Department of Physics, Chemistry and Biology

Master's Thesis

Optical properties of cubic silicon carbide

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Linköping, January 1, 2015

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Abstract

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Contents

1 Introduction

This thesis describes the growth and optical characterization of cubic silicon carbide (*SiC*). SiC is a semiconductor which has attracted academic interest since the 19:th century, when it was first fabricated and used as an abrasive [1]. SiC has been found to be a very stable material. It exhibits a high chemical inertness [2], and is currently commonly used in high power and high temperature applications due to its ability to survive in such environments [Citation?].

SiC is a material which exists in a large number of different polytypes, the most common of which are hexagonal, cubic and rhombohedral. The work described in this thesis deals with the only cubic polytype, denoted *3C*. This is one of the structurally most simple polytypes. Compared to the hexagonal counterparts 4H and 6H, the 3C polytype has for a long time been difficult to fabricate in good quality single crystal form, and is therefore less studied than the hexagonal types [Citation needed]. Recently a method of fabricating good quality material has been reported, using sublimation epitaxy [3]. The method, called fast sublimation growth process (*FSGP*), has been used to grow the samples used in the work described in this thesis.

Cubic SiC has many interesting material properties, which have given rise to several proposals of applications for 3C. Some of these proposed applications are not possible to create with the hexagonal polytypes, but are unique for the cubic polytype. One such application is the use of boron doped 3C in an impurity photovoltaic solar cell (*IPV*). This is suitable for 3C due to its band gap size together with the binding energy of boron as an acceptor in the material, which is almost ideal for photovoltaic cell material. This would give a significant increase in photovoltaic cell efficiency compared to the currently commercially available alternatives [4][Current efficiencies citation needed]. Another proposed application of 3C is as a photo-electrode in a photoelectrochemical cell used for water splitting [5, 6], where solar energy is used in the decomposition of water into hydrogen and oxygen gas.

This thesis deals with characterization of the optical properties of boron doped

3C-SiC. This is done using absorption spectroscopy, photoluminescence spectroscopy, ... Chapter 2.3 gives an introduction to silicon carbide, its structure and properties. Chapter 3 describes the process of growing the material. Both growth of undoped and boron doped material is described here. In chapter 4 a description of the different characterization methods is given, together with a theoretical description of what the measurements can tell about material properties. Chapter 5 describes how the experiments were done and chapter 6 describes the results obtained from the experiments. The results are discussed in chapter 7. Chapters 8 and 9 discuss what has been learned about the material and how the work should be continued in the future.

2

An introduction to silicon carbide

This chapter describes the relevant properties of SiC. Section 2.1 describes the atomic arrangement in the material, and some different arrangements are discussed. Section 2.2 discusses the energy band structure of 3C-SiC. Finally section 2.3 describes the mechanism and some effects of doping in 3C-SiC.

2.1 Crystal structure

Silicon carbide is a crystalline material consisting of silicon and carbon atoms. The crystalline nature of the material means that the atoms are arranged in a periodically repeating structure called a *lattice*. For given chemical elements there may be several different ways to arrange the atoms in a lattice, i.e. different chemical compounds of the same types of atoms. This is called *polytypism*, where the different lattice structures are called *polytypes* of the material. SiC has a large number of different polytypes. There are more than 250 known polytypes of SiC [7]. The different polytypes can be described as different stacking orders of layers of atoms [8]. Figure 2.1 shows one such layer. Here each circle symbolizes one carbon and one silicon atom, displaced a small distance from each other. This pair of atoms is called the *base* of the crystal.

The marked hexagon in figure 2.1 marks an area of the crystal which can be used to define the different polytypes. Figure 2.2 shows the same area but with different placements of the base atoms. Again each sphere is one crystal base. The three different placements A, B and C describe how each layer is placed compared to the one above. It should be noted that the plane in figure 2.1 is the same as A in figure 2.2.

The stacking orders of three of the most common polytypes is shown in figure 2.3. The depicted orders of the layers refers to one period in the periodic structure. The names for the different polytypes are stated at the top of the figure. The digit in

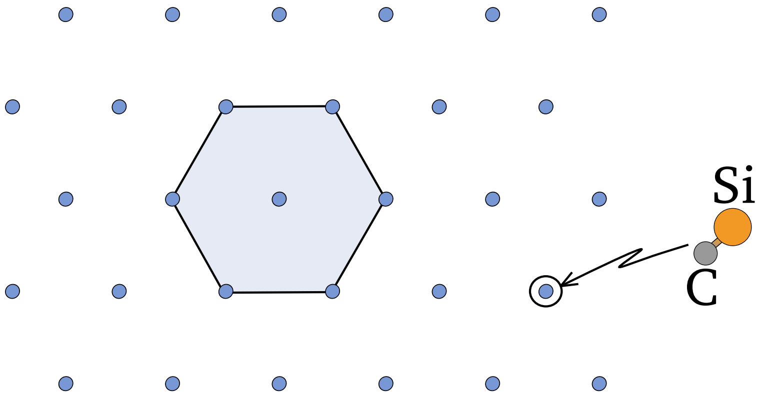

Figure 2.1: Atomic arrangement of the atoms in each layer. Here each sphere corresponds to one carbon and one silicon atom, as shown by the arrow.

