

EFTEM and EELS Studies of the Interface Structure of Ni/MgO

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Ni thin films growing epitaxially on some substrates, for example, on single crystal MgO, are of great interests recently due to their special magnetic properties that may lead to some new applications. Although MgO substrate and Ni have a large lattice mismatch of $\sim 16.4\%$, cube on cube (CC) epitaxial growth has been successfully conducted [1]. Theoretical investigations predict that Ni interacts strongly with MgO [2], i.e., Ni is easy to be oxidized. Moreover based on the measurement of the magnetic property, polarized neutron reflectivity and high-resolution X-ray diffraction studies, it was speculated that there probably forms an ordered NiO thin layer (~ 5 nm) at the interface [1]. Nevertheless, it is still not clear whether or not such a thin NiO layer is formed at the Ni/MgO interfaces. A detailed study of the local electronic structure of the interface is needed.

The growth of a thin (about 50 nm) Ni film on MgO (001) substrate was conducted in a MBE VG 80 M system. The sample was annealed at 300 °C after growth. More detailed descriptions can be found in reference [1]. A JEOL-2010F STEM/TEM was used for the study that can be performed in both TEM and STEM modes at 200 kV. A Gatan Image Filter (GIF) system is attached to this microscope that can be used for electron energy loss spectroscopy (EELS) [3] and energy filtered transmission electron microscope (EFTEM) [4]. EFTEM images were recorded at an 8k magnification using a CCD camera at 2 \times binning (512 \times 512 pixels). The lens conditions were set to define probe sizes of 0.2 nm for both high-angle annual dark-field (HAADF) imaging and EELS.

Figure 1 shows EFTEM elemental mapping results. From Fig.1 (a) it can be clearly seen that an interfacial layer (~ 5 nm thick) is formed at the interface of Ni/MgO that has distinct interfaces with both the substrate and the epitaxial thin film. To identify the structure of such a thin layer, elemental mapping was performed for both Ni and O elements across the interface of Ni/MgO. The Ni- (Fig. 1 (b)) and O- (Fig. 1 (c)) maps show that distributions of Ni and O elements all cover such a thin layer. This suggests that the thin layer consists of both Ni and O elements that can also be clearly seen from the RGB map reconstructed from the two elemental maps (Fig.1 (d)). Although we have not succeeded in acquiring a high quality Mg map from the same area due to that Mg has a relatively high energy core-loss peak (*K* edge), conclusion can still be made that the formed thin layer at the interface is NiO layer. Diffusion of Ni atoms down to several nanometers into the MgO substrate is not possible under the present experimental conditions.

Figure 2 (a) clearly shows the CC epitaxial growth of a high quality Ni thin film on the MgO substrate. A thin layer with lattice matching well with the MgO substrate is clearly seen. Due to that both NiO and MgO have fcc (Fm3m) structures with similar lattice parameters (0.4177 and 0.4213 nm, respectively), it is not possible to resolve them from HREM images. To obtain electronic structure information from the interface, EELS profile (O: *K* edge and Ni: *L*₂₃ edges were used) was performed in STEM mode that are displayed in Fig. 2 (b) and (c). Because the white-line intensity ratio (*L*₃/*L*₂) for the Ni oxide is a little bit larger than that for the Ni metal [5], we can extract the

valance state information of Ni by calculating the white-line intensity ratios of the spectra. Measurement of the L_3/L_2 intensity ratios in second derivative mode gives the intensity ratios of 3.3-3.5 (for the spectra acquired from position **a**) and 3.6-4.0 (for the spectra acquired from position **b**), respectively. This further confirms that the interfacial thin layer is oxidized, i.e., a thin NiO layer is formed. Further studies involving using high-energy resolution atomic resolved EELS and electron spectroscopic imaging (ESI) techniques are ongoing. More information about the bonding in the Ni/NiO and the NiO/MgO interfaces as well as the MgO side structure will be provided.

References

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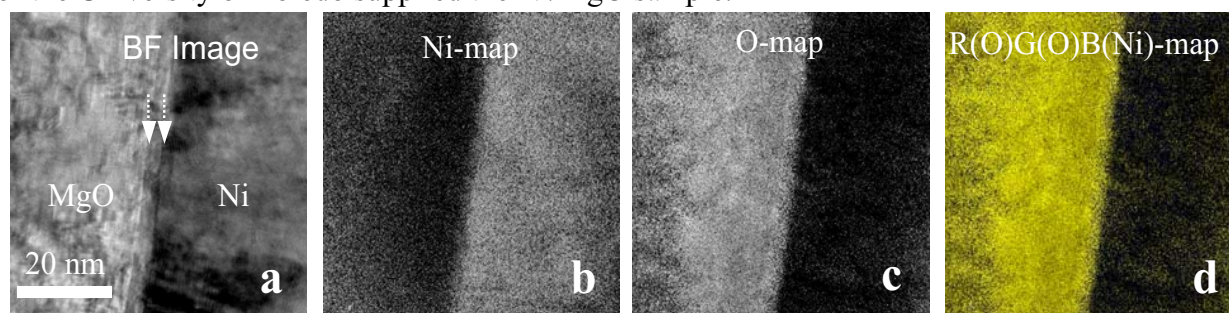


FIG. 1. (a) – (d) display BF, Ni-map, O-map and the generated RGB-map, respectively, obtained from the Ni/MgO interface.

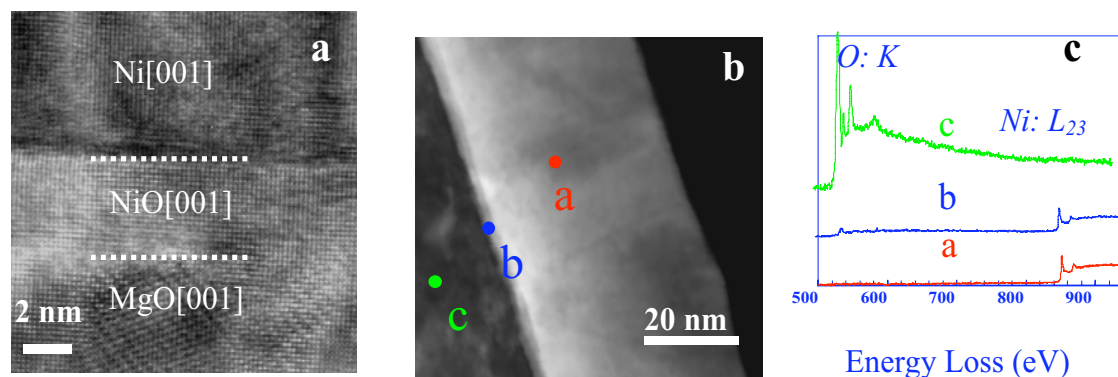


FIG. 2. (a) HREM image showing the interface structure of the Ni/MgO; (b) HAADF image with three positions marked from which corresponding EEL spectra were acquired shown in (c). The EEL spectra were background removed by fitting the background to a power law of the form Ae^{-r} and then were normalized to the energy range of 900-950 eV. They were vertically shifted for clarity.