Thickness and surface-termination effects on magnetocrystalline anisotropy of FeRh(001) thin films

Soyoung Jekal, S. H. Rhim, Soon Cheol Hong
Department of Physics and EHSRC, University of Ulsan, Ulsan, Korea

A. B. Shick
Institute of Physics, ASCR, Na Slovance 2, Prague, Czech Republic

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Outline

✓ Introduction to AFM spintronics
✓ What are interesting for FeRh?
✓ Our calculational results
✓ Conclusions
Advantages of AFM spintronics

✓ Robust to external magnetic field
✓ No stray field
✓ No shape anisotropy
✓ Faster dynamics
  Low critical current for STT switching
✓ Abundance of AFM materials
  Most magnetic semiconductors are AFM

A. H. MacDonald and M. Tsoi, Phil. Trans. R. Soc. A 369, 3098 (2011)
Switching time: \(~20 \text{ ns at } 0.5 \text{ V}\)
Two paradigms for spintronics

"Mott" two-spin-channel model of ferromagnets

"Dirac" relativistic spin-orbit coupling

Tomas Jungwirth, Institute of Physics, ASCR
Antiferromagnetic MATERIALS playing ACTIVE role in spintronics

Mott with ferromagnet

Dirac with ferromagnets

Mott with antiferromagnets

Dirac with antiferromagnets

Tomas Jungwirth, Institute of Physics, ASCR
What are interesting for FeRh?
What are interesting in FeRh alloys

- Transition temperature of AFM$\rightarrow$FM: $T_{tr} \approx 340$ K
  - MM(Fe) $\approx 3.1$ $\mu_B$, MM(Rh) $\approx 1.0$ $\mu_B$ in FM
- Relatively high Curie temperature: $T_C \approx 670$ K
- Heat assisted magnetic RAM
- A good candidate for a magnetocaloric refrigerator
Room-temperature antiferromagnetic memory resistor
Electric-field control of magnetic order above room temperature

\( \alpha = \mu_0 \Delta M / E = 1.6 \times 10^{-5} \text{ sm}^{-1} \)

At least one order larger than previous reports
Fe Spin Reorientation across the Metamagnetic Transition in Strained FeRh Thin Films


(a) FeRh//MgO
(b) FeRh//IBAD MgO

Magnetic hyperfine field (T)
Magnetization (kA/m)

(c) Heating
(d) Cooling

Magnetocrystalline anisotropy (meV/μm²)

Temperature (K)

0.985 0.990 0.995 1.000 1.005 1.010 1.015 1.020

AFM
FM

Our story on FeRh(001) thin films
Microscopic understanding of MCA

Origin of MCA: Spin-orbit coupling

The SOC perturbed Hamiltonian:

$$H = H^0 + H^{sl} = H^0 + \xi(r) \sigma \cdot \mathbf{L}$$

The SOC induced change of the total energy:

$$E^{sl} = E(H^0 + H^{sl}) - E(H^0)$$

$$\xi(r) = \frac{1}{4c^2r} \frac{\partial V}{\partial r}$$

$$\langle xz | L_z | yz \rangle = 1$$
$$\langle x^2 - y^2 | L_z | xy \rangle = 2$$
$$\langle z^2 | L_x | xz, yz \rangle = \sqrt{3}$$
$$\langle xy | L_x | xz, yz \rangle = 1$$
$$\langle x^2 - y^2 | L_x | xz, yz \rangle = 1$$

**Fe bcc**

easy axis: (100)

\[ K_1 = 4.8 \times 10^4 \ J / m^3 \]
\[ = 2.4 \ \mu eV / \text{atom} \]

**Co hcp**

easy axis: (0001)

\[ K_1 = 4.1 \times 10^5 \ J / m^3 \]
\[ = 45 \ \mu eV / \text{atom} \]

**Ni fcc**

easy axis: (111)

\[ K_1 = -5.5 \times 10^3 \ J / m^3 \]
\[ = -0.3 \ \mu eV / \text{atom} \]

