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Substrate Surface Roughness-Induced Antiphase Boundaries and Strain Relaxation in Cufe₂o₄ Films on Mgal₂o₄ (001) Substrates

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Spinel ferrites have great potential applications in microwave devices and spintronics because of their high saturation magnetization, high spin polarization and low loss performance at high frequencies [1]. Among the spinel ferrites, $CuFe_2O_4$ has been widely investigated due to its interesting physical properties. $CuFe_2O_4$ has two structural polymorphs: a high-temperature cubic and a low-temperature tetragonal. The Cu^{2+} ions tend to occupy octahedral sites and the Fe^{3+} ions occupy both octahedral and tetrahedral sites. It was found that cation distribution and phase stability of $CuFe_2O_4$ can be affected by the growth parameters for the thin-film fabrication, which induces a profound impact on the magnetic, electric and optical properties of the films [2]. In addition, antiphase boundaries (APBs) in epitaxial films have significant effects on the physical properties. Recently, it was reported that the rough substrate can introduce APBs into the functional oxide films [3]. In this work, we investigate the microstructure of epitaxial $CuFe_2O_4$ films on rough $MgAl_2O_4$ (001) substrates. Our studies mainly focus on the origin of APBs and strain relaxation in the $CuFe_2O_4/MgAl_2O_4$ (001) system.

The $CuFe_2O_4$ thin films were fabricated on single crystalline $MgAl_2O_4$ (001) substrates by magnetron sputtering deposition. The growth condition was at substrate temperature 600 ℃ and under the pressure of 0.05 mbar with a mixed atmosphere of Ar_2 and O_2 in the ratio of 1:1. Cross-sectional transmission and scanning transmission electron microscopy (TEM/STEM) specimens were prepared by focus ion beam (FIB) technique (FEI Dual Helios Nano-lab 600i). FIB lamellae were cut along the ⟨100⟩ and ⟨110⟩ direction of the $MgAl_2O_4$ substrate. Low-magnification bright-field (BF) TEM images and selected-area electron diffraction (SAED) patterns were acquired on a JEOL-2100 microscope. High-angle annular dark-field (HAADF) imaging was performed on an aberration-corrected JEOL-ARM200F microscope. The lattice distortion at the dislocation cores and APBs in the film was analyzed by the geometrical phase analysis (GPA) technique [4].

Figure 1a displays a low-magnification BF-TEM image showing the cross-sectional overview of the $CuFe_2O_4/MgAl_2O_4$ (001) heterostructure, viewed along the [100] $MgAl_2O_4$ zone axis. The film thickness is determined to be about 20 nm and the contrast variation within the film is visible, as indicated by oblique white arrows. Figure 1b shows a typical SAED pattern of the $CuFe_2O_4$ film and part of the $MgAl_2O_4$ substrate taken along the [100] $MgAl_2O_4$ zone axis. The splitting of the $0\bar{6}\bar{2}$ reflection along both in-plane and out-of-plane direction is discerned, as shown by the magnified part in the inset in Figure 1b, indicating that the strain relaxation occurs between the film and the substrate. Figure 1c shows a low-magnification HAADF image of the heterostructure, viewed along the [100] $MgAl_2O_4$ zone axis. It is found that the substrate surface is not flat and the maximal surface roughness is measured to be about 3.4 nm. The APBs display the dark lines within the film, which bound the dislocations and connect to the hump on the rough substrates, as marked by oblique white arrows in Figure 1c. The

HAADF results are coincident with the BF-TEM results in Figure 1a. The density of the humps on the rough substrate surface is measured to be about 5.16×10^5/cm.

The APBs originate in the film-substrate interface and obliquely penetrate the whole film as shown in Figures 2a and 2b, viewed along the [100] $CuFe_2O_4$ zone axis. In Figure 2b, the *a*/2[010] dislocation dissociates to two partials (*a*/4[011] and *a*/4[01$\bar{1}$]) at the interface, and each partial dislocation bounds an APB. In some cases, APBs bounding the dislocations of *a*/4[011] and *a*/4[01$\bar{1}$] may interact within the films, as shown in Figure 2c. It should be noted that the two APBs do not terminate inside the film but penetrate each other. Strain analysis has been performed on Figure 2c using the GPA technique. Figure 2d and 2e displays the in-plane strain (e_{xx}) and out-of-plane strain (e_{yy}) map of the HAADF image in Figure 2c, respectively. The strain variation is obvious at the interfacial dislocation in both e_{xx} and e_{yy}. On the basis of the e_{yy} map, the out of-plane lattice parameter of the $CuFe_2O_4$ film is larger than that of $MgAl_2O_4$ substrate. In the e_{xx} and e_{yy} map, the contrast variation appears around the APBs, as marked by oblique white arrows, which indicates that the translation vector across the APBs may be not equivalent to the *a*/4⟨011⟩ of $CuFe_2O_4$ unit cell. The rough substrate can introduce lattice distortions into the APBs in the film close to the heterointerface. Our results indicate that the rough substrate can result in the formation of APBs and strain relaxation in the $CuFe_2O_4$/$MgAl_2O_4$ system [5].

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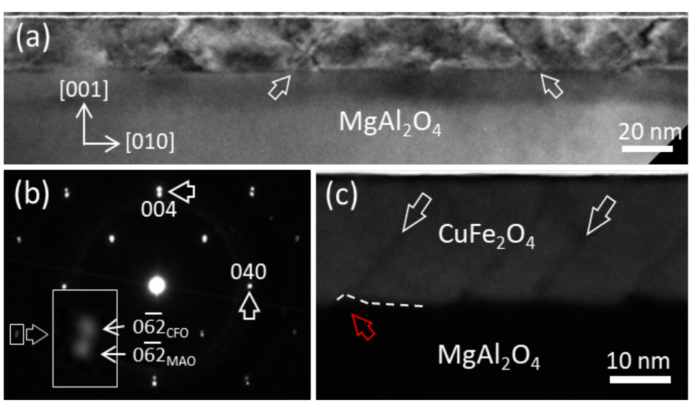

Figure 1. (a) Low-magnification BF-TEM of the $CuFe_2O_4$/$MgAl_2O_4$ heterostructure. (b) A superposed SAED pattern of the heterostructure, viewed along [100] $MgAl_2O_4$ zone axis. (c) Low-magnification HAADF image of the $CuFe_2O_4$/$MgAl_2O_4$ heterostructure.

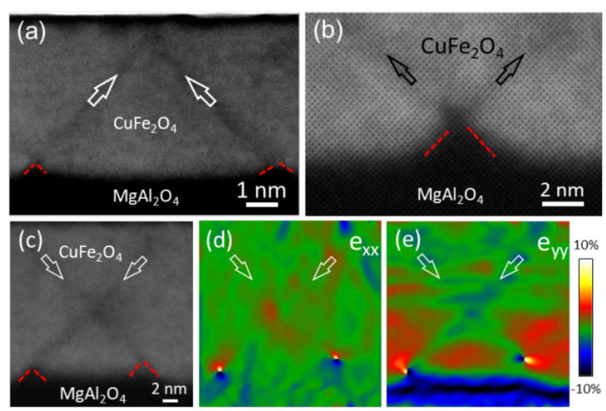

Figure 2. (a-c) HAADF images showing the APBs in the $CuFe_2O_4$ film and the humps on the substrate surfaces. (d,e) The GPA maps of in-plane strain (e_{xx}) and out-of-plane strain (e_{yy}) of (c), respectively.

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