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Ultrathin SiO_2-films on 4H-SiC(0 0 0 1) studied by angle-scanned photoelectron diffraction

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Abstract

X-ray photoelectron spectroscopy and angle-scanned photoelectron diffraction were used to investigate thermally grown ultrathin SiO_2 films on 4H-SiC(0 0 0 1). Due to the chemical sensitivity of the applied methods it was possible to study different aspects of the films. A chemically shifted component in the Si 2p photoemission spectrum was ascribed to Si emitter atoms at the interface and allowed a determination of the interface structure between the ultrathin SiO_2 film and the SiC substrate. The photoelectron diffraction pattern of another chemically shifted Si 2p component contained information about the local environment of near-interface Si emitters in the oxide film. This information was made accessible by means of an extensive comparison between experimental and simulated data. In the simulations the use of the cluster radius as a fitting parameter turned out to provide information about the range of local order in the oxide film. A chemically shifted component in the C 1s photoemission spectrum was used to study the structural properties of carbon contaminations, which were detected in the SiO_2 layer after special preparation procedures.

Keywords: Photoelectron diffraction; XPD; Silicon carbide; Semiconductor surfaces and interfaces

1. Introduction

Silicon carbide is a wide bandgap semiconductor with promising possibilities for applications in semiconductor devices. It can be applied in devices operated at high temperatures, with high currents, or with high voltages. It is advantageous for the device processing, that SiC can be, as silicon, thermally oxidized to form an insulating SiO_2 film. However, the properties of these films prepared by thermal oxidation are not as good as those of SiO_2 films on silicon surfaces. The density of states in the SiC bandgap is much higher, which reduces the electrical quality of the interface. The reasons for this are not yet completely understood, although in the recent years a lot of investigations were conducted and numerous results were obtained [1–3]. There seem to exist two main sources of an increased density of states in SiO_2 films on SiC, namely carbon contaminations in the oxide film or at the interface and structure defects at the SiO_2 side of the interface. Seemingly, carbon contaminations are the origin of electronic states in the lower part of the SiC bandgap while structure defects in the silicon oxide cause defect states in the upper part of the SiC bandgap [4,3].

It is experimentally demanding to achieve information about the structural origins of these two types of defects. Especially, an experimental access to the interface structure is difficult. Photoemission spectroscopy with its element specificity and chemical sensitivity is one of the very few techniques which provide a possible access to the interface below the film. The same advantages apply to photoelectron diffraction, which extends the possibilities of photoelectron spectroscopy and allows the determination of the local atomic structure around the respective emitter atoms. Both techniques were used in this work to study ultrathin films of thermally grown SiO_2 on 4H-SiC(0 0 0 1) surfaces. The Si 2p photoemission signal consists of three chemically shifted components which can be ascribed to emitters in the SiC bulk, the SiO_2 film, and at the interface [5–8]. Therefore, the photoelectron diffraction of this signal could be used to study the interface and the local atomic environment of the near-interface Si emitters inside the SiO_2 film. In order to extract the structure information from the experimental data, a comprehensive simulation-experiment comparison was necessary and a comparison to experimental data recorded for ordered silicate layers on SiC surfaces proved to be useful. A systematic variation of the cluster radius in the simulations was applied for the first time in this work. It provided a useful tool to gain information about the size of locally ordered regions at the interface. Further, we

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provide a study of carbon contaminations, which were present on some samples depending on the preparation conditions. They could be detected by their chemical shift in the C 1s signal and studied by photoelectron diffraction.

2. Experiment

All experiments were conducted in a μ-metal shielded UHV chamber with a base pressure below 5×10^{-11} mbar. Photons were provided by the U41-PGM beamline at BESSY 2 in Berlin. The overall energy resolution (photons and analyzer) was set to about 100 meV at a photon energy of $h\nu = 180$ eV and to about 190 meV at a photon energy of $h\nu = 330$ eV. With these settings the energy resolution allowed to separate the individual components in the spectra and the photon flux was sufficient to record angle-scanned full 2π XPD data.

