Optical characterization of 4H-SiC by far ultraviolet spectroscopic ellipsometry

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We have developed a far UV spectroscopic ellipsometer system working up to 9 eV, and applied it to the characterization of three 4H-SiC samples with different surface conditions [i.e., as-received and chemical mechanical processing (CMP) processed 4H-SiC bulk substrates and a 4H-SiC epi sample]. Pseudodielectric functions \( \varepsilon_1 \) and \( \varepsilon_2 \) clearly demonstrate the excellent surface sensitivity of the far UV ellipsometry system as it distinguishes the improvements provided by CMP process. Simulation results of ellipsometer data indicate the existence of a damaged subsurface layer in the as-received 4H-SiC bulk substrate. The investigation of sample surfaces using atomic force microscopy confirms the results of ellipsometry measurements. © 2001 American Institute of Physics. [DOI: 10.1063/1.1384895]

Silicon carbide (SiC) has been given great attention in high-power, high temperature, and high frequency device applications due to its large band gap energy, large electric breakdown field, high saturated electron drift velocity, and large thermal conductivity. For the full utilization of these superior material properties in the device operation, however, high quality substrates are required. Despite great progress in SiC substrate growth technology, currently existing defects such as micropipes and dislocations on bulk substrates and subsequently grown epitaxial layers have delayed the development of commercially available SiC-based devices.\(^1\)-\(^4\) Besides these defects, surface and interface roughness are another important issue since a rough junction interface reduces the blocking voltages. In addition, the rough surface reduces the channel mobility or causes the early breakdown of the oxide in metal-oxide-semiconductor field effect transistors.\(^5\),\(^6\) Various approaches to minimize the surface and interface roughness have been tried including conventional surface oxidation followed by HF etching, hydrogen etching,\(^7\),\(^8\) and chemical mechanical polishing (CMP).\(^4\)

As a very sensitive nondestructive optical characterization tool, ellipsometry has provided valuable information especially in thin film, surface, and interface studies.\(^9\),\(^10\) In this study, we extended the spectral scanning range of ellipsometry from the conventional 6.5 up to 9 eV by developing a far UV spectroscopic ellipsometer, and we applied it to the study of 4H-SiC surfaces. This extension in the scanning range of the spectroscopic ellipsometer is useful in the characterization of SiC substrates since major peaks in the imaginary part of dielectric functions of all SiC polytypes occur above 6.5 eV and below 8 eV.\(^11\) The basic setup of our far UV spectroscopic ellipsometer is that of a fixed polarizer and a rotating analyzer, as is typical for conventional ellipsometers. In order to avoid the absorption of UV light by oxygen and its radicals below 190 nm, the main system was placed inside a glove box purged by nitrogen gas, and optical components were specially selected for UV use. The details will be discussed elsewhere. The samples were also investigated using atomic force microscopy (AFM) to better understand these ellipsometry results.

In this work, we investigated three 4H-SiC samples with different surface conditions. We compare an as-received and a CMP processed bulk substrate as well as an epi sample. Both the as-received and the CMP-processed bulk substrate samples are n type \((n = 3.7 \times 10^{17} \text{ cm}^{-3})\) with \((0001)\) Si face and 8° off-axis. The epilayer is 4 μm thick with an n-type doping (nitrogen) of approximately \(5 \times 10^{15} \text{ cm}^{-3}\). The CMP process used in this study is similar to that of Zhou et al.\(^12\) A Strasbaugh model R6DE-DC-4 polisher was used with Rodel regular poli tex polishing pads and full strength Logitech SF1 colloidal silica polishing solution. The wafer was polished for 1 h under 2000 g pressure at a speed of 200 rpm. Unlike Zhou et al., there was no intentional heating of the wafer during polishing. Typical removal rates for unheated polishing were found to be approximately 150 Å/h but this rate was found to have a significant error and to depend on a number of parameters including the age of the polishing pad and the pH of the polishing solution. The wafer was rinsed in deionized water immediately after polishing to prevent matter from sticking to the surface.