S. Kaya, *Sci. Reports Tohoku Univ.* 17, 639 (1928)
Methods to calculate MCA energy

\[ E_{\text{MCA}} = E_{\text{tot}}(\theta=90^\circ) - E_{\text{tot}}(\theta=0^\circ) \]

**FLAPW- Torque:**

\[ E(\theta) = k_1 \sin^2 \theta + k_2 \sin^4 \theta; \quad E_{\text{MCA}} = E(90^\circ) - E(0^\circ) = k_1 + k_2 \]

\[ \frac{\partial E(\theta)}{\partial \theta} \bigg|_{\theta = 45^\circ} = k_1 + k_2 \]

\[ E_{\text{MCA}} = \langle \Psi_i \left| \frac{\partial H}{\partial \theta} \right| \Psi_i \rangle \bigg| \theta = 45^\circ \]

FLAPW and VASP methods

Two methods:

Full Potential Linearized
Augmented Plane-wave (FLAPW)
All-electron (core+valence )
- Very accurate method
- Slow computation
- For small systems and for confirmations

Vienna Ab initio Simulation Package (VASP)
Pseudopotential Method
- Less accurate than all-electron
- Fast computation (?)
- For large systems (?)

\[ \lambda_{001} = \frac{2}{3} \frac{dE_{MCA}/d(c/c_0)}{d^2E_{tot}/d(c/c_0)^2} \]

<table>
<thead>
<tr>
<th></th>
<th>FLAPW</th>
<th>VASP</th>
<th>Exp.</th>
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<tbody>
<tr>
<td>bcc Fe</td>
<td>2.84</td>
<td>2.85</td>
<td>2.87</td>
</tr>
<tr>
<td></td>
<td>2.23</td>
<td>2.20</td>
<td>2.22</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>19</td>
<td>21</td>
</tr>
<tr>
<td>fcc Co</td>
<td>3.52</td>
<td>3.54</td>
<td>3.53</td>
</tr>
<tr>
<td></td>
<td>1.67</td>
<td>1.72</td>
<td>0.62</td>
</tr>
<tr>
<td></td>
<td>69</td>
<td>79</td>
<td>-52</td>
</tr>
<tr>
<td>fcc Ni</td>
<td>3.52</td>
<td>3.53</td>
<td>3.53</td>
</tr>
<tr>
<td></td>
<td>0.62</td>
<td>0.61</td>
<td>-49</td>
</tr>
</tbody>
</table>
Four different magnetic structures

Magnetic unit cell: $a^* = \sqrt{2} \ a$, $c^* = 2c$
Total energies of different magnetic states

![Graph showing total energies of different magnetic states, with lines and markers for FM, A-AFM, C-AFM, and G-AFM. The y-axis represents energy in eV, and the x-axis represents lattice in Å.]
Magnetic moments of different magnetic states of bulk FeRh

<table>
<thead>
<tr>
<th></th>
<th>A-AFM</th>
<th>C-AFM</th>
<th>G-AFM</th>
<th>FM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>3.144</td>
<td>3.129</td>
<td>3.122</td>
<td>3.168</td>
</tr>
<tr>
<td>Rh</td>
<td>0.000</td>
<td>0.015</td>
<td>0.000</td>
<td>1.031</td>
</tr>
</tbody>
</table>
DOS of bulk FeRh
Interlayer spacings of thin films

Fe-terminated

Rh-terminated
ΔE = E - E_{G-AFM}

Fe-terminated

Rh-terminated

Ground magnetic states
Fe-terminated films: G-AFM, Rh-terminated films: FM
A-AFM state is also more stable than the G-AFM for thinner film than 7-ML.
DOS of thin film FeRh
Magnetic moments ($\mu_B$) of Fe and Rh atoms of the Fe-terminated FeRh(001) in G-AFM

