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doi:10.1017/S143192761300367X
Microsc. Microanal. 19 (Suppl 2), 2013

MnMn/O Interface Termination at the $Co_2Mn_\alpha Si$/MgO Interface in Magnetic Tunnel Junctions Investigated by Scanning Transmission Electron Microscopy

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We have discovered MnMn/O and CoCo/O interface terminations at the MgO/Co_2MnSi (CMS) interfaces in CoFe/MgO/$Co_2Mn_\alpha Si$ (α = 0.80, 1.0 and 1.29) magnetic tunnel junctions (MTJs) from high-resolution STEM images. The existence of MnMn/O and CoCo/O interface termination explains the high tunnel magnetoresistence (TMR) obtained in similar CoFe/MgO/$Co_2Mn_{1.29}Si$ MTJs [1] because simulation shows that only the metastable MnMn/O interface termination gives 100% spin polarization across the CMS/MgO interface [2]. Steps in the MgO barrier induce switching of the interface termination between MnMn/O and CoCo/O terminations. We also found that increasing Mn concentration in the CMS electrodes increased the fraction of MnMn/O termination. Other interface terminations like SiSi/Mg were not observed in the MTJs. The mixed terminations we found at the CMS/MgO interface provide a key to understand the high TMR and strong temperature dependence of these MTJs [1].

Figure 1(a) is an HRSTEM image of the MTJ multilayer structure consisting of (from the lower side) CoFe/MgO/$Co_2Mn_{1.29}Si$. Steps at the CMS/MgO are visible due to the very flat MgO tunnel barrier. Figure 1(b) shows CoCo/O and MnMn/O terminations on the left and right side of image, respectively. The changes of the interface terminations are associated with the steps of the MgO tunnel barrier labeled by the orange arrows in Figure 1(b). Away from the interface, the $L2_1$ structure with the Mn and Si positions interchanged in subsequent MnSi planes is visible in the line profiles in Figure 1(c). At the interface, all the atomic columns have the same intensity. The distances in Figure 2(a) and (b) between the last CMS and first MgO layers are 0.20±0.01 nm and 0.25±0.01 nm for the CoCo/O and MnMn/O terminations, respectively, which are in good agreement with calculations by Hülsen *et al*. [2]. They disagree with simulated images based on a disordered MnSi/O interface [3].

The intensity of the atom columns at the interface is suppressed by interfacial strain [4], as shown by Figure 2(b)-(d). We increased the HAADF detector angles to suppress the interfacial strain contrast in the STEM images at CMS/MgO interface. The difference between the intensity of the Mn column in the CMS electrode and that of Mn at the interface decreases with increasing the detector angles. Figure 2(e) and (f) shows the simultaneously acquired HAADF and ABF STEM images at the CMS/MgO interface. SiSi/Mg interface termination can be excluded due to the metal-oxygen bonding shown in Figure 2(f).

Our results indicate that the metastable MnMn/O termination is favored by nonequilibrium sputter deposition with excess Mn in the CMS. The Mn concentration in the CMS also affects the interface terminations at CMS/MgO interface. Saito *et al.* reported MnSi/O interface termination at CMS/MgO interface with a Mn deficient CMS electrode [5], although they did not consider MnMn/O in detail. Figure 3 shows the fraction of the MnMn/O termination increases with the increasing Mn concentration. We also found MnSi/O interface termination in the MTJ with $Co_2Mn_{0.80}Si$ electrode, but CoCo/O and MnMn/O terminations are still the dominant species in our MTJs [6].

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[6] The authors acknowledge funding from the US Department of Energy, Basic Energy Sciences (contract DE-FG02-99ER45777). This work was supported in part by the C-SPIN Center, one of six centers supported by the STARnet phase of the Focus Center Research Program (FCRP), a Semiconductor Research Corporation program sponsored by MARCO and DARPA. The work at Hokkaido University was partly supported by a Grant in-Aid for Scientific Research (A) (Grant No. 23246055) from MEXT, Japan.

