

Epitaxial single crystal MgO buffers on Si (100)

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The integration of functional metal oxides with silicon has been a persistent challenge due to the thermodynamic instability of their resulting interfaces [1]. Crystalline oxide buffer layers have been used as a solution by providing a thermodynamically stable transition layer. Magnesium oxide (MgO) buffers have been shown to work as effective pseudo-substrates for metal oxide epitaxy [2, 3], and its deposition on silicon has been shown to be stable [4].

In this talk we report an extensive study of high-quality MgO buffer layers using molecular beam epitaxy (MBE) on Si(100) substrates. The buffers were grown through electron-beam evaporation of single crystal MgO, which was deposited at 300°C under an oxygen partial pressure of 3.7×10^{-5} Torr. The reflection high-energy electron diffraction (RHEED) pattern (Figure 1.a) reveals a modulated pattern along the MgO[100] direction, indicating the beginning of small island formation and surface faceting. The thickness dependence on the films' crystallinity was studied through the FWHM of the (200) MgO Bragg peak rocking curve as seen in Figure 1.b. The trend suggests an improvement in the crystallinity as the layers become thicker. Figure 1.c shows the scanning transmission electron microscopy (STEM) image of a cross section of the MgO/Si interface, revealing an in-plane epitaxial relationship of MgO $\langle 100 \rangle \parallel$ Si $\langle 100 \rangle$ with a 4:3 coincident site arrangement between the MgO and Si conventional unit cells. The figure also reveals the presence of tilted MgO grains and small-angle grain boundaries. The interface layer observed in Figure 1.c was investigated using x-ray photoelectron spectroscopy (XPS), suggesting the formation of Mg-O-Si bonds at the interface. Additionally, the measured band alignment at the MgO/Si interface and its relation to first principles calculations of various interface models will be discussed.

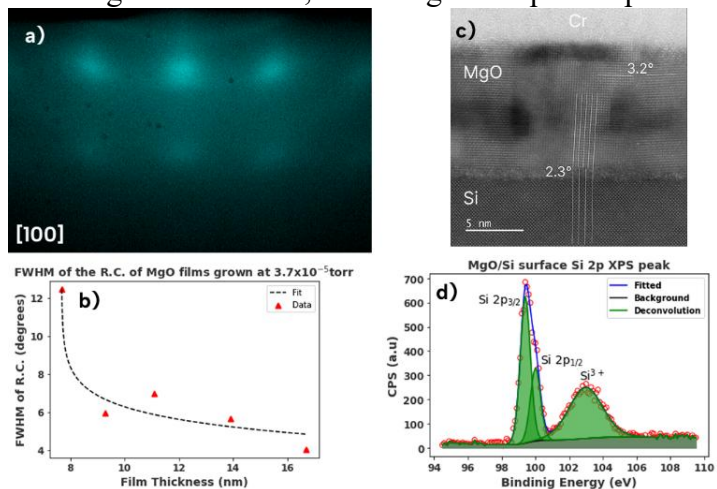


Figure 1. (a) RHEED pattern of MgO, (b) FWHM trend of the rocking curve for the (200) Bragg peak of MgO, (c) STEM image of MgO/Si structure, (d) XPS measurement of the Si oxidation state at the interface.

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Supplementary information:

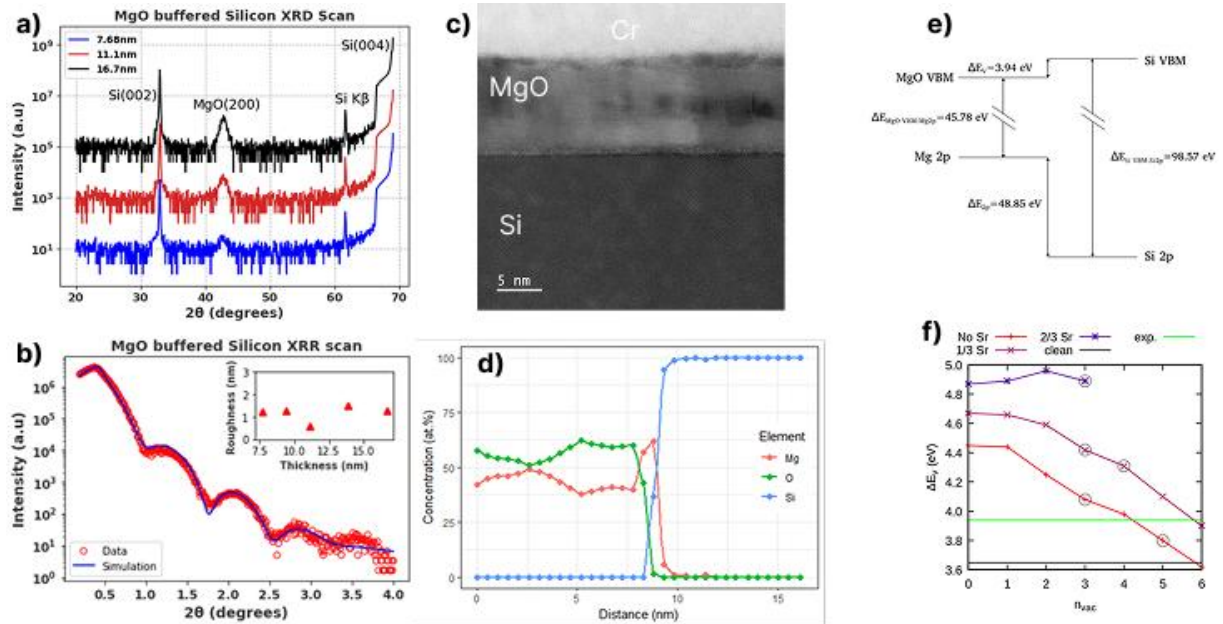


Figure 2. (a) XRD scan of MgO films on Si showing a clear MgO(200) Bragg peak, (b) XRR scan of an MgO film, the inset shows the roughness trend with respect to film thickness, (c) STEM image of a large, uniform MgO grain, (d) EELS concentration line profile showing a silicate interface, (e) band alignment measurement showing the valence band, (f) DFT+U calculation of the valence band offset of MgO/Si.