



Comparison Among GAAS and SiC: Energy Dispersion Study

KEYWORDS

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ABSTRACT This paper compares the characteristics of SiC and GaAs with respect to physical parameters. There are number of factors that contribute to the reliability of SiC – wide band gap. Typical features include high power, high frequency, high thermal conductivity and higher doping concentration, small depletion width results in reduction of specific “on” resistance. These properties equip SiC with high breakdown voltage and higher efficiency. A comparative study of typical properties of SiC and GaAs is done and it is observed that SiC is superior.

I. INTRODUCTION

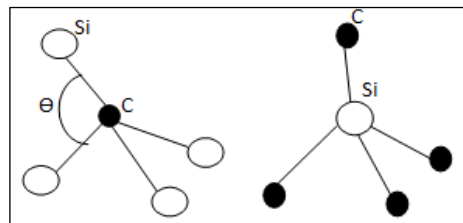
Silicon carbide was first observed in 1824 by a Swedish scientist, Jons Jacob Berzelius, [1] while naturally occurring SiC was discovered by Henri Moissan in 1905, he found small hexagonal platelets in a meteorite. The mineral is now called Moissanite [1]. This has also become the name of commercial gemstones made from SiC. The history of man-made SiC starts dates back to 1891, when Acheson produced SiC. Later, in the 1950s, when research on solid state electronic devices has started, SiC was one of the semiconductor materials studied. In 1955[1] Lely introduced a crystal growth technique to produce high quality bulk SiC, but fabrication was not possible. Later, in 1978 seeded sublimation epitaxy or modified Lely method was developed by Tairov and Tsvetkov[1]. Recently the most commonly used technique for epitaxial growth of SiC is the vapour phase epitaxy (VPE) which is usually found in a chemical vapor deposition (CVD) reactor.

1.1 General Silicon Carbide Information

Silicon carbide is composed of tetrahedral of carbon and silicon atoms with strong bonds in the crystal lattice. This produces a very hard and strong material. This is not attacked by any acids or alkalis or molten salts up to 800°C. In air, SiC forms a protective silicon oxide coating at 1200°C which can be used up to 1600°C [6]. The high thermal conductivity coupled with low thermal expansion and high strength gives this material exceptional thermal shock resistant qualities. Chemical purity, resistance to chemical attack at temperature, and strength retention at high temperatures have made this material very popular as wafer tray supports and paddles in semiconductor furnaces [6]. The electrical conduction of the material has led to its use in resistance heating elements for electric furnaces, and as a key component in thermostats (temperature variable resistors) and in varistors (voltage variable resistors).

1.2 Structure and Polytypes

SiC has a crystalline structure and its polytypic in nature. The influence of polytypism on the physical properties of SiC is presented.



(a) (b)
Figure 1 Basic elements of SiC crystals: Tetrahedrons containing (a) one C and four Si (b) one Si and four C atoms.

SiC is a binary compound containing equal amount of Si and C, where Si-C bonds are nearly covalent, with an ionic contribution of 12% (Si positively, C negatively charged). The smallest building element of any SiC lattice is a tetrahedron of a Si (C) atom surrounded by four C (Si) atoms (Fig.1) in strong sp^3 -bonds. Therefore the first neighbor shell configuration is identical for all atoms in any crystal-line structure of SiC. The tetrahedral bond angle θ , as depicted in Fig. 1, is 70.529° for the ideal bond configuration. The most important characteristic properties of SiC is polytypism – a one dimension-type polymorphism. Upto date 250 different polytypes of SiC are known [2].

1.3 Physical properties

The different poly-types have wide ranging physical properties. 3C-SiC has the highest electron mobility and saturation velocity because of reduced phonon scattering resulting from the higher symmetry. The band gaps differ widely among the poly-types ranging from 2.3 eV for 3C-SiC to 3 eV in 6H SiC to 3.3 eV for 2H-SiC. In general, the greater the quartzite component, the larger the band gap. Among the SiC poly-types, 6H is most easily prepared and best studied, while the 3C and 4H poly-types are attracting more attention for their superior electronic properties. The poly-typism of SiC makes it nontrivial to grow single-phase material, but it also offers some potential advantages - if crystal growth methods can be developed sufficiently, then hetero junctions of different SiC poly-types can be prepared and applied in electronic devices.[6]

1.4 Electrical properties

The basic parameters and their reference values for different polyphases of SiC is listed in Table 1 at reference temperature 300o k.

