Resolving Atomic-Scale Complex Magnetic Order in an Antiferromagnetic Ultrathin Film by Spin-polarized Scanning Tunneling Microscopy

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Introduction

a) Non-colinear magnetic order

Heisenberg exchange interaction

$H_{HEI} = -J_{ij}\boldsymbol{S_i}\cdot\boldsymbol{S_j} \rightarrow$ ↑↑↑ or ↑↓↑

Dzyaloshinskii-Moriya interaction

$H_{DMI} = -\boldsymbol{D}_{ij}\cdot(\boldsymbol{S_i}\times\boldsymbol{S_j}) \rightarrow$ ↑ ⟹ ↓

Flat Spin Spiral (SS)

$\vec{S}_{ss} = \cos(\boldsymbol{q}\cdot\boldsymbol{r}_i)\hat{x} + \sin(\boldsymbol{q}\cdot\boldsymbol{r}_i)\hat{y}$

$\boldsymbol{q}$: wave vector of magnetic order
$\boldsymbol{r}_i$: location of atom

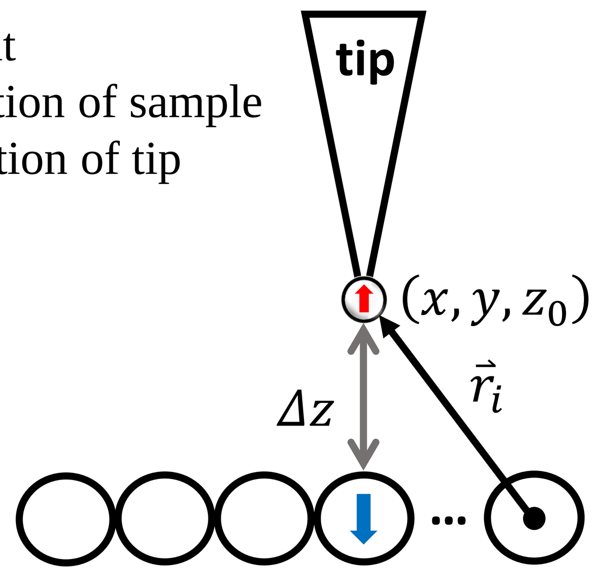
b) Spin-polarized Scanning tunneling microscopy

$I(\vec{r},\theta) \propto e^{-\kappa|\vec{r}|}\,(1 + P_s P_t\cos(\theta))$

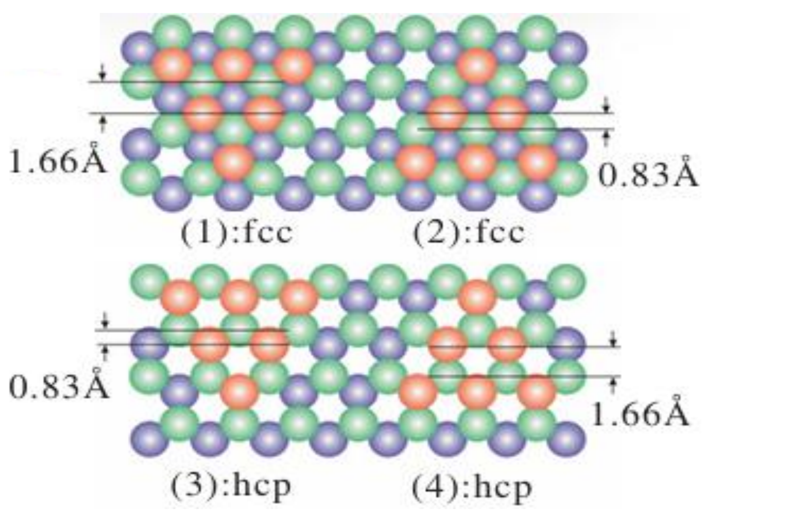
Spin Average   Spin polarized

κ: decay constant
P_s: spin polarization of sample
P_t: spin polarization of tip

$$I_{total}(x,y,z_0) = \sum_i e^{-\kappa|\vec{r}_i|}\,(1 + P_{s,i}P_t\cos(\theta_i))$$
$$\approx I_0(z_0) + \frac{dI_0}{dz}\Delta z$$



c) 120° Néel structure - ML Mn/Ag(111)