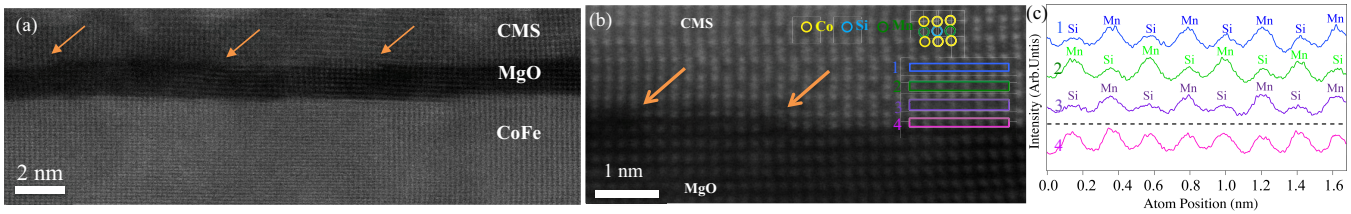

Figure 1 (a) STEM image of the MTJ structure, CoFe/MgO/$Co_2Mn_{1.29}Si$, with steps at the MgO/CMS interface indicated by arrows. (b) Z-contrast image of the MgO/CMS showing two different interface terminations. (c) Horizontal profiles taken on the numbered MnSi planes in (b) show $L2_1$ ordering within the film but not at the interface.

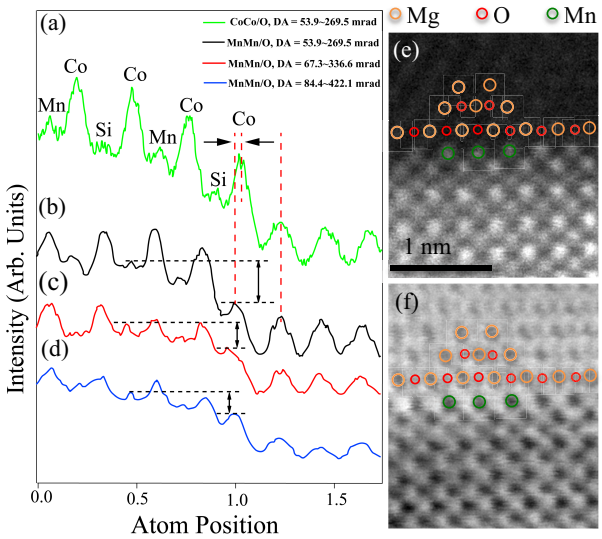

Figure 2 Intensity profiles taken vertically in Figure 1(b) at (a) CoCo/O terminated interface, (b) MnMn/O terminated interface. (c) and (d) show that at larger detector inner angle, the intensity drop across the interface is smaller. (e) Z-contrast STEM and (f) ABF STEM images of interface along the [100] zone axis of CMS.

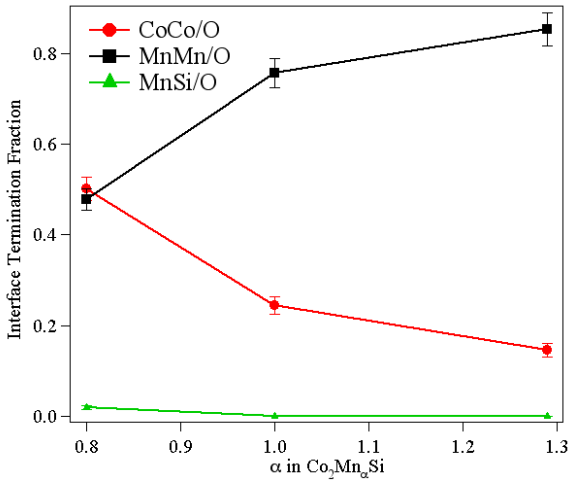

Figure 3 Fraction of CoCo/O, MnMn/O and MnSi/O interface terminations as a function of Mn concentration in $Co_2Mn_\alpha Si$.

https://doi.org/10.1017/S143192761300367X Published online by Cambridge University Press