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ZnO Epitaxy on (111) Silicon using Intervening Bixbyite Oxide Buffer Layers

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ZnO has attracted intense interest of research in recent years due to possible replacement for GaN for photodiode [1] and lasing applications [2]. ZnO has a comparable band gap to GaN, 3.37 eV, while having a two-fold increase in exciton binding energy, 60 meV vs. 20 meV, allowing for brighter emission at lower thresholds. The commercial availability of bulk ZnO single crystals could also substantially reduce the cost of ZnO-based devices relative to that of GaN-based devices. One significant hurdle in developing ZnO based multifunctional devices, however, has been integration with silicon (Si). Direct growth of ZnO on Si has proven extremely difficult, resulting almost exclusively in polycrystalline and textured films, due to the formation of oxide layers on the Si surface, reactivity between ZnO and Si, a large lattice mismatch (15.4 %), and a large mismatch in thermal expansion (60 %). These effects, though, can be mitigated through the employment of a buffer layer.

Bixbyite oxides are one such candidate for buffering ZnO growth on Si. They have the cubic structure (space group $Ia\bar{3}$) in the stoichiometry M_2O_3 (M = Sc, Lu, Y, Gd) which are nonreacting and thermodynamically stable with both Si and ZnO. In this work the epitaxial thin films of Sc_2O_3, Lu_2O_3, and Gd_2O_3 with thicknesses varying from 1 to 100 nm were grown on (111) p-Si by reactive molecular beam epitaxy. ZnO thin films with thicknesses ranging from 300 nm to 2 μm were then grown with two steps by pulsed laser deposition. A low-temperature nucleation layer (~10 nm) was grown at 240 °C, followed the growth of a high temperature thick film at 600 °C. Microstructure and defects of ZnO films were then studied using high-resolution transmission electron microscopy (TEM), photoluminescence (PL) spectroscopy, and x-ray diffraction (XRD). The orientation relationship is found to be $(0001)[1\bar{2}10]_{ZnO} \parallel (111)[\bar{1}10]_{M_2O_3} \parallel (111)[1\bar{1}0]_{Si}$.

Figs. 1(a-c) show the microstructure of the ZnO films grown on Si substrates with the Sc_2O_3, Lu_2O_3, and Gd_2O_3 buffer layers, respectively. All films consist of smooth surface and sharp interfaces. A thin amorphous layer of SiO_x was observed between Si and the M_2O_3 buffer layers despite the epitaxial nature of the buffers and ZnO films (Fig. 2). These amorphous layers are not present, though, before ZnO deposition (Fig. 3), and can thus be concluded to have formed during subsequent ZnO growth by oxygen diffusion through the buffer layers. PL and XRD reveal excellent optical and structural properties compared with ZnO films grown on other substrates such as saphhire [3,4].

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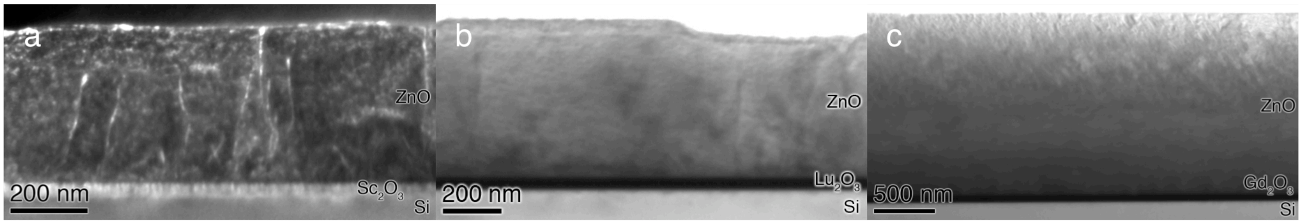

FIG. 1. TEM survey micrographs of ZnO films on (a) Sc_2O_3, (b) Lu_2O_3, and (c) Gd_2O_3 buffer layers.

