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Characterization of major in-grown stacking faults in 4H-SiC epilayers

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ABSTRACT

The optical properties of major in-grown stacking faults (IGSFs) in 4H-SiC epilayers have been characterized by micro-photoluminescence (micro-PL) spectroscopy and its intensity mapping. Strong PL emissions from the IGSFs are observed even at room temperature. Three kinds of IGSFs have been identified in the samples based on the micro-PL spectra. Each kind of IGSF shows the distinct PL emission peak located at 460, 480, and 500 nm, respectively. The micro-PL intensity mapping at the emission band of each IGSF has been performed to spatially profile the IGSF. The shapes, distributions, and densities of IGSFs in the epilayers are then presented. The microstructure of each IGSF has been revealed by high-resolution transmission electron microscopy observations. The stacking sequences of three IGSFs are determined as (4,4), (3,5), and (6,0) in the Zhdanov's notation, respectively, which apparently differ from the perfect 4H-SiC, (2,2). Three identified IGSFs are then classified as quadruple Shockley SFs, triple Shockley SFs, and double Shockley SFs, respectively, based on the shear formation model.

1. Introduction

Silicon carbide (SiC), as a wide bandgap semiconductor, is an attractive material for developing high-power, high-temperature, and high-frequency devices, owing to its superior properties [1]. However, there are several critical issues related to the crystalline quality (defects) needed to be solved before the full commercialization of SiC devices. Considering that micropipe defects, known to be the most harmful defects for device performance, are no longer a major problem, other defects, particularly various types of stacking faults (SFs) remain a challenge. This challenge becomes even more challenging with increasing the thickness of epilayers, because the area of the SFs is proportional to the epilayer's thickness. In recent years, SFs in SiC received increasing attention due to their negative impacts on the performance of 4H-SiC devices and on the long-term operation stability [2–6].

SiC can crystallize in over 200 different polytypes. The multiplicity of structures is the consequence of the very low energy necessary to locally change the stacking sequence in any of the crystalline forms of SiC. The formation energy of SFs in SiC, e.g., in 4H-SiC, is experimentally determined to be only 14.7 mJ/m^2 [7], which is about an order of magnitude lower than the energies of corresponding defects in other semiconductors, such as diamond (280 mJ/m^2) [8], Si (55 mJ/m^2) [9], or GaAs (45 mJ/m^2) [10]. Due to the lower formation energy it is relatively easy to generate SFs in 4H-SiC polytype. SFs in 4H-SiC can appear spontaneously during the growth (so-called in-grown SFs, IGSFs) [11,12] or in some later processing steps like annealing [13], oxidation [14], implantation or even in electrically stressed p-i-n diodes [15]. There are several types of IGSFs reported in 4H-SiC epilayers. However, there are still lack of systematic studies on the IGSFs in 4H-SiC epilayers, especially in the one-to-one correlation between the optical property and the microstructure of IGSF. The aim of this paper is to characterize the IGSFs in 4H-SiC epilayers using the micro-photoluminescence (PL) mapping method. The room-temperature micro-PL spectrum from each kind of IGSF is firstly collected to reveal its band energy, and then micro-PL mapping at this band energy is performed to spatially profile the distribution, shape, and density of each IGSF. High-resolution transmission electronic microscopy (TEM) observations are then carried out to determine the stacking sequences of IGSFs. The formation process of IGSFs is also discussed using the shear formation model.

2. Experimental

4H-SiC epilayers were grown on 8° off-axis 4H-SiC (0 0 0 1) n^+ substrates (doping concentration: $5-6\times10^{18}\,\mathrm{cm}^{-3}$) by horizontal hot-wall chemical vapor deposition in a SiH_4–C_3H_8–H_2 system [16]. Epitaxial growth was performed at 1650 °C with a reactor pressure of 80 Torr and the C/Si ratio of 0.9. The growth rate was 12–25 μm/h, and the thickness of epilayer was approximately

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55 μm. The epilayer was intentionally doped with the nitrogen donors to 1.5×10^{15} cm^{-3}. Micro-PL spectroscopy and PL intensity mapping were performed on the samples by using a *PLMicro-SiC* by *Nanometrics Inc*. [17]. PL was excited by the 25 mW, 325 nm line of a He–Cd laser, dispersed with a grating monochromator, and detected by a photomultiplier. The excitation beam was chopped and a lock-in amplifier was used to extract the weak PL signal. The extensive efforts were performed on the optics and detection channels in order to provide enhanced sensitivity in the UV spectral region. The laser beam was focused to a spot with a diameter of about 0.8 μm using a sapphire objective lens. The sample was mounted on a XYZ stage with a spatial resolution of 0.5 μm. The set-up can acquire data in a single wavelength mode (PL intensity mapping mode) or in a full spectral scanning mode (PL spectroscopy mode), with the spectral resolution of 1 nm. TEM studies were carried out on a JEOL microscope operating at 300 kV.

3. Results and discussion

Fig. 1 shows the micro-PL spectra from a 4H-SiC epilayer with and without IGSFs at room temperature. At the 4H-SiC matrix (without IGSFs), only one peak located at 390 nm is observed. This peak (3.18 eV) corresponds to the near band-edge emission of 4H-SiC. At the IGSF position, the intensity of the near band-edge emission is greatly reduced, and a new band appears. This indicates that the IGSF manifests itself as a carrier recombination center in 4H-SiC, in accordance with the quantum well model [18]. Three IGSFs are successfully identified with the additional emission wavelengths located at 460 nm (IG-I), 480 nm (IG-II), and 500 nm (IG-III), respectively, as shown in Fig. 1.