Parameters	3C-SiC	4H-SiC	6H-SiC
Breakdown field	$\sim = 10^6$ V/cm	$(3\div 5) \times 10^6$ V/cm	$(3\div 5) \times 10^6$ V/cm
Electrons Mobility	≤ 800 cm ² V ⁻¹ s ⁻¹	≤ 900 cm ² V ⁻¹ s ⁻¹	≤ 900 cm ² V ⁻¹ s ⁻¹
Holes Mobility	≤ 320 cm ² V ⁻¹ s ⁻¹	≤ 120 cm ² V ⁻¹ s ⁻¹	≤ 90 cm ² V ⁻¹ s ⁻¹
Diffusion coefficient electrons	≤ 20 cm ² /s	≤ 22 cm ² /s	≤ 90 cm ² /s
Diffusion coefficient holes	≤ 8 cm ² /s	≤ 3 cm ² /s	≤ 2 cm ² /s
Electron thermal velocity	2.0×10^5 m/s	1.9×10^5 m/s	1.5×10^5 m/s
Hole thermal velocity	1.5×10^5 m/s	1.2×10^5 m/s	1.2×10^5 m/s

1.5 Polymorphs of Silicon Carbide

Many compound materials exhibit polymorphism i.e. they can exist in different structures called polymorphs. Silicon carbide (SiC) is unique in this regard as more than 250 polymorphs of silicon carbide had been identified. The polymorphs of SiC include various amorphous phases observed in thin films and fibers, as well as a large family of similar crystalline structures called poly-types. The atoms of those layers can be arranged in three configurations, A, B or C, to achieve closest packing. The stacking sequence of those configurations defines the crystal structure, where the unit cell is the shortest periodically repeated sequence of the stacking sequence.

1.6 Categorizing the poly-types

A shorthand has been developed to catalogue the literally infinite number of possible poly-type crystal structures: Let us define three SiC bi-layer structures (that is 3 atoms with two bonds in (Figure 2, 3, 4) in the pictures below) and label them as A, B and C. Elements A and B do not change the orientation of the bi-layer (except for possible rotation by 120°, which does not change the lattice and is ignored hereafter); the only difference between A and B is shift of the lattice. Element C, however, twists the lattice by 60°(6).

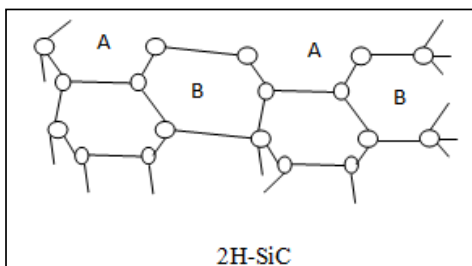


Fig. 2

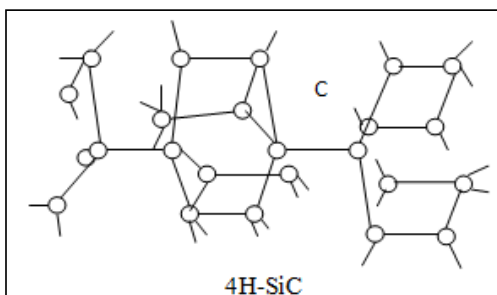


Fig. 3

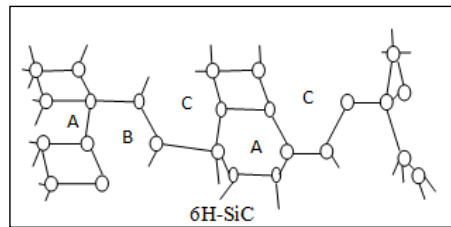


Fig. 4

Polymorphs of Silicon carbide

Using those A, B, C elements, any SiC poly-type can be formed (for example of the hexagonal poly-types 2H, 4H and 6H). The 2H-SiC structure is equivalent to that of quartzite and is composed of only elements A and B stacked as ABABAB. The 4H-SiC unit cell is twice longer, and the second half is twisted compared to 2H-SiC, forming the ABCB stacking. The 6H-SiC cell is triple that of 2H and the stacking sequence is ABCACB. The cubic 3C-SiC has ABC stacking.

