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Polarities of AlN films and underlying 3C-SiC intermediate layers grown on (1 1 1) Si substrates

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Abstract

The hydride vapor phase epitaxy (HVPE) of {0 0 0 1} AlN films on {1 1 1} Si substrates covered with epitaxial {1 1 1} cubic SiC (3C-SiC intermediate layers) was carried out. 3C-SiC intermediate layers are essential to obtain high-quality AlN films on Si substrates, because specular AlN films are obtained with 3C-SiC intermediate layers, whereas rough AlN films are obtained without 3C-SiC intermediate layers. We determined the polarities of AlN films and the underlying 3C-SiC intermediate layers by convergent beam electron diffraction (CBED) using transmission electron microscopy. For the first time, the polarities of the AlN films and the 3C-SiC intermediate layers were determined as Al and Si polarities, respectively. The AlN films were hardly etched by aqueous KOH solution, thereby indicating Al polarity. This supports the results obtained by CBED. The result is also consistent with electrostatic arguments. An interfacial structure was proposed. The 3C-SiC intermediate layers are promising for the HVPE of AlN films on Si substrates.

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1. Introduction

Aluminum nitride (AlN) is the primary candidate for deep ultraviolet emitters and advanced electronic devices due to its wide band gap and high thermal conductivity. Since there is a lack of native substrates on which AlN can be grown, it is grown on foreign substrates. Typically, hexagonal silicon carbide (6H-SiC) or sapphire is used as a substrate for AlN growth. However, these substrates are small in area and expensive (6H-SiC), and they have low thermal conductivity (sapphire). Moreover, the chemical stability and hardness of these substrates hinder their removal after AlN growth. In contrast, silicon (Si) substrates are large in area and inexpensive, and they have high thermal conductivity. In addition, they can be easily removed after AlN growth. This feature of Si substrates, in particular, provides good flexibility in the design and fabrication of electronic devices. The growth of AlN on Si substrates, therefore, is an attractive method to circumvent the above-mentioned hindrances. However, such growth leads to large lattice mismatch (19%) and a large difference between the thermal expansion coefficients of AlN and Si (47%). These mismatches in turn generate dislocations and stresses that deteriorate the AlN grown on Si.

On the other hand, {1 1 1}-oriented cubic (3C)–SiC has a lattice structure close to that of {0 0 0 1} AlN—the basal plane of AlN. The lattice mismatch and difference between the thermal expansion coefficients of {0 0 0 1} AlN and {1 1 1} 3C-SiC is 1% and 18%, respectively, which are much smaller than those between AlN and Si—19% and 47%, respectively. Thus, it is expected that high-quality

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AlN could be obtained by using 3C-SiC as the intermediate layer between AlN and Si. Previously, our group and two other research groups reported the growth of GaN on Si using 3C-SiC intermediate layers [1–6]. However, there is no report on the growth of AlN on Si using 3C-SiC intermediate layers to date. The lattice mismatch and difference between the thermal expansion coefficients of AlN and 3C-SiC is 1% and 18%, respectively, which are much smaller than those between GaN and 3C-SiC—3% and 24%, respectively. Therefore, AlN grown on Si using 3C-SiC intermediate layers is a promising alternative. Table 1 summarizes the material properties of the various components of this system. The hydride vapor phase epitaxy (HVPE) [7] of AlN on Si using 3C-SiC intermediate layers has been performed for the first time.

The most common growth direction for AlN is that normal to the basal plane {0 0 0 1}, along the direction ⟨0 0 0 1⟩. AlN lacks inversion symmetry along ⟨0 0 0 1⟩ and the two directions [0 0 0 1] and [0 0 0 $\bar{1}$] are distinct [8–10]. This property is called the "polarity" of a crystal, and it can be explained in terms of the bond configuration.