<table>
<thead>
<tr>
<th></th>
<th>3-ML</th>
<th>5-ML</th>
<th>7-ML</th>
<th>9-ML</th>
<th>11-ML</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe(S)</td>
<td>3.065</td>
<td>3.122</td>
<td>3.140</td>
<td>3.145</td>
<td>3.141</td>
</tr>
<tr>
<td>Rh(S-1)</td>
<td>0.000</td>
<td>0.036</td>
<td>0.036</td>
<td>0.035</td>
<td>0.025</td>
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<tr>
<td>Fe(S-2)</td>
<td>-</td>
<td>3.008</td>
<td>3.044</td>
<td>3.075</td>
<td>3.123</td>
</tr>
<tr>
<td>Rh(S-3)</td>
<td>-</td>
<td>-</td>
<td>0.001</td>
<td>0.005</td>
<td>0.017</td>
</tr>
<tr>
<td>Fe(S-4)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>3.102</td>
</tr>
<tr>
<td>Rh(S-5)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.001</td>
</tr>
</tbody>
</table>
Magnetic moments ($\mu_B$) of Fe and Rh atoms of the Rh-terminated FeRh(001) in FM

<table>
<thead>
<tr>
<th></th>
<th>3-ML</th>
<th>5-ML</th>
<th>7-ML</th>
<th>9-ML</th>
<th>11-ML</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rh(S)</td>
<td>1.026</td>
<td>1.082</td>
<td>1.105</td>
<td>1.117</td>
<td>1.092</td>
</tr>
<tr>
<td>Fe(S-1)</td>
<td>3.116</td>
<td>3.173</td>
<td>3.174</td>
<td>3.179</td>
<td>3.184</td>
</tr>
<tr>
<td>Rh(S-2)</td>
<td>-</td>
<td>1.043</td>
<td>1.052</td>
<td>1.054</td>
<td>1.054</td>
</tr>
<tr>
<td>Fe(S-3)</td>
<td>-</td>
<td>-</td>
<td>3.193</td>
<td>3.189</td>
<td>3.196</td>
</tr>
<tr>
<td>Rh(S-4)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
<td>1.036</td>
</tr>
<tr>
<td>Fe(S-5)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
Magnetocrystalline anisotropy energies

Fe-termination

Rh-termination

![Graphs showing magnetocrystalline anisotropy energies for Fe- and Rh-termination.](image-url)
Layer (element-specific) and the total MCA energy

<table>
<thead>
<tr>
<th></th>
<th>5-ML</th>
<th>7-ML</th>
<th>9-ML</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rh(S)</td>
<td>2.97</td>
<td>3.75</td>
<td>3.67</td>
</tr>
<tr>
<td>Fe(S-1)</td>
<td>-1.17</td>
<td>-1.63</td>
<td>-1.49</td>
</tr>
<tr>
<td>Rh(S-2)</td>
<td>0.15</td>
<td>0.075</td>
<td>0.23</td>
</tr>
<tr>
<td>Fe(S-3)</td>
<td>-</td>
<td>0.04</td>
<td>-0.21</td>
</tr>
<tr>
<td>Rh(S-4)</td>
<td>-</td>
<td>-</td>
<td>0.01</td>
</tr>
<tr>
<td>Total</td>
<td>1.65</td>
<td>2.24</td>
<td>2.22</td>
</tr>
</tbody>
</table>
Surface formation energy

\[ E_{surf} = \frac{1}{2} \left[ A_{2n+1} - (B_{2n-1} + 2A_1) \right] \]
Thickness effect on switching barrier of AFM to FM
Conclusion

- Ground magnetic states of Rh-terminated FeRh thin films are different from its bulk.

- The GKA rule on the superexchange interaction is crucial in determining the magnetic ground phases of FeRh bulk and thin films.

- The Zener-type direct-interaction and energy gain by Rh magnetization play partly in determining the ground magnetic states.

- Rh-terminated FeRh thin films show strong perpendicular MCA energy, +2.1 meV/□.

- $T_C$ can be engineered by thickness and surface-termination of FeRh.