Morphology and structure evolution of ZnO nanocrystallites deposited on 4H-SiC and SiO₂/Si substrates

<u>I. Tsiaoussis¹</u>, J. Stoemenos¹, V. Khranovskyy², R. Yakimova²

1. Solid State Physics Section, Department of Physics, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

2. Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-58183 Linköping, Sweden

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ZnO nanocrystals were grown by atmospheric pressure metalorganic chemical vapor deposition (APMOCVD) on 4H-SiC and SiO₂/Si substrates. In the first case commercial 4H-SiC [0001] substrates were miscut by 8° off the c- axis to $[11\bar{2}0]$ and then a p-SiC layer was grown by sublimation epitaxy. In the second case the growth followed a two- step procedure, allowing at the first step deposition of a continuous ZnO layer (seeding layer) followed by discontinuous nanostructures growth. The substrate temperature was kept at 500 °C. The structural characteristics of ZnO nanocrystals epitaxially grown on p-type 4H-SiC(0001) and Si (100) were studied by conventional transmission electron microscopy (TEM) and high resolution transmission electron microscopy (HRTEM).

The deposited ZnO nanocrystallites on 4H-SiC substrate are shown in the low magnification, cross-section TEM micrograph in fig.1a. The size of the nanocrystallites varies from 200 to 350nm and their height from 120 to 200nm. The crystallites seem to touch each other; this is an artifact because all the crystallites encountered by the electron beam are projected on the plain of the screen. The ZnO nanocrystals were formed at the terraces of 8° miscut toward the $[11\overline{2}0]$ direction of the 4H-SiC substrate. They have the shape of hexagonal nanopillars with their edges parallel to the $<11\overline{2}$ 0> directions and a top c-plane facet reflecting the crystal symmetry of ZnO. The free surface between the hexagonal nanopillars was covered by a very thin highly defected epitaxial ZnO film strongly suggesting Stranski-Krastanov mode of growth. It is worth noticing that the nanocrystallites grow between adjacent steps of the substrate, as shown by arrows in fig.1b.The steps were formed along the $[11\overline{2}0]$ 4H-SiC crystallographic direction and their height was about 25nm as expected. Most of the crystallites are in perfect epitaxial relation with the substrate having the $[0001]_{ZnO} / [0001]_{4H-SiC}$ and the $[1010]_{ZnO} / [1010]_{4H-SiC}$ as shown in the selected area diffraction (SAD) pattern (fig.1c). The misfit between the crystallites and the SiC substrate on the basal plane is 5.6% so that the (1010) reflections of ZnO and 4H-SiC are well distinguished in the (SAD) patern. Figure 1d shows a high-resolution TEM (HRTEM) micrograph from the ZnO / 4H-SiC interface. Lattice fringes of the (0001) type from the 4H-SiC substrate and (0001)* lattice fringes of the ZnO overgrown are evident.

In the second case massive nanopillar growth was observed, as shown in the SEM micrograph (fig.2a). The crystallites have conical shape with mean height from the top to the interface of about 110nm and a mean width 160nm, as shown in the LM micrograph (fig.2b). The ZnO overgrown was formed on the SiO₂ layer, about 5nm thick. The conical crystallites exhibit strong preferred orientation having the c-axis almost perpendicular to the substrate, as shown in the selected area diffraction (SAD) pattern (fig.2c). Thus, during the early stage of growth a high number of small nucleus is formed covering the SiO₂ surface, as shown in the

HRTEM micrograph (fig.2d). From them only these having the c-axis perpendicular to the substrate survive. Accounting for the high optical quality and the availability of p-n junctions, the structures prepared in this study can be considered as a promising key element for nano-optoelectronics.



Figure 1: a) Cross-section TEM micrographs of the deposited on 4H-SiC substrate ZnO nanocrystallites, b) The nanocrystallites grow between adjacent steps of the substrate, steps were formed along the [1120] 4H-SiC crystallographic direction and their height was about 25nm as expected. c) Most of the crystallites are in perfect epitaxial relation with substrate having the the $[0001]_{ZnO} / [0001]_{4H-SiC}$ and the $[10\overline{1}0]_{ZnO}//[1010]_{4H-SiC}$, d) A high-resolution TEM (HRTEM) micrograph shows the ZnO / 4H-SiC interface.



Figure 2: a) SEM micrograph, a massive nanopillar growth was observed, b) LM micrograph, the crystallites have conical shape with mean height of about 110nm and a mean width 160nm c) The conical crystallites exhibit strong preferred orientation, d) HRTEM micrograph ,during the early stage of growth a high number of small nucleus is formed.