Table 1
Lattice parameters (at 300 K) and averaged thermal expansion coefficients of various semiconductor materials

Material	Symmetry	Lattice parameter (Å)	Linear thermal expansion coefficient (K^{-1})
AlN (wurtzite)	Hexagonal	$a = 3.1114$	5.3×10^{-6}
		$c = 4.9792$	4.2×10^{-6}
GaN (wurtzite)	Hexagonal	$a = 3.189$	5.6×10^{-6}
		$c = 5.185$	3.2×10^{-6}
(1 1 1) 3C-SiC	Cubic	$a = 4.3589$	4.5×10^{-6}
		$a^* = 3.082$	
(1 1 1) Si	Cubic	$a = 5.4309$	3.6×10^{-6}
		$a^* = 3.840$	

a^* is a virtual lattice parameter that corresponds to the a-axis in a hexagonal lattice. It is calculated by using $a^* = 1.4142a/2$ in order to compare the lattice parameters for different symmetries.

For single bonds along ⟨0 0 0 1⟩ from cations (Al) to anions (N), the polarity is defined as "Al polarity" and its direction is [0 0 0 1]. On the contrary, for single bonds along ⟨0 0 0 1⟩ from anions (N) to cations (Al), the polarity is defined as "N polarity" and its direction is [0 0 0 $\bar{1}$]. Further, as mentioned previously, {1 1 1} 3C-SiC has a lattice structure close to that of {0 0 0 1} AlN. By a similar argument, in the case of {1 1 1} 3C-SiC, for single bonds along ⟨1 1 1⟩ from cations (Si) to anions (C), the polarity is defined as "Si polarity" and its direction is [1 1 1]. On the contrary, for single bonds along ⟨1 1 1⟩ from anions (C) to cations (Si), the polarity is defined as "C polarity" and its direction is [$\bar{1}$ $\bar{1}$ $\bar{1}$]. The crystal structures of AlN and 3C-SiC are shown in Fig. 1a and b, respectively.

AlN exhibits different properties depending on the polarity. For example, the etching of AlN using an aqueous alkaline solution (KOH and NaOH) with Al polarity resulted in a smooth surface, while that using a solution with N polarity resulted in a rough surface [9,10]. Further, the polarization of AlN is dependent on the polarity. Precise determination and control of polarity is therefore crucial to device fabrication [8]. However, there are few reports on the polarity of AlN [9,10]; moreover, the polarity of AlN grown on Si using 3C-SiC intermediate layers is unknown. In this paper, for the first time, we have determined the polarity of AlN grown on Si using 3C-SiC intermediate layers. The polarity was determined by convergent beam electron diffraction (CBED) using transmission electron microscopy (TEM) [11] and by etching AlN using an aqueous KOH solution [9,10].

2. Experimental procedure

Prior to sample preparation, (1 1 1) Si substrates were subjected to thermal cleaning at a temperature of 1100 °C with hydrogen in a horizontal reactor. Carbonization of Si substrates was performed using C_3H_8 at a temperature of 1100 °C. The carbonized Si substrates served as a template for subsequent SiC growth [12,13]. 3C-SiC intermediate layers with a thickness of 1 μm were prepared on the Si

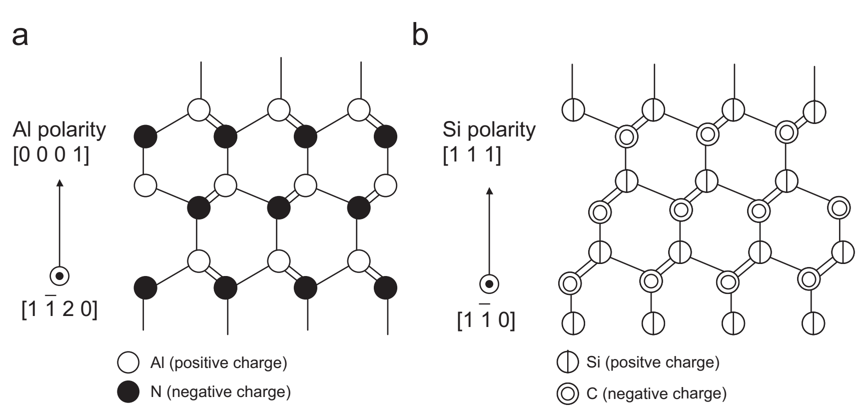

Fig. 1. Crystal structure of (a) AlN and (b) 3C-SiC projected along [1 1 $\bar{2}$ 0] and [1 $\bar{1}$ 0], respectively. Arrows indicate the direction of [0 0 0 1] (Al polarity) for AlN as well as the direction of [1 1 1] (Si polarity) for 3C-SiC.