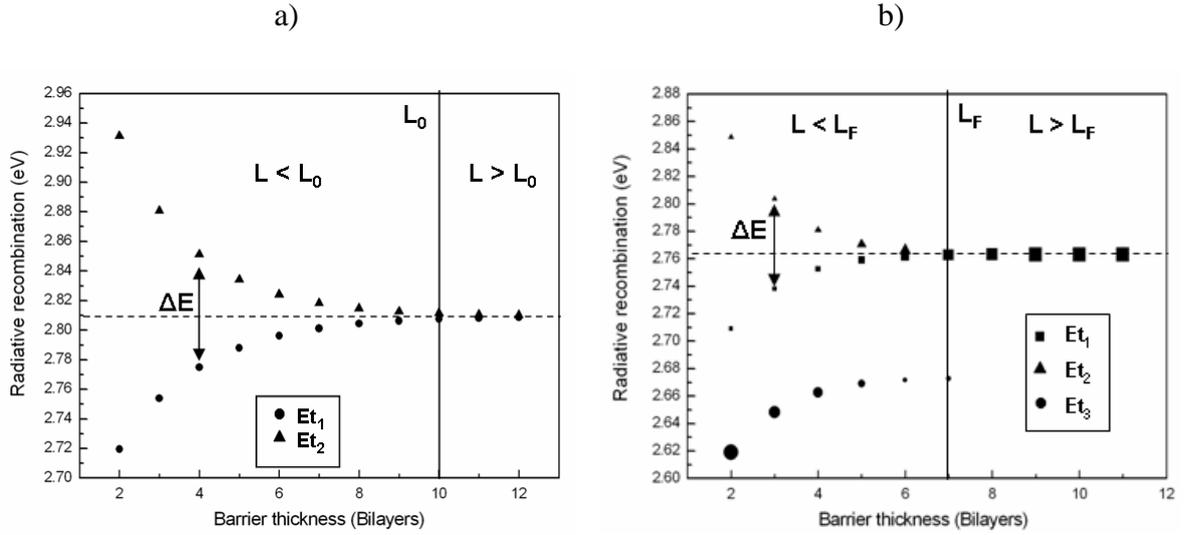


Figure 4: Recombination energies calculated for a type-II heterostructure of the type 4H/3C/4H/3C/4H without a) an electrical field and with b) an electrical field of about 1.2 MV/cm. Both panels are given versus the thickness (L) of the intermediate barrier which separates the two 3C QWs. In panel a), the black circles represent the radiative transition energy (E_{t1}) of electrons confined at the fundamental energy level of the 3C QWs with holes in the 4H barriers. The black triangles represent the radiative transition energy (E_{t2}) of electrons at the excited state with holes in the 4H barriers. ΔE is the energy difference between E_{t1} and E_{t2} . In panel b) before coupling, only one transition manifests. Upon coupling, three transitions start to appear. E_{t1} and E_{t2} represent the radiative transition energies from the fundamental state (E_1) and the excited state (E_2) to the top valence band on the left side of the left and right 3C QWs respectively. E_{t3} is a new feature that appears because of inter-well coupling. In both cases, L_0 and L_F are guides for the eyes. They indicate a critical value of the intermediate 4H barrier thickness from which ΔE is very small.

Polytype	$m_e(m_0)$	Gap (meV)	ΔE_c (meV)	ΔE_v (meV)
3C-SiC	0.316	2390	-943	-70
4H-SiC	0.330	3263	0	0
8H-SiC	0.428	2860	-368	-35

Table 1: Summary of parameters used in the computation for 3C, 4H and 8H polytypes. This includes the electron effective mass (m_0), the bandgap energy at low temperature, the conduction offset (ΔE_c) and the valence offset (ΔE_v).