

# STUDY OF THE POSSIBILITY OF POLYTYPE 3C SILICON CARBIDE BULK CRYSTALS GROWING FOR USE IN POWER DEVICES

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## ABSTRACT

Due to its electro-physical parameters, the silicon carbide is a promising material for power devices, including the microwave range. In recent years there has been considerable progress in the development of power devices, based on SiC. Serious problem, which hinders the widespread commercialization of SiC bipolar power devices, is the p-n structures degradation during high densities of passing forward current. In 1981 the blue SiC LED's emission spectrum over time degradation was detected. Later, after the creation of power rectifier diodes, based on SiC, it was found that their characteristics are also deteriorated with increase of operating time. It was found that the cause of degradation are the so-called "Stacking Faults" (SF) -i.e., the formation of cubic SiC layers inside the hexagonal SiC diodes during direct current flow through them. However, it is easy to assume that this degradation mechanism is absent in devices, completely based on cubic polytype 3C-SiC. This study is dedicated to the study of possibility of creating device heterostructures based on 3C-SiC. It is shown that the heterojunction between SiC polytypes may be more structurally perfect than heterojunctions between semiconductors with different chemical nature. The conclusion on perspective of SiC-based heterostructures application in modern electronic devices is made.

**Keywords:** Cubic Silicon Carbide, Polytype, Sublimation Epitaxy, Hetero-Polytype Structure, 3C-SiC

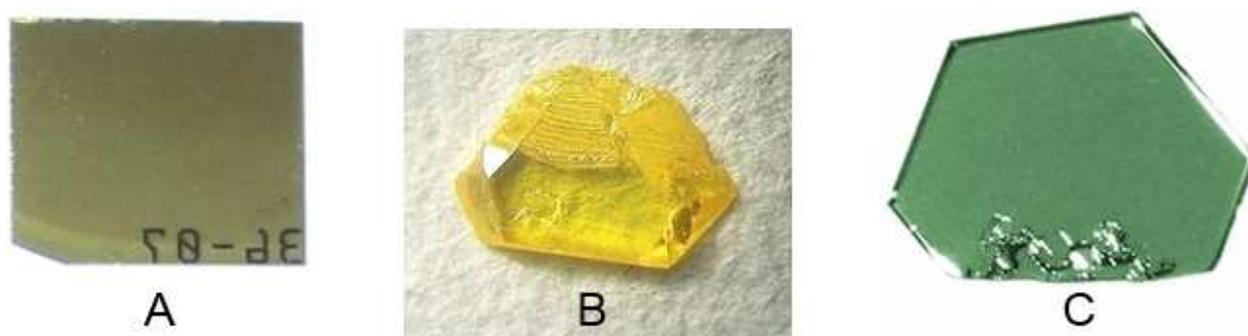
## 1. INTRODUCTION

It is known that due to its electro-physical parameters, the silicon carbide is a very promising material for manufacturing power devices, including the HF range. SiC has a high breakdown energy ( $E_{br} \sim 3 \text{ MV/cm}$ ), high thermal conductivity ( $\sim 3.8 \text{ W/cm deg}$ ) and high electrons saturation velocity ( $\sim 2.5 \cdot 10^7 \text{ cm sec}^{-1}$ ). Furthermore, SiC-based devices are capable to operate at high temperatures ( $850^\circ\text{C}$ ). In recent years there has been considerable progress in the development of power devices, based on SiC of microwave range (Cooper *et al.*, 1998). In addition to its unique electrical properties, the silicon carbide has the ability to crystallize in different modifications (polytypes). Polytypes of SiC, having the same chemical nature, can

vary greatly in their electro-physical parameters and appearance (**Fig. 1**). In recent years, the world's interest in the obtaining and investigation of hetero-polytype structures, based on silicon carbide, increased.

Serious problem, which hinders the widespread commercialization of SiC bipolar power devices, is the p-n structures degradation during high densities of passing forward current. Zeither and Theeis (1981) the blue SiC LED's emission spectrum over time degradation was detected. In the emission spectrum the peak in the green region of the spectrum appeared, which was also spatially localized on the diode working plane. The authors explained their results by the formation of 3C-SiC inclusions inside 6H-SiC polytype in the p-n structures under the influence of forward current.

