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## Influence of interface termination layer on temperature dependence of tunneling magnetoresistance of Co<sub>2</sub>MnSi/MgO-based magnetic tunnel junctions

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We have recently demonstrated giant tunneling magnetoresistance (TMR) ratios ( $\beta$ ) of up to 1995% at 4.2 K and up to 354% at 290 K for epitaxial Co<sub>2</sub>MnSi (CMS)/MgO/CMS magnetic tunnel junctions (MTJs).<sup>1</sup> If we use parameter  $\gamma = \beta(4.2 \text{ K})/\beta(290 \text{ K})$  to represent the degree of temperature (*T*) dependence of  $\beta$ ,  $\gamma$  for the CMS MTJs that showed a high  $\beta$  of 1910% at 4.2 K was 5.4, resulting in a lower  $\beta$  of 354% at 290 K than the 604% at RT for a CoFeB/MgO/CoFeB MTJ that exhibited a much lower  $\beta$  of 1144% at 5 K ( $\gamma = 1.9$ ).<sup>2</sup> The purpose of the present study was to investigate the possible origin of the strong *T* dependence of  $\beta$  of CMS/MgO-based MTJs. In this study, we prepared epitaxial MTJs having a CMS electrode in combination with a Co<sub>50</sub>Fe<sub>50</sub> (CoFe) electrode and a MgO barrier and prepared three kinds of MTJ layer structures on MgO(001) substrates: (1) MTJ-1: (from the lower side) CoFe/MgO/CMS (3 nm), (2) MTJ-2: CoFe-buffer/CMS (3 nm)/MgO/CoFe (3 nm), and (3) MTJ-3: CoFe/MgO/ultrathin CoFe inserted layer (1.1 nm)/CMS (3 nm). We used Mn-rich CMS electrodes<sup>3,4</sup> having a film composition of Co<sub>2</sub>Mn<sub>1,29</sub>Si<sub>1,0</sub> for MTJ-1 and a film composition of Co<sub>2</sub>Mn<sub>1,35</sub>Si<sub>0.88</sub> for MTJ-2 and MTJ-3.

Figure 1 shows  $\beta$  as a function of *T* from 4.2 K to 290 K for these three kinds of MTJs. We first compare the *T* dependence of  $\beta$  for MTJ-1 and MTJ-2. It has been experimentally shown that harmful Co<sub>Mn</sub> antisites are strongly suppressed for Mn-rich CMS electrodes,<sup>1,3,4</sup> suggesting that the bare tunneling spin polarizations that are determined by the majority- and minority-spin density of states at the Fermi level are close for the Mn-rich CMS electrodes having the almost identical film compositions used in this study. Then, the higher  $\beta$  value at 4.2 K for MTJ-1 than MTJ-2 has been attributed to the enhanced coherent tunneling contribution arising from the larger misfit dislocation spacing for MTJ-1.<sup>4</sup> According to the theory by Zhang *et al.*,<sup>5</sup> if the bare tunneling spin polarizations and the properties of thermally excited magnons are close for MTJ-1 and MTJ-2,  $\gamma$  should be close. Note that, however, MTJ-1 showed much stronger *T* dependence of  $\beta$  ( $\gamma = 3.3$ ) than MTJ-2 ( $\gamma = 2.6$ ), resulting in a slightly lower  $\beta$  of 311% at 290 K for MTJ-1 than the 340% for MTJ-2 although the latter exhibited a markedly lower  $\beta$  at 4.2 K.

To clarify the origin of the difference in the *T* dependence of  $\beta$ , we investigated the interface structure of these MTJs by high-resolution Z-contrasted scanning transmission electron microscopy. We found that the termination layer at the CMS/MgO interface for MTJ-2 mainly consisted of MnMn/O termination layer<sup>6</sup> which has been theoretically predicted to be thermodynamically unstable.<sup>7</sup> On the other hand, we found that the termination layer for MTJ-1 consisted of coexisting MnMn/O and CoCo/O terminations with one

monolayer steps probably caused by the very flat interface in MTJ-1. Given the observation of CoCo/O terminations coexisted with MnMn/O terminations, we attribute the stronger T dependence of MTJ-1 to the theoretically predicted strong spin fluctuation of Co atoms in the Co plane of CMS in the interfacial region with a MgO barrier.<sup>8</sup>

To further evidence this understanding, we prepared MTJ-3 in which an ultrathin CoFe layer (1.1 nm) was inserted between the MgO barrier and the upper CMS electrode. Most importantly, the *T* dependence of  $\beta$  was significantly weakened ( $\gamma = 2.5$ ). This resulted in a much higher  $\beta$  of 448% at 290 K. The markedly enhanced  $\beta$  at RT for MTJ-3 can be explained by the elimination of the CMS/MgO interface, including in particular, the CoCo/O termination, observed in MTJ-1.

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Fig. 1. TMR ratios as a function of *T* from 4.2 K to 290 K for a CoFe/MgO/CMS (MTJ-1), a CoFe-buffered CMS/MgO/CoFe (MTJ-2) and a CoFe/MgO/CoFe (1.1 nm)/CMS (MTJ-3). For comparison, TMR ratios as a function of *T* for an identically fabricated CoFe/MgO/CoFe are plotted.