Ellipsometry parameters \( \Psi \) and \( \Delta \) were measured from 3 to 9 eV. Although the actual measurements were performed from 3 eV, the data below 4.78 eV were not considered in the extraction of dielectric functions \( \varepsilon_1 \) and \( \varepsilon_2 \) because of the lack of accuracy below that energy. The inaccuracy of the...
data below 4.78 eV is most likely due to the interference by the second order scattered light from higher photon energy region. Figure 1 shows pseudodielectric functions $\varepsilon_1$ and $\varepsilon_2$ of the as-received and CMP processed 4H-SiC bulk substrates and 4H-SiC epi sample. As expected, $\varepsilon_1$ and $\varepsilon_2$ of the CMP processed sample have somewhat higher peaks than those of as-received sample. This means the CMP step improved the surface quality of the bulk substrate, since the smoother surface shows higher peaks in $\varepsilon_1$ and $\varepsilon_2$. The epi sample exhibits lower $\varepsilon_1$ and $\varepsilon_2$ than those of our bulk substrates. The significant differences in $\varepsilon_1$ and $\varepsilon_2$ between the bulk substrate samples and the epi sample strongly suggest that the epi sample has a surface problem such as step bunching, etc.

Those samples were next investigated using AFM to clarify the situation. AFM measurement of the as-received substrate shows many scratch lines on the surface from the polishing process, and about 3.9 Å rms roughness on unscratched areas of the surface. The AFM image of the CMP processed bulk substrate shows that all those scratch lines are removed after the CMP process. The rms roughness is less than 1 Å. The results of AFM scanning confirm the excellent sensitivity of the far UV spectroscopic ellipsometry in that it clearly distinguishes substrates with a few angstroms difference in the roughness. The AFM image of the epi sample demonstrates the appearance of macrosteps with size of 200–500 nm width and 30–40 nm height as observed in other studies.13–15 It is speculated that those structures are formed in the process of the surface free energy minimization.13,14 It is also observed that a few hundred angstrom size balls most likely made of diamond exist all over the sample surface. The existence of those macrosteps as well as those balls increases the rms roughness of the epi sample and thus decreases the heights of peaks in $\varepsilon_1$ and $\varepsilon_2$ as observed in the ellipsometer measurement.

We performed further simulations to better understand the SiC material quality under study. First, the data by Cobet et al.11 were used to estimate the surface roughness and other properties of the two bulk samples. In this simulation, the Bruggeman effective medium approximation was used and a single overlayer was modeled in a mixture of SiC and oxide. The results showed a larger roughness for the as-received than for the CMP sample, 2.4 Å for the CMP sample and 3.7 Å for the as-received sample, which is in agreement with the AFM data taken for the same samples. Next, applying the surface roughness and mixture derived by the earlier simulation to the CMP sample, a bulk dielectric response was extracted for the CMP substrate. The simulation using this bulk spectrum to analyze the as-received data resulted in a similar value for the thickness of the rough layer, but with a reduced rms error compared with the results using Cobet et al.’s data. This demonstrated that our dielectric response is closer to that of the as-received material than was the Cobet result for epitaxial SiC. However, there still remained a systematic error that appeared too large for the thickness of this thin overlayer. Therefore, in order to further investigate, a three-layer model with the following structure was tried. We fixed a surface roughness layer similar to the one found earlier, using the bulk dielectric spectrum from the CMP sample as the substrate for the as-received sample. Then, all remaining discrepancy between the model and the experiment was attributed to a third layer with 45 Å thickness between the bulk SiC and the rough surface. This layer was allowed to vary to improve the agreement between theory and experiment. Simulation results show a clear and significant further broadening of the critical points, as shown in Fig. 2. Furthermore, in this case the epsilon 2 peak was reduced as well as broadened. These results persisted through variations in thickness and surface roughness parameters, indicating that it is not an artifact of the simulation. We conclude that a subsurface layer with dielectric response that differs from that of the substrate and even more from “perfect” epitaxial material exists. This layer is below the rough surface layer that can also be observed by an AFM. Further study will be required to establish whether this is a uniform feature of as-received substrates, the types of CMP, plasma, or other treatments required to remove it, and the effect it may have upon electrical properties.

In summary, we have developed a far UV spectroscopic ellipsometer working up to 9 eV. We applied it to the study of three 4H-SiC samples with different surface conditions:
As-received and CMP processed bulk substrates as well as an epi sample with macrosteps. The measurement results demonstrate the excellent surface sensitivity of the far UV spectroscopic ellipsometry. It clearly distinguishes substrates with a few angstroms difference in surface roughness, and further indicates the existence of a damaged subsurface layer in as-received bulk substrate.

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