MITSUBISHI ELECTRIC

SiC Lecture series

3. Crystal Structure and Energy Band of SiC

Crystal Structure and Energy Band of SiC

Silicon Carbide (SiC), a semiconductor material, is a crystal composed of silicon (Si) and carbon (C) in a stoichiometric ratio of 1:1, making it a type of compound semiconductor. Since both silicon and carbon are Group IV elements, each atom has four covalent bonding orbitals. Silicon and carbon atoms alternate in a tetrahedral coordination to form the crystal structure.

The crystal structure of SiC consists of the densest possible stacking of unit structures, each composed of a pair of Si and C atoms. SiC has numerous stable crystal forms (polytypes) that differ in the stacking sequence of these unit structures. Figure 1 illustrates the stacking methods for the densest possible arrangement of unit structures composed of Si and C atoms in a planar configuration. When stacking one planar structure on top of another, there are two possible stacking positions: site B or site C on plane A. This allows for many possible stacking sequences. Additionally, in SiC, the energy differences due to variations in stacking sequences are relatively small, resulting in the existence of crystals with different stacking structures (periods).

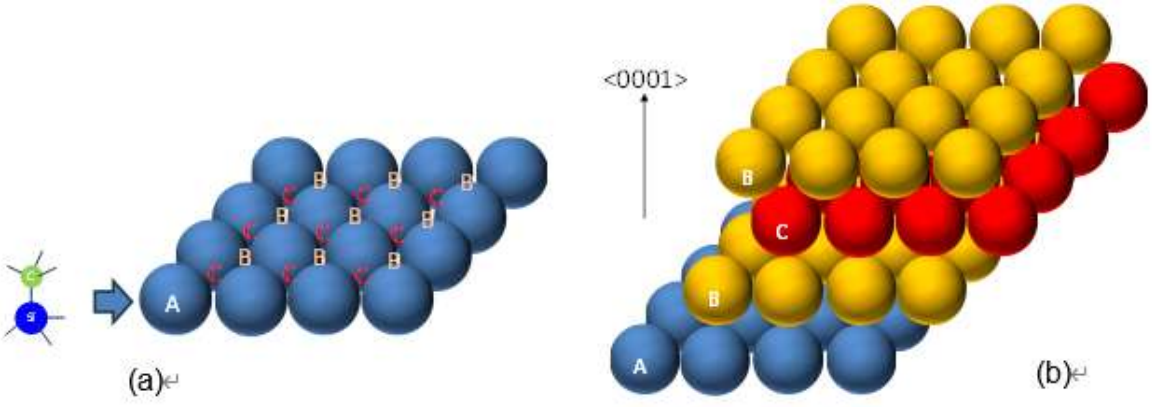

Figure 1 (a) Unit structure of Si-C pairs arranged in a plane and the sites for stacking additional unit structures on top of it (b) Stacking sequence of 4H-SiC

Representative polytypes of SiC include 3C, 4H, and 6H. Here, the numbers indicate the stacking period, with C representing cubic and H representing hexagonal. The dominant polytype formed is determined by the conditions, such as temperature, during the crystal growth process. The stacking sequence of 4H-SiC is shown in Figure 1 (b), and the stacking sequences of various polytypes are summarized in Table 1.

Table 1 Stacking Sequences of Various SiC Polytypes

Polytype	Stacking sequence
2H	AB‥
3C	ABC‥‥
4H	ABCB‥‥
6H	ABCACB‥‥‥
15R	ABCACBCABACABCB‥

Silicon carbide (SiC) is a semiconductor with an indirect transition energy band structure, and its bandgap energy varies depending on the polytype. For example, in the case of 4H-SiC, the bandgap energy is approximately three times that of silicon (Si), measuring 3.26 eV.

Incidentally, the energy of visible light ranges from 1.7 eV to 3.3 eV, making high-purity 4H-SiC crystals transparent to visible light. High-concentration n-type SiC crystals have many carrier electrons in the conduction band. These electrons absorb specific energies of visible light due to the band structure, causing SiC substrates used in device fabrication to exhibit yellow to green colors.

In general, the bandgap energy of a semiconductor tends to increase as the bonding distance (atomic radius) between constituent atoms decreases. For example, the bandgap energy of SiC is larger than that of Si (1.1 eV) but smaller than that of C (diamond) (5.5 eV). Additionally, since the atomic distance in GaN is 0.192 nm and that in SiC is 0.189 nm, their bandgap energies are close, with GaN having a bandgap energy of 3.4 eV.

A larger bandgap energy indicates that more energy is required to generate electron-hole pairs through electron excitation from the valence band to the conduction band. In other words, it signifies a higher electric field required to cause dielectric breakdown, which determines the performance of power devices. Consequently, SiC has a higher voltage tolerance compared to the mainstream material Si, making it desirable as a semiconductor for power devices. Table 2 shows the bandgap energies of various SiC polytypes.

Table 2 Bandgap Energies of Different SiC Polytypes

Polytype	Band gap energy
2H	3.33 eV
3C	2.39 eV
4H	3.26 eV
6H	3.02 eV
15R	2.99 eV

Among the stable polytypes, 4H-SiC is typically used for power devices in power conversion applications due to its high dielectric breakdown field strength and low anisotropy in electrical characteristics. Today, most commercially available SiC substrates for power devices are n-type conductive 4H-SiC, and devices are fabricated on the 4° off-axis (0001) plane (the plane where the Si dangling bonds extend vertically from the surface).

Within SiC crystals, there can be crystal defects known as stacking faults, where the stacking sequence of Si-C layers is locally incorrect. When the stacking sequence changes, the energy levels of the conduction band and valence band also change. For example, if a different stacking sequence partially intrudes into 4H-SiC, the energy gap in this region becomes smaller than that of the surrounding area, forming a well-like potential. When bipolar current flows through this region, the

carrier electrons and holes can be trapped, affecting the electrical conduction of the SiC device, such as by increasing the on-resistance. Therefore, careful consideration is required when fabricating devices. Mitsubishi Electric addresses these issues through various tests and the design of proprietary device structures.

January 2025
Power Device Works