Atomically resolved MgO(100) surfaces and supported earth metals

C. L. Pang, A. Sasahara, and H. Onishi
Department of Chemistry, Faculty of Science, Kobe University, Kobe 657-8501, Japan
pang@kobe-u.ac.jp

Mixed oxide systems play a tremendously important role in industry. As an example, dispersed BaO is the storage component in NO_x storage/reduction automobile catalysts, which use γ-alumina as the support [1]. Although high resolution images [2] including atomically resolved images [3] have been obtained on ultra-high vacuum (UHV) cleaved MgO(100) crystals, sputter-annealed samples may offer crucial advantages depending on the intended applications. For example, as a support for the growth of nano-particles, it is likely that the crystal will be annealed to follow sintering processes or to create continuous films. With a cleaved sample, upon heating, Ca would segregate to the surface complicating such studies. On the other hand, the amount of segregated Ca can be significantly reduced with repeated sputter-anneal cycles [4]. With this in mind, we present UHV NC-AFM studies of sputter-annealed MgO(100) crystals with varying quantities of supported CaO_x and BaO_x.

The MgO(100) crystals were prepared with sputter-anneal cycles up to ~1700 K, giving good quality 1×1 low energy electron diffraction patterns and atomically resolved images in both constant height and constant frequency shift modes, an example being displayed in fig. 1(a). Bright spots in such images can correspond to Mg cations or O anions depending on the nature of the tip apex, as evidenced by a contrast inversion following a tip-change (not shown). At the upper step-edges (not shown), undercoordinated ions give rise to spots with an enhanced brightness as observed previously for NaCl(100) thin films [5]. Figs. 1(a) and (b) show that CaO_x particles, with sizes down to individual Ca adatoms, remain on the surface from bulk segregation. Scanning Kelvin probe microscopy (SKPM) images indicate a decrease of the work function over the CaO_x particles, suggestive of an electron transfer from Ca to the MgO(100) substrate.

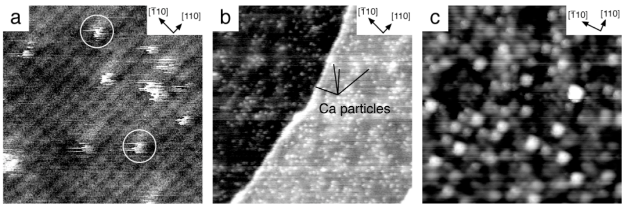

Fig. 1 Unfiltered NC-AFM images of MgO(100) recorded with a JSPM-4500A microscope (*JEOL*). Δf ranges from -17 Hz to -128 Hz. **(a)** (50 Å)^2 constant height (detuning) image. The circles indicate individual adatoms assigned to Ca. **(b)** (1000 Å)^2 constant Δf (topographic) image. CaO_x particles are indicated with the step-edges almost completely decorated with CaO_x. **(c)** (5000 Å)^2 topographic image with supported BaO_x.

Finally, BaO_x was grown on MgO(100). Ba was evaporated in UHV from an *SAES* getter source onto a MgO(100) sample held at ~900 K and subsequently annealed both in UHV and in an O_2 flow (~1×10^{-5} mbar) up to ~1300 K. Flat-topped, cuboid particles were formed with widths up to ~300 Å and heights up to ~80 Å, as shown in fig. 1(c). The boundaries of these particles are aligned to the {110} directions of the MgO(100) substrate.

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