2. Wide Band gap materials

Table 2 shows some characteristic properties of different wide bandgap semiconductors, selected from the viewpoint of Microelectronics applications. Silicon and GaAs are also included for comparison. Having a large bandgap (2.3–6.2 eV), it is much more difficult to thermally excite electrons from the valence band to the conduction band. For example in SiC the probability of thermal excitation of an electron over the bandgap is 10-26 at room temperature, i.e. there are no thermally excited electrons in the conduction band. The wide bandgap is also accompanied by considerably higher breakdown voltage as compared to silicon and GaAs. This means that for power devices with similar blocking voltage capabilities, the one made of silicon must have about 100 times lower doping level in a 10 times thicker layer, as compared to a SiC device. Thick layers with low doping levels will have high resistance, increasing the power loss and heat generation in the device. Therefore, the use of wide bandgap materials, like SiC, gives the possibility to increase the blocking voltages for high power devices, as well as to make devices smaller and to reduce power losses. For switching devices, the high saturation drift velocity of carriers in combination with the high breakdown voltage, makes the wide bandgap semiconductors superior to most of the common semiconductor materials when it comes to impedance matching, output power and switching loss. As the power losses are much lower than in silicon, and the thermal conductivity and thermal stability are much higher, the need for surrounding cooling system is reduced. With superior material properties, SiC power devices show great potential for high-power density, high temperature switching applications. SiC is a wide band gap semiconductor which is very attractive for specific high power, high frequency and high temperature applications.

2.1 SiC-Break down Voltage

The greater higher breakdown electrical field of SiC compared to other semi conductors enables reduction of drift region thickness by nearly 10 times which combined with 10 times higher doping concentration permits a roughly 100 times decrease in the drift region resistance that dominates the total ON resistance. It is seen that break down voltage decrease with increasing doping concentration [1]. 4H-SiC has higher doping concentration depletion width in 4H-SiC is smaller because of larger doping concentration results in reduction in the specific ON resistance.

Critical electrical field for breakdown in silicon is given by $EC = 4010 \text{ ND}^{1/8}$ and for 4H-SiC is given by $EC = 3.3 \times 10^4 \text{ ND}^{1/8}$. [1]. For Same doping concentration the critical field in 4H-SiC is 8.2 times larger than silicon. The larger critical field results in larger Balligas figure of merit [1].

2.2 SiC –High Efficiency

The wide band gap as well the high breakdown electrical field of SiC permits faster switching that increases switching frequency which improves system efficiency with a fixed switching frequency [1], the energy losses when a device is conducting current or blocking voltage are much smaller as well due to 100 times lower on resistance and much lower leakage current than SiC and GaAs which further improves the circuit efficiency by reduction energy losses when device stays ON and OFF[1]. Among the wide band gap material, SiC and GaAs the comparable materials properties to SiC such as band gap, electron mobility, saturation velocity lower resistance, cheap substrates like Si and sapphire, further more native oxide can be grown on SiC etc. makes SiC the wider used materials.

Table 2 Properties of wide bandgap semiconductors

Property	Si	GaAs	4H-SiC
Bandgap at 300K (eV)	1.11	1.43	3.26
Lattice parameters (Å)	5.43	5.65	a=3.08 c=10.08
Lower intrinsic carrier concentration (n _i cm ⁻³)	1.5*10 ¹⁰	1.8*10 ⁶	8.2*10 ⁻⁹
Melting point (°C)	1410	1240	Sublimes > 2800
Electron mobility (10 ⁻⁴ m ² /Vs)	1400	8500	900
Hole mobility (10 ⁻⁴ m ² /Vs)	600	400	40
Breakdown electric field 10 ⁸ V/m	0.3	0.4	2.2
Thermal conductivity (W/m K)	150	54	490
Saturation drift velocity (10 ⁵ m/s)	1.0	2.0	2.7
Dielectric constant	11.8	12.8	10
Mohs Hardness	7	4.5	9.2-9.3
Figure of merit = $E_s / (\mu_n E_c^2)$	23.15	68*10 ⁻⁹	7.9*10.3

3. Energy Dispersion in SiC and GaAs

The conduction and valence band energy dispersion is studied for GaAs and SiC for the Miller indices vector (1 0 0). The study parameters are listed in Table 3.

