Magnetic tunnel junctions using Co-based Heusler alloy electrodes
Half-metallic Heusler alloy thin films for spintronic devices

(1) Half-metallic nature theoretically predicted for some of these alloys.
(2) High Curie temperatures well above RT.

Co$_2$YZ: L2$_1$ structure

Consisting of four fcc sublattices

Coherent tunneling can be fully utilized in Heusler alloy/MgO heterostructures along with the half-metallicity

-5.1% between Co$_2$MnSi and MgO

$\sqrt{2}a_{\text{MgO}} = 0.5957$ nm

$a_{\text{Co}_2\text{MnSi}} = 0.5654$ nm

DOS

Energy gap

Purpose

To clarify the key factors that determine the spin-dependent tunneling characteristics of Heusler-alloy Co$_2$MnSi/MgO-based MTJs
The suppression of detrimental Co$_{\text{Mn}}$ antisites is essential to obtain the half-metallicity of Co$_2$MnSi (CMS).

1. The lower TMR ratios for MTJs with Mn-deficient CMS electrodes were explained by the formation of Co$_{\text{Mn}}$ antisites that lead to minority-spin in-gap states around $E_F$ as theoretically predicted by Picozzi et al.

2. Consistent with this, the higher TMR ratio for MTJs with Mn-rich CMS electrodes was explained by suppressed Co$_{\text{Mn}}$ antisites.

(1) T. Ishikawa et al., APL 95, 232512 (2009). (2) M. Yamamoto et al., JPCM 22, 164212 (2010)
Formula unit composition model for nonstoichiometric Co$_2$MnSi

Assuming the antisite formation, not the vacant site formation

**Mn-deficient** $\text{Co}_2\text{Mn}_{0.69}\text{Si}_{1.0}$

$$[\text{Co}_2][\text{Mn}_{0.75}\text{Co}_{0.17}\text{Si}_{0.08}][\text{Si}_{1.0}]$$

**Co$_{\text{Mn}}$ antisite (detrimental)**

**Mn-rich** $\text{Co}_2\text{Mn}_{1.29}\text{Si}_{1.0}$

$$[\text{Co}_{1.86}\text{Mn}_{0.14}][\text{Mn}][\text{Si}_{0.93}\text{Mn}_{0.07}]$$

**Mn$_{\text{Co}}$ antisite (not harmful)**

M. Yamamoto et al., JPCM 22, 164212 (2010)
Enhancement of coherent tunneling contribution for Co$_2$MnSi/MgO MTJs

A CoFe-buffer and a thin Co$_2$MnSi lower electrode was introduced

Key points: (1) A smaller lattice misfit of -4.3% between CoFe and MgO
(2) The thin 3-nm-thick CMS lower electrode is lattice-matched to the CoFe buffer

Co$_{2.0}$Mn$_{\alpha}$Si$_{0.96}$
$\alpha$: 0.72 (Mn-deficient) $\sim$ 1.57 (Mn-rich)

1. All layers were grown epitaxially and were single crystalline.
2. Atomically flat and abrupt interfaces were formed.
3. There were no clear lattice misfit dislocations between the CoFe buffer and the lower CMS electrode.
4. (111) spots for the upper CMS electrode were clearly observed.
Structural quality of the interfacial regions of the CoFe-buffered CMS MTJ was improved in terms of misfit dislocation density.

<table>
<thead>
<tr>
<th>MTJ layer structure</th>
<th>Lower CMS/MgO (nm)</th>
<th>MgO/upper CMS (nm)</th>
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</thead>
<tbody>
<tr>
<td>CoFe-buffered CMS MTJs</td>
<td>6.4 (1.0)</td>
<td>6.2 (1.4)</td>
</tr>
<tr>
<td>MgO-buffered CMS MTJs *</td>
<td>4.4 (0.8)</td>
<td>4.2 (0.7)</td>
</tr>
</tbody>
</table>

Values in brackets are the standard deviations.

The CoFe-buffered $\text{Co}_2\text{MnSi}$ MTJ layer structure showed larger misfit dislocation spacing, i.e., smaller density of misfit dislocation at the lower and upper MgO interfaces than the MgO-buffered $\text{Co}_2\text{MnSi}$ MTJs.

Misfit dislocation spacing at the lower and upper interfaces with a MgO.
Giant TMR ratios of 1995% at 4.2 K and 330% at RT were demonstrated.

1. These TMR ratios are much higher than the 1135% at 4.2 K and 236% at RT for MgO-buffered Co$_2$MnSi MTJs.

2. This can be attributed to enhanced coherent tunneling contribution arising from the increased misfit dislocation spacing.
Giant TMR ratios of up to 1995% at 4.2 K and up to 330% at RT were demonstrated, clearly indicating the half-metallicity of Co$_2$MnSi electrodes.

The observed giant TMR ratios are due to:
1. Enhanced half-metallicity obtained by the suppression of harmful Co$_{\text{Mn}}$ antisites.
2. Enhanced coherent tunneling contribution evidenced by the comparison of the MgO-buffered and CoFe-buffered MTJs.

Conclusion

1. The suppression of detrimental $\text{Co}_{\text{Mn}}$ antisites is essential to obtain half-metallicity of $\text{Co}_2\text{MnSi}$. This can be achieved by using Mn-rich composition.

2. Giant TMR ratios of up to about 2000% at 4.2 K and up to 354% for $\text{Co}_2\text{MnSi}/\text{MgO}/\text{Co}_2\text{MnSi}$ clearly indicate the half-metallicity of Mn-rich $\text{Co}_2\text{MnSi}$ electrodes.