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**Fig. 1.** SiC crystals of different polytypes (a) 4H-SiC (b) 3C-SiC (c) 6H-SiC

Later, after the creation of power rectifier diodes, based on SiC, it was found that their characteristics were also deteriorated with increasing operating time. This is reflected in the increase of leakage currents, lowering of breakdown voltage during the reverse inclusion and increase of diode forward resistance (Bergman *et al.*, 2001).

Research of this phenomenon has been the subject of many publications and it has been found that the cause of degradation are the so-called “Stacking Faults” (SF), i.e., the formation of cubic SiC layers inside the hexagonal SiC of 4H or 6H polytypes during the forward current flowing through it (Mao *et al.*, 2001). It turned out that the energy, dissipated during non-radiative recombination of electron-hole pair in SiC, is sufficient to overcome the barrier, corresponding to a shift of an atom in a different position. I.e., there was a rearrangement of hexagonal polytype lattice-displacement of the atom from hexagonal positions the crystal lattice into cubic ones-the formation of cubic polytype layer. As a starting point of SF growth served the dislocation, located in the volume of the epitaxial layer or at the interface between epitaxial layer and substrate. SF is actually a quantum well of more narrow-bandgap 3C-SiC inside hexagonal SiC, causing intense recombination and consequently, a decrease in the lifetime and increase of the device’s base region series resistance. Under the influence of direct current the linear dimensions of SF increased rapidly, parallel to the crystal axis of the crystal. When SF reaches the metallurgical boundary of p-n transition a complete degradation of the device occurs.

The degradation, associated with the formation of SF, is currently one of the major problems in the development of bipolar devices, based on SiC. However, it is easy to assume that this degradation mechanism will not be present in devices, based on 3C-SiC. A cubic

silicon carbide is the most narrow-bandgap polytypes of SiC and, in any case, the structural defects cannot form quantum wells in it. However, until now this assumption has no reliable experimental confirmation. For this there are two main reasons:

- Lack of 3C-SiC substrates of considerable size available on the market
- Very low structural perfection of the 3C-SiC layer, grown by CVD method on Si substrates or hexagonal SiC polytypes

It is planned to develop the technology of 3C-SiC substrates manufacturing, which can be used for the production of power devices, based on silicon carbide that would be unaffected by the degradation, associated with the formation of SF.

Thus, it will fix the problem that hinders wide industrial production of power devices, based on silicon carbide.

## 2. SiC POLYTYPICITY

The progress in the development of silicon carbide technology, achieved in past 20 years, allowed the creation almost of all types of semiconductor devices on its basis. Along with an established industrial manufacturing of SiC substrates the producing of Schottky diodes with a breakdown voltage of 600 V and direct currents up to 20 A have started in recent years. It is expected that commercially available high-frequency FET-MESFET will be the next device, produced serially.

Due to the large bandgap, high thermal conductivity, high thermal, chemical and radiation resistance, SiC was considered primarily as a promising material for power electronics. At the same time, silicon carbide has the ability to crystallize in different modifications

(polytypes) that have the same chemical composition but different electrical parameters. This makes silicon carbide a promising material in terms of creating different types of heterostructures as well.

The existence of various crystalline modifications of SiC was discovered in (Baumhauer, 1912). Later, this phenomenon was called polytypism, i.e., polymorphisms in the single direction (Schneer, 1955). Silicon carbide is among the best example of polytype compounds.

Actually, the term “polytypism” has been introduced specifically to it, due to the fact that different crystalline forms of SiC are very similar to each other structurally. Currently, there are more than 200 known crystal modifications of SiC (Verma and Krishna, 1966).