The samples were cut from a 4H-SiC(0 0 0 1) wafer which had a miscut of about 8°, they were mounted in the sample holder, and transfered to UHV. The oxide layer was removed by an anneal at 1100 °C in a silicon flux, which was provided by an electron beam evaporator. A reduction of the annealing temperature to 800 °C led to the formation of the $(\sqrt{3} \times \sqrt{3})R30°$ reconstruction of the clean Si-terminated 4H-SiC(0 0 0 1) surface. All samples were prepared this way. This procedure was the starting point for the following oxidation processes. Depending on the oxidation conditions, diverse silicon oxide films were prepared. A thermal annealing of the sample at 800 °C in an ambient of 1×10^{-4} mbar of O_2 resulted in an ultrathin silicon oxide film, in which no carbon contaminations could be detected by XPS and no long-range periodicity was shown by LEED. An oxidation of the sample at a temperature around 1200 °C and at a low oxygen pressure of 1×10^{-8} mbar also resulted in an ultrathin SiO_2 film without long-range order. However, under these conditions carbon contaminations are formed, as can be observed by XPS. Finally, an ordered silicate layer could be prepared by an oxidation at around 900 °C in an atmosphere of oxygen, which contained water. It could be shown [9] that this ordered silicate layer is the same as had been prepared and investigated by Bernhardt et al. [10].

The photoelectron diffraction data were measured in the angle-scanned mode. Therefore, the sample was rotated both around the Θ- and the Φ-angle, denoting the polar- and

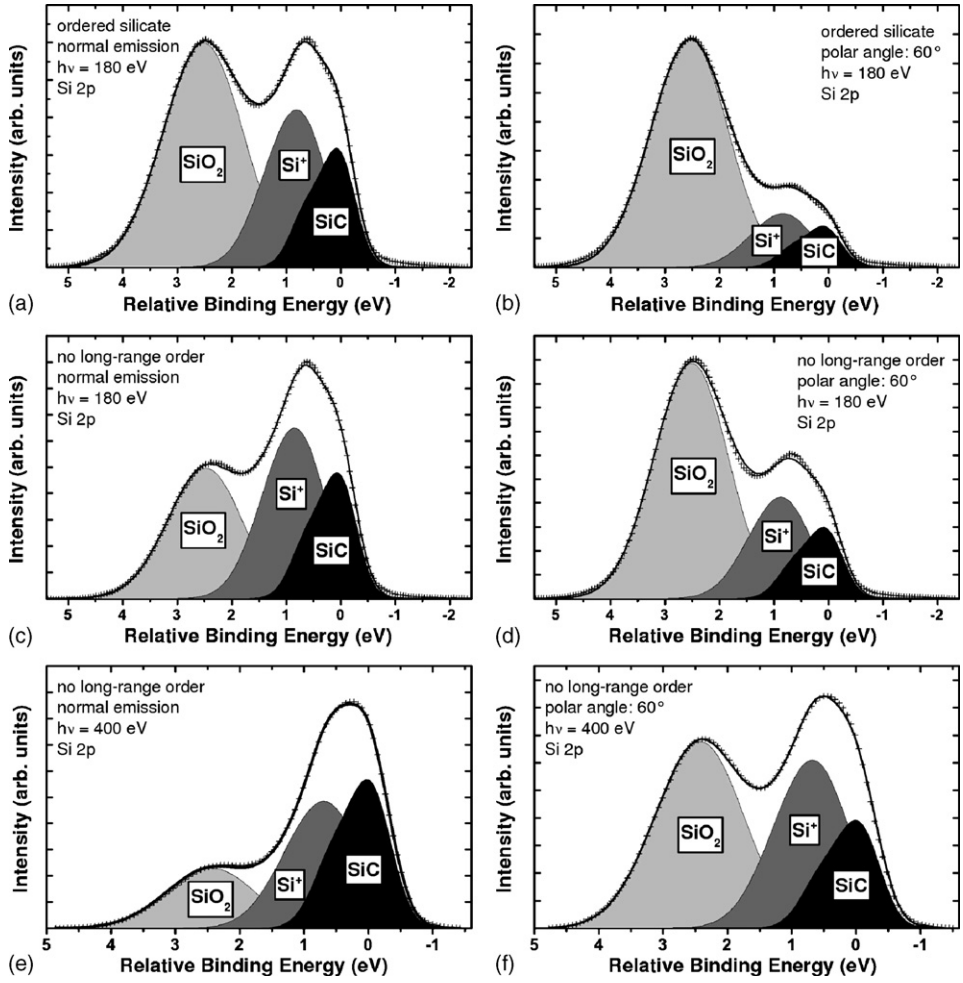

Fig. 1. X-ray photoelectron spectra of the Si 2p signal. Each component consists of the spin orbit split $2p_{1/2}$ and $2p_{3/2}$ peaks. Spectra (a) to (d) were recorded with a photon energy of 180 eV, resulting in a kinetic energy of the photoelectrons of approximately 80 eV, spectra (e) and (f) with a photon energy of 400 eV ($E_{kin} \approx 300$ eV). The spectra of the ordered silicate layer are depicted in (a) and (b) while (c) to (f) display spectra of a nonordered layer without any long-range order.