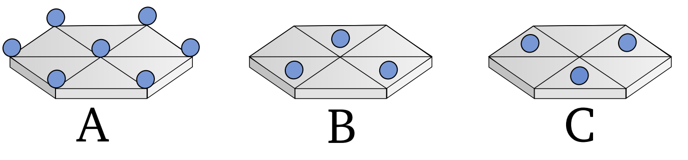

Figure 2.2: Different atomic placements for the layers

the name refers to the number of layers of a period and the letter denotes the crystal symmetry. The letter *H* denotes the hexagonal polytypes, whereas *C* stands for the cubic polytype. Another common polytype is the 6H-SiC, which thus is a hexagonal structure with a period of six base layers. It should be noted that the 2H structure is the wurtzite structure and the 3C is the zincblende structure.

2.2 Band structure

2.3 Doping in 3C

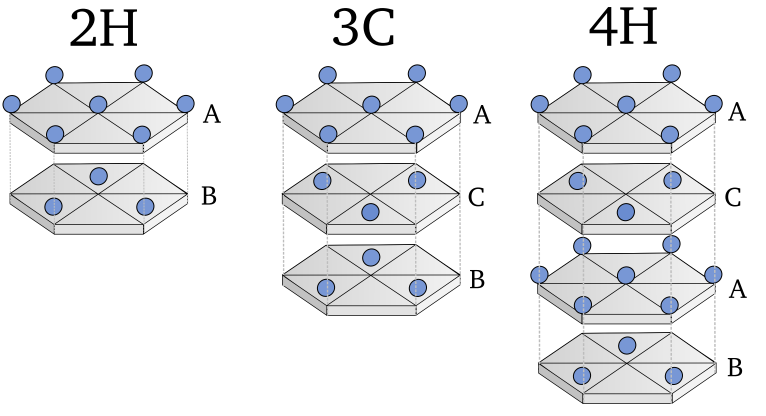

Figure 2.3: Stacking order for the three most simple polytypes.

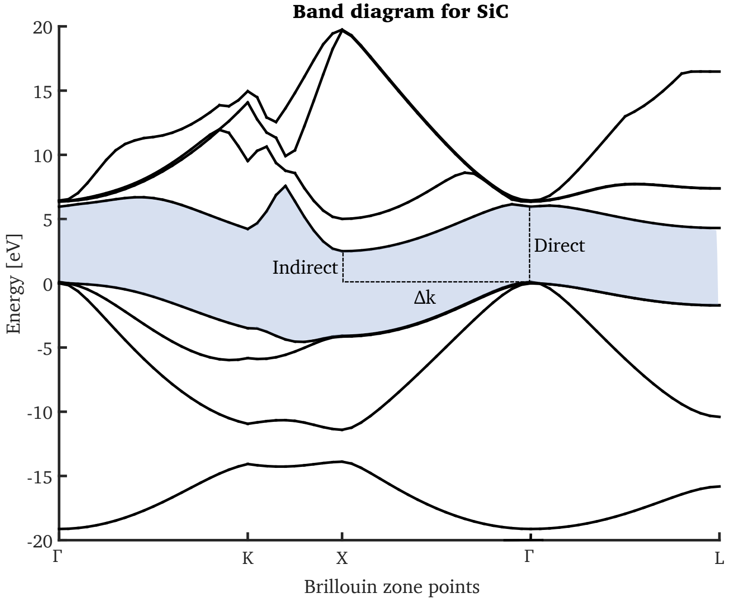

Figure 2.4: The band diagram of SiC at ambient conditions for different positions in the Brillouin zone. The indirect and direct band gaps are marked in the figure. The marked area is the band gap. The energy levels have been obtained using the pseudopotential method, as described in [9].

3

Growth techniques

This chapter describes the growth technique.

4

Characterization techniques

This chapter will describe the different characterization techniques.

4.1 Absorption measurements

Here will follow a description of how the absorption measurements were done.

5 Experimental setup

Here the setups for the various experiments will be described.

6 Results

This chapter describes the results obtained from the experiments.

7

Discussion

In this chapter I will discuss the results of the work.

8 Conclusion

The conclusions drawn from this work are described here.

9

Future work

In this chapter I will write some of my thought of what is to be done in the future concerning these topics.

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