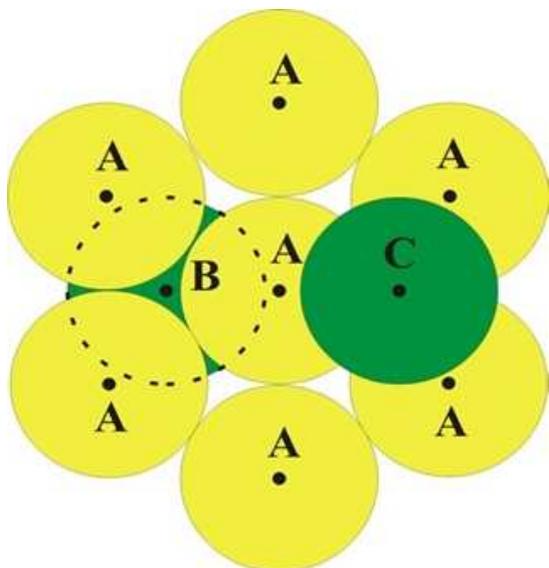


Fig. 2. Scheme of atom centers positions in the various layers crystal of lattice

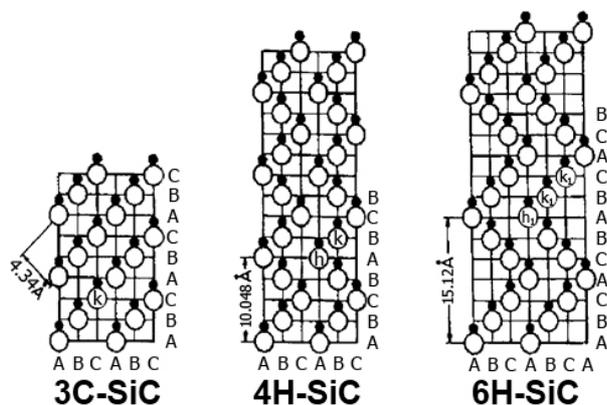


Fig. 3. Periodicity of the SiC crystal lattice of different polytypes

Figure 2 shows the positions of the atoms centers in a dense spherical packing. If the centers of all spheres in first layer are located in the points A, then for the second layer the position of the centers at points B or C are already possible. Which of the possible positions will be occupied by the atoms in the second and subsequent layers determines the structure of the polytype.

To characterize the polytype the Ramsdell notation is also used often (Ramsdell, 1947). It consists of a natural number equal to the number of layers in the period in the direction, perpendicular to the base plane (Fig. 3) and an alphabetic character, characterizing the syngony of Bravais lattice: C-cubic, H-hexagonal, R-rhombohedral, for example, 3C, 4H, 6H.

### 3. PROSPECTS OF 3C-SiC IN POWER ELECTRONICS

Among more than two hundred of silicon carbide polytypes one of the most interesting is the cubic polytype 3C-SiC. It has a maximum mobility of  $1200 \text{ cm}^2/\text{V sec}$  (Levinshtein *et al.*, 2001), among SiC polytypes, the value of which does not depend on crystallographic direction. This greatly simplifies the manufacturing technology of power devices, because does not require precise positioning of the plates to the apparatus substructures. The magnitude of the bandgap substantially depends on the polytype and varies from 2.39 eV for 3C SiC and to 3.3 eV for 2H-SiC. Thus, the difference in the values of the forbidden zones ( $\Delta E_g$  [HC]) between a Cubic (3C) and pure Hexagonal (2H) SiC polytypes is  $\sim 0.9 \text{ eV}$ .

Other parameters of 3C-SiC (critical electric field, the maximum operating temperature, electrons saturation velocity and thermal conductivity) are differ slightly from the parameters of the hexagonal polytypes (Table 1).