Table 3 Parameters used in Simulation Study

S.No	Parameter	Silicon Carbide (SiC)	Gallium Arsenide (GaAs)
1.	gap energy [eV]	$E_g = 2.36$	$E_g = 1.424$
2.	valence dipole energy [eV]	$E_p = 17.667$	$E_p = 28.8$
3.	luttinger parameter #1	$g_1 = 4.23$	$g_1 = 6.79$
4.	luttinger parameter #1	$g_2 = 0.31$	$g_2 = 1.924$

5.	luttinger parameter #1	$g_3 = 1.46$	$g_3 = 2.782$
6.	spin orbit coupling energy [eV]	$\Delta = 0.341$	$\Delta = 0.341$
7.	conduction band mass [m ₀]	$m_c = 0.32$	$m_c = 0.065$
8.	valence band initial energy [eV]	$E_v = 0$	$E_v = 0$
9.	conduction band initial energy [eV]	$E_c = E_v + E_g$	$E_c = E_v + E_g$
10.	speed of light [m/sec]	$c = 3e8$	$c = 3e8$
11.	free electron mass [eV*sec ² /m ²]	$m_0 = 0.51e6/c^2$	$m_0 = 0.51e6/c^2$
12.	Planck's constant [eV*sec]	$h = 4.135e-15$	$h = 4.135e-15$
13.	\hbar [eV*sec]	$\hbar = h/(2*\pi)$	$\hbar = h/(2*\pi)$
14.	\hbar [eV*m ²]	$\hbar_m = \hbar/m_0$	$\hbar_m = \hbar/m_0$
15.	lattice const [m]	$a = 4.3596e-10$	$a = 5.6532e-10$

The energy dispersion of carriers (both electrons & holes) and conduction band is obtained through simulation study (in MATLAB). The sequence of steps are given below;

Step1: The input parameters are energy gap, valence dipole energy, luttinger parameter, spin orbit coupling energy, conduction band mass, valence band initial energy, conduction band initial energy, speed of light, free electron mass, planks constant and lattice constant. The values are listed in Table 3

Step 2: Initial values are calculated.

Step3: Miller indices values are calculated using $k = (-0.22*\pi/a); (0.01*2*\pi/a); (0.1*2*\pi/a)$ where a = lattice constant.

Note: k-x, k-y & k-z is calculated.

Step4: Forming matrices using the values.

Step5: Conduction and Valence band energy dispersion for electrons, heavy holes, light holes graphs are plotted.

4. Results and Discussion

From the simulation results the SiC possession good conduction and valence band energy dispersion, for electrons, heavily doped heavy hole, light hole, which leads to good wide band gap with high power density, high temperatures, fast switching, high efficiency high breakdown voltage than GaAs. Electron mobility is about 900 x 10⁻⁴ m²/Vs in case of SiC and 8500 x 10⁻⁴ m²/Vs in case of GaAs, The hole mobility is about 40 x 10⁻⁴ m²/Vs in case of SiC and 400 x 10⁻⁴ m²/Vs in case of GaAs, since electron and hole mobility is high in the case of SiC, high Breakdown electrical field of about 2.2 x 10⁸ V/m is achieved. Two SiC polytypes are popular in SiC research: 6H – SiC and 4H-SiC (6H SiC being dominant). But recently 4H-SiC have become more dominant poly because of lattice anisotropy, which mean the mobilities of the material in the vertical and horizontal planes are not the same where as the mobilities in 4H – SiC are identical along the two planes. From the above discussion it is observed that SiC is a superior material. The plots are shown in figure 5 and figure 6 (Appendix - I)

5. Conclusion

In this paper, the energy dispersion behaviour for the

carriers (both electrons & holes) in SiC & GaAs materials by considering physical parameters effects is presented. These two materials are studied extensively for high speed, high frequency and high power switching applications.

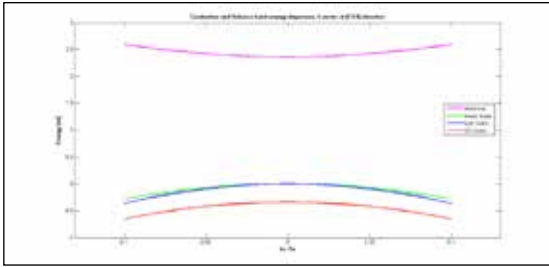


Fig. 5 The Conduction and Valence band energy dispersion , k vector at (1 0 0) for GaAs

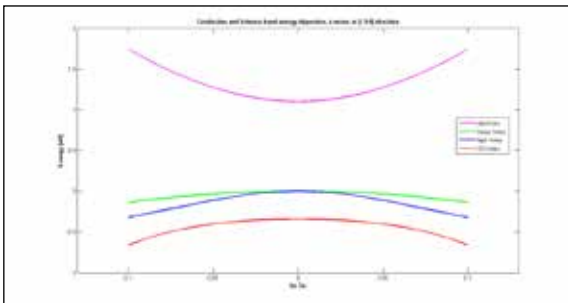


Fig. 6 The conduction and Valence band energy dispersion ,k vector (1 0 0) for SiC

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