In order to reveal the spatial profile of these IGSFs, the micro-PL mapping at the additional wavelengths (the band energy of IGSF) was performed, as shown in Fig. 2. The contrasted color areas correspond to the IGSF, which suggests that the additional emission is related to the IGSF. The PL intensity of the contrast decreases toward the direction opposite to the wafer offcut, i.e., in the direction opposite to the step flow [11–20]. For IGSFs residing on the basal planes of 4H-SiC, this corresponds to the increasing distance from the surface of the structure. For the IG-I, the right-angled triangular shape of the emission areas was clearly identified, and composed of the dislocation lines along [11–20] and [10–10], or [11–20] and [01–10], as shown in Fig. 2(a). The length of the right-angled triangles along the off-axis direction of [11–20] is approximately 400 μm, which corresponds to the projected length of the basal plane in the epitaxial layer (55 μm/ tan 8° ≈ 400 μm). IG-I is the dominant IGSF in the sample, with a density of ~50 cm^{-2}. The formation of IG-I was found to be very sensitive to the initial growth process. The density of IG-I can be greatly reduced to below 10 cm^{-2} after the growth conditions at the initial stage were optimized. IG-II also has the right-angled triangular shape, similar with the IG-I, as shown in Fig. 2(b). However, its size is obviously smaller than IG-I, especially the width vertical to the step flow direction. The typical density of the IG-II is about 1–5 cm^{-2}. The shape of IG-III is close to the rectangle. Its density is similar to that of IG-II.

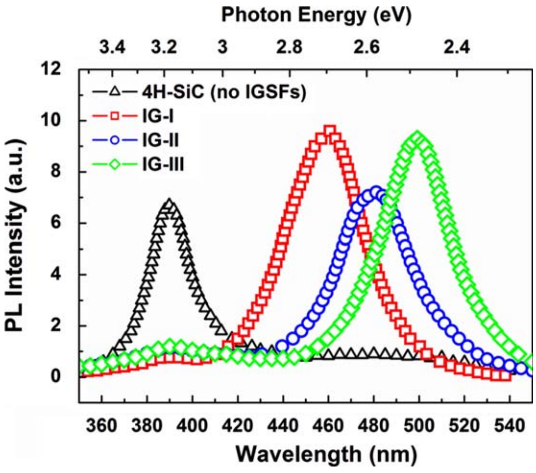

Fig. 1. Micro-PL spectra from the 4H-SiC epilayer without and with IGSFs.

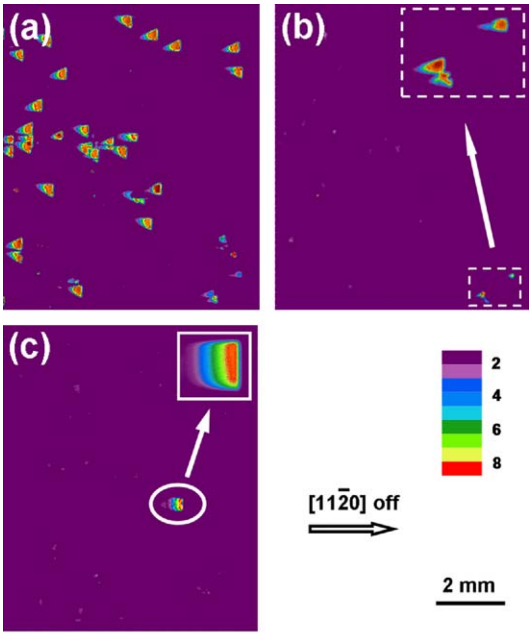

Fig. 2. Micro-PL intensity mapping at (a) 460 nm (IG-I), (b) 480 nm (IG-II), and (c) 500 nm (IG-III) (the same area in the sample).

We prepared the cross-sectional TEM specimens for each IGSF using focused ion beam micro-machining. The sample containing IGSFs was first etched in molten KOH at 500 °C for 5–10 min. This step produced two etching pits corresponding to two basal plane dislocations and a groove corresponding to the intersection of IGSF with the epilayer surface for each IGSF, as shown in Fig. 3. (Before KOH etching, IGSF is featureless in the optical microscopy image.) The TEM specimens were then cut from the part of the IGSF where the defect intersected the surface. Fig. 4 shows the high-resolution TEM images of the IGSFs. The stacking sequences of the IG-I, IG-II, and IG-III shown in Fig. 4 are (4,4), (3,5), and (6,0) in the Zhdanov's notation, respectively, which apparently differ from the perfect 4H-SiC, (2,2).

A common formation mechanism of stacking faults in SiC polytypes is by shear, where part of the crystal above the shear plane is rigidly shifted by the vector connecting the A, B, or C locations in the basal plane. The stacking faults caused by the shear are called Shockley faults. Starting from the perfect 4H polytype, one can produce two different types of stacking sequences by shear of each one of *h* and *c* bi-layers in the right direction, as shown in Fig. 5. The transformation can be denoted as (2,2)→(1,3) and (2,2)→(3,1) in the Zhdanov's notation ((3,1) is not shown). Accordingly, we call these two SFs single Shockley SFs (1SSFs). If we shear both *h* and *c* bi-layers (layer 11 and 10) in the same direction, we can produce a new SF, called double Shockley SFs (2SSFs). The transformation of 2SSFs can be denoted as (2,2)→