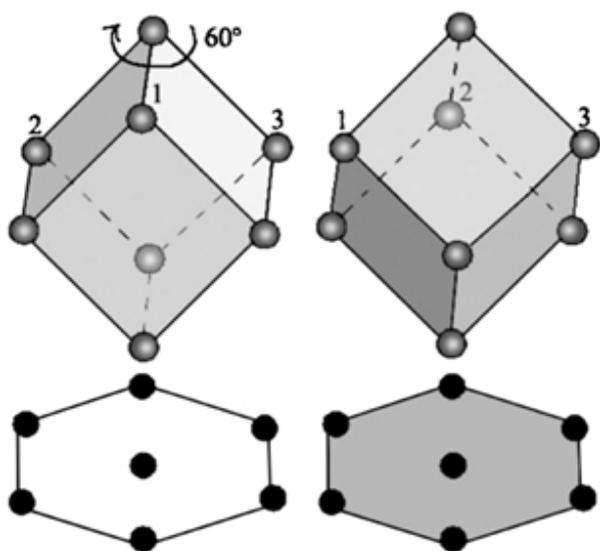
Heterojunctions are the contacts between two semiconductors with different chemical nature or two different crystal polytypes of one semiconductor. The latter are called hetero-polytype.

From the point of view of power devices production technology the hetero-polytype structures are characterized by the following advantages:

- Lack of heteropair component mutual diffusion
- A slight mismatch in the lattice constants
- The same chemical properties
- The possibility of creating a heterojunction in already grown structure

**Table 1.** Selected properties of SiC of different polytypes

Parameter	2H-SiC	4H-SiC	6H-SiC	3C-SiC
Stacking order	AB	ABCB	ABCACB	ABC
Jagodzinskii notation	h	hc	hcc	c
Percentage "hexagonality", $\gamma$ (%)	100	50	33	0
Lattice constant (Å)	a = 3.076 c = 5.048	a = 3.073 c = 10.053	a = 3.08 c = 15.117	4.34
Band gap (eV)	3.33	3.26	3	2.39
Thermal conductivity ( $\text{W cm}^{-1} \text{ }^\circ\text{C}^{-1}$ )		3-4	3-4	3-4
Critical breakdown field strength, $E_{\text{cr}}$ ( $\text{MV cm}^{-1}$ )		2-3	2-3	>1.5
Electron mobility, $\mu_n$ ( $\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ) (300 K)		≤850	≤450	≤1000
Saturation rate, $V_s$ ( $\times 10^7 \text{ cm sec}^{-1}$ )		2	2	2.7
Hole mobility, $\mu_p$ ( $\text{cm}^2 \text{ V}^{-1} \text{ sec}^{-1}$ ) (300 K)		≤120	≤100	≤40

**Fig. 4.** Scheme of integration of 3C-SiC cubic lattice into a hexagonal lattice

The most promising is the creation of heterostructures between cubic and one of hexagonal nH-SiC silicon carbide polytypes. To imagine the incorporation of a cubic lattice in a hexagonal one, you should look down on the cube standing on one of its vertices. The projection of this cube on the horizontal plane will have the form of a hexagon (**Fig. 4**). Wherein the growing layer of 3C-SiC will have a different crystal orientation than nH-SiC, used for the growth of substrate. If the initial hexagonal substrate had the orientation of (0001), the grown epitaxial layer will have an orientation of (111).

These crystallographic features of 3C-SiC layers growing, based on nH-SiC substrates, lead to the so-

called "pseudomorphic growth" (Fissel *et al.*, 2000; Takagi *et al.*, 2004). This means that the lattice constants of cubic and hexagonal polytypes are practically identical (lattice mismatch <0.1%) in the plane of growth. In the same time in the direction, perpendicular to the plane of growth, the lattice constants of the cubic and hexagonal polytypes will be different. It shows the theoretical possibility of obtaining near-perfect heterostructures between SiC polytypes. Thus, the 3C-SiC polytype is the most interesting.

#### 4. METHODS OF GROWING LAYERS AND BULK CRYSTALS OF 3C-SiC

Lely method and modified Lely method, used for the obtainment of bulk crystals of SiC hexagonal polytypes, do not allow to grow 3C-SiC. In the 70 s of past century, the technology of producing monocrystals of 3C-SiC by thermal decomposition of trichlorosilane in hydrogen on a heated graphite substrate. However, this method did not allow obtaining crystals with sizes more than a few millimeters. Later, the technology of gas-phase epitaxy of 3C-SiC layers on the surface of silicon substrates was proposed. With this procedure it is possible to obtain the cubic silicon carbide layers of a larger area, but due to the significant mismatch of crystal lattices (~20%) and low growth temperature, limited by silicon melting point, the structural perfection of the produced layers remains low. It is not possible to apply the obtained 3C-SiC layers for the industrial production of semiconductor devices.