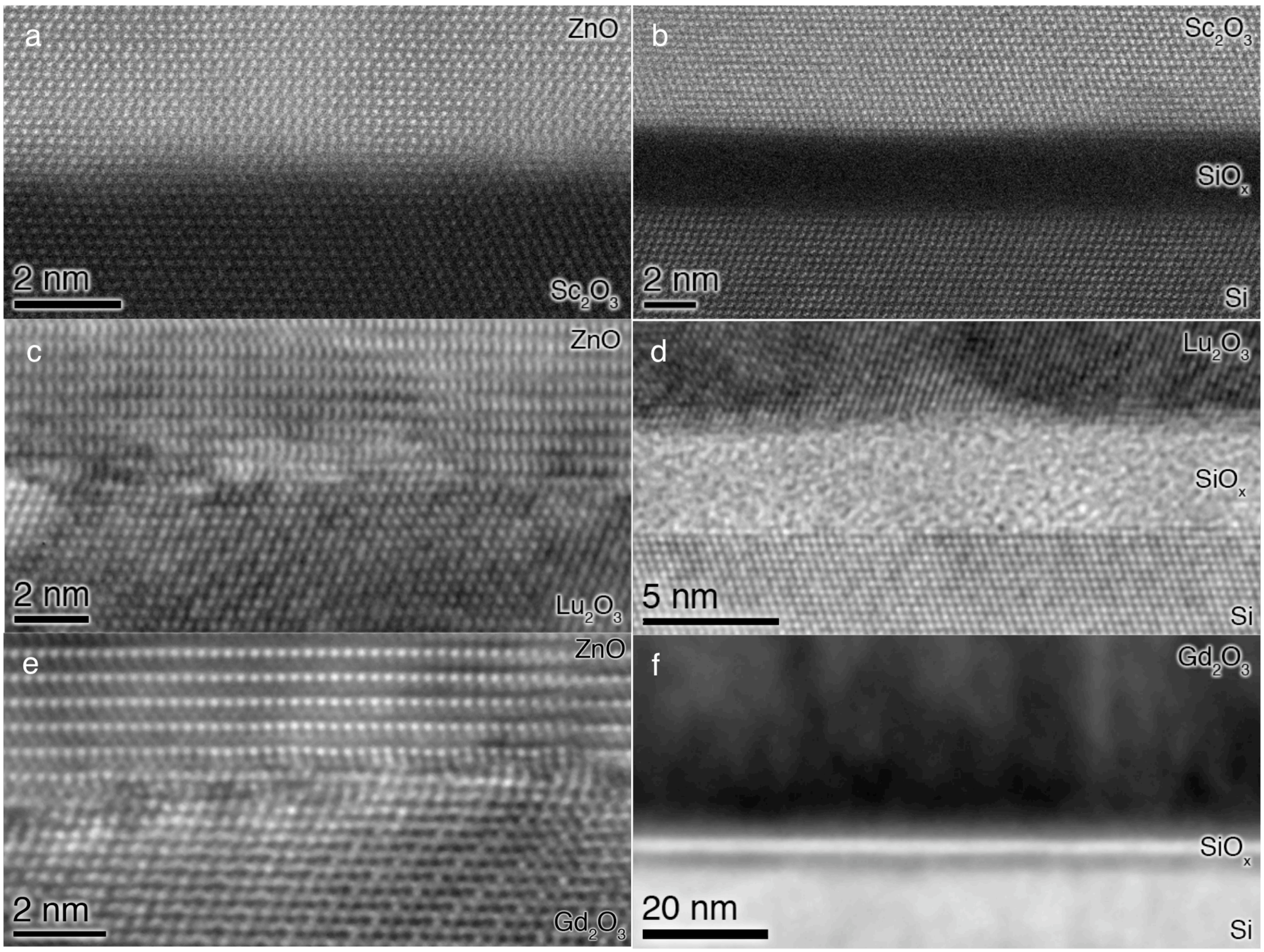

FIG. 2. HR-STEM and HR-TEM micrographs of the ZnO/M_2O_3 and M_2O_3/Si interface regions for (a, b) Sc_2O_3, (c, d) Lu_2O_3, and (e, f) Gd_2O_3 buffer layers, respectively.

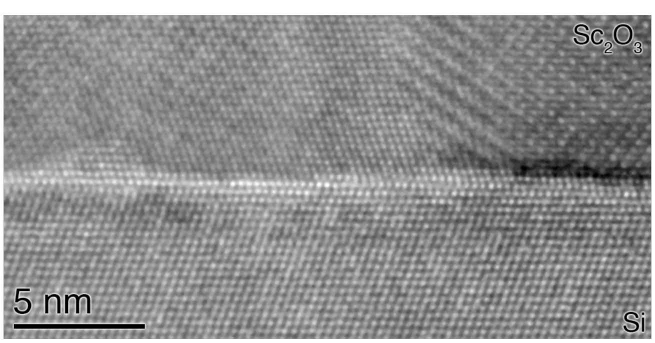

FIG. 3. HR-TEM image of the Sc_2O_3/Si interface before subsequent ZnO growth, showing no amorphous SiO_x layer.

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