Alternative technology of growing the epitaxial layers of cubic silicon carbide is the Sublimation Epitaxy in Vacuum (SEV) 3C-SiC based on substrates of hexagonal polytypes 4H-SiC, 6H-SiC. Previously, it was shown that for obtainment of thick epitaxial layers of 3C-SiC with

good structural perfection based on substrates of different hexagonal silicon carbide polytypes (Lebedev, 2007) with area of  $\sim 0,5-0,8 \text{ cm}^2$ .

SEV method actually is a simplified high-temperature option of molecular beam epitaxy. The advantages of this method include:

- Epitaxy is performed at temperatures of 2100-2300 K, which is a more “natural” conditions for the growth of SiC crystals (spontaneous birth of SiC crystals on the walls of the graphite furnace is observed at 2500-2800 K) and leads to a sharp decrease in the probability of structural defects formation
- SEV method allows to perform the sublimation etching “in situ” before growth to obtain atomically smooth surface and, as a result, get a perfect interface between the epitaxial layers
- Growth occurs in a high vacuum, which reduces uncontrolled doping and its influence on the process of hetero-polytypeepitaxy

Using the SEV method the homo-epitaxial p-n 3C-SiC structures, based on 6H-SiC substrates were obtained (Lebedev *et al.*, 2003). A disadvantage of sublimation epitaxy in general and SEV in particular, is that the growth source is not renewed in the process of growth. With the passage of time this leads to changes in the Si/C ratio in a growth zone and as a result, to poor controllability of epitaxy process. This can lead to appearance of SiC layers, which have finely twinned structure or to formation of lightly doped regions of p-3C-SiC inside n-3C-SiC layer (Savkina *et al.*, 2002; 2003). Nevertheless, the possibility of obtaining high-quality epitaxial 3C-SiC layers, based on 6H-SiC substrates, polytype-homogeneous, thick ( $>100 \text{ m}$ ), of good structural perfection and with a minimum diameter of 25 mm is shown. Given the reach of growth rates  $\sim 200 \text{ m h}^{-1}$ , the thickness of these layers during multiple processes can be increased to a size typical for bulk SiC ingots.

More promising is the use of these structures as seeds for growing ingots of bulk 3C-SiC by modified method Lely, where the growth rate still several times higher. Such ingot can further be separated into monocrystalline substrate with the help standard techniques, which is used for producing the bars of hexagonal silicon carbide. Thus, there are prerequisites for the development of technology for producing bulk crystals of 3C-SiC for commercial use.

## 5. CONCLUSION

It should be expected that hetero-polytype structures will have a higher structural perfection than heterojunctions between semiconductors with different chemical nature. SiC is noyable among other polytype compounds as by having a large number of stable polytypes, by a large difference in their electrophysical properties and by high thermal, chemical and radiation resistance. Thus, we can assume that the creation of devices based on SiC hetero-polytype structures will be one of the most important trends in semiconductor electronics in the near future.

## 6. FINDINGS

In recent years a considerable progress in the development of power devices, based on SiC, including microwave range was achieved. Works in this direction are stimulated by the unique electro-physical properties of silicon carbide: High critical strength of the field (breakdown field), high thermal conductivity, high electrons saturation velocities, the ability to operate at high temperatures. The main problem hindering the widespread commercialization of power devices made of silicon carbide is the degradation of p-n structures during the passing of a direct current of high density. The reason to this is the formation of cubic SiC layers inside the hexagonal due to the displacement of an atom from the hexagonal positions of crystal lattice to cubical. This occurs at a value of direct current, sufficient to overcome the barrier, which corresponds to a displacement of an atom in a different position. Natural is the assumption that this effect will be absent in hetero-polytype structures of 3C-6H SiC, therefore the cubical silicon carbide polytype is the most promising material for the manufacturing of power electronics devices. However, this requires experimental confirmation.

## 7. ACKNOWLEDGEMENT

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