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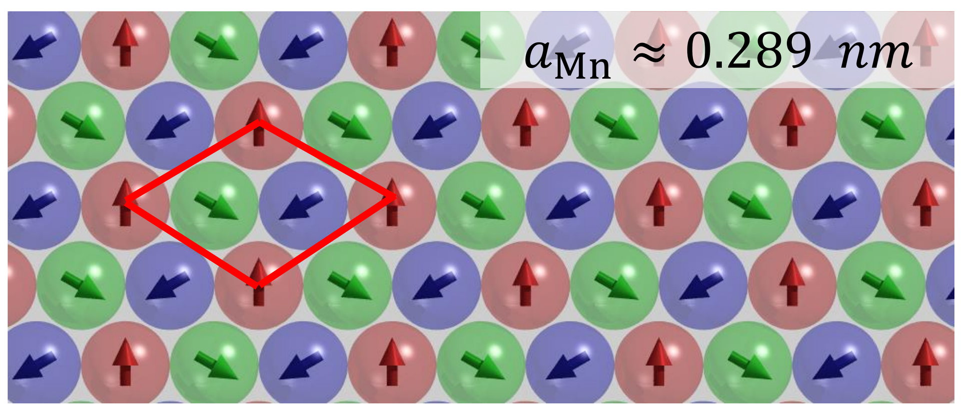
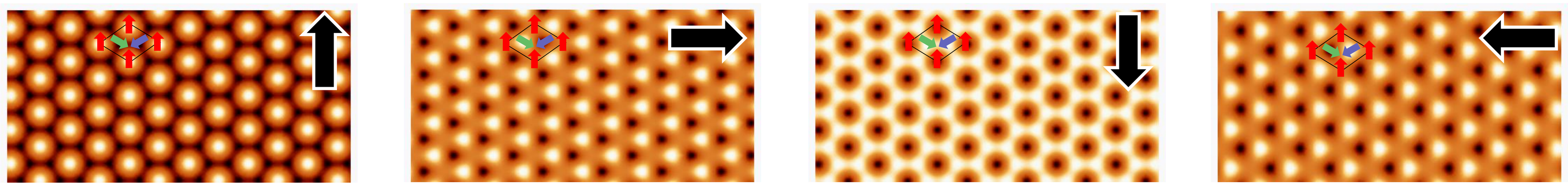
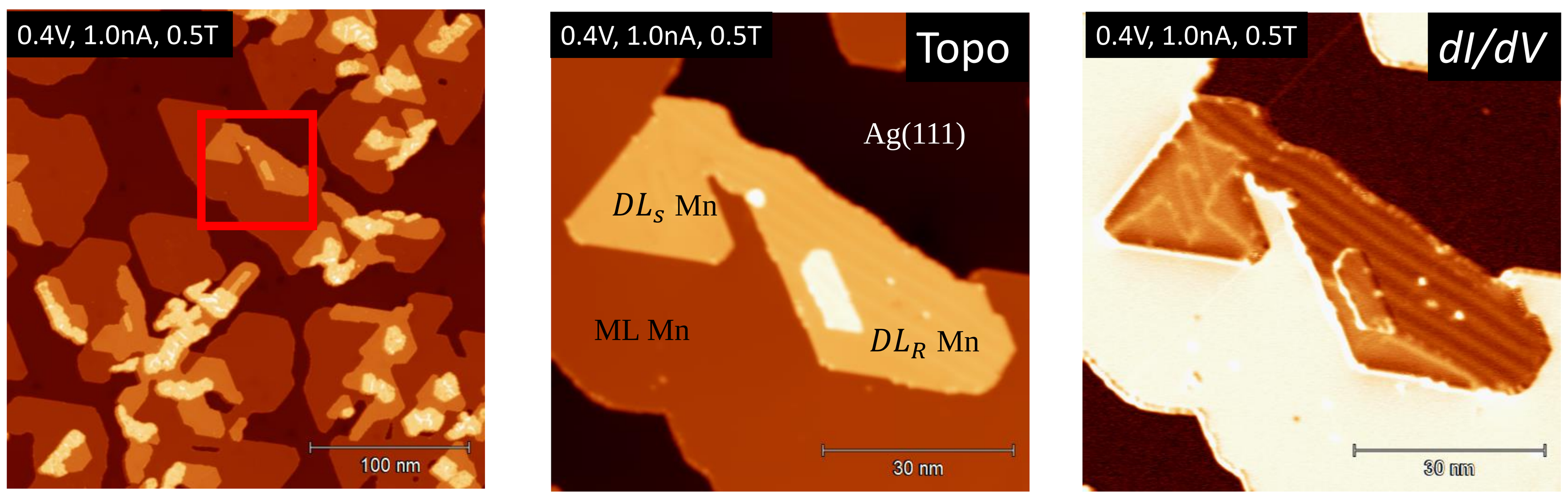


$(\sqrt{3}\times\sqrt{3})R30°$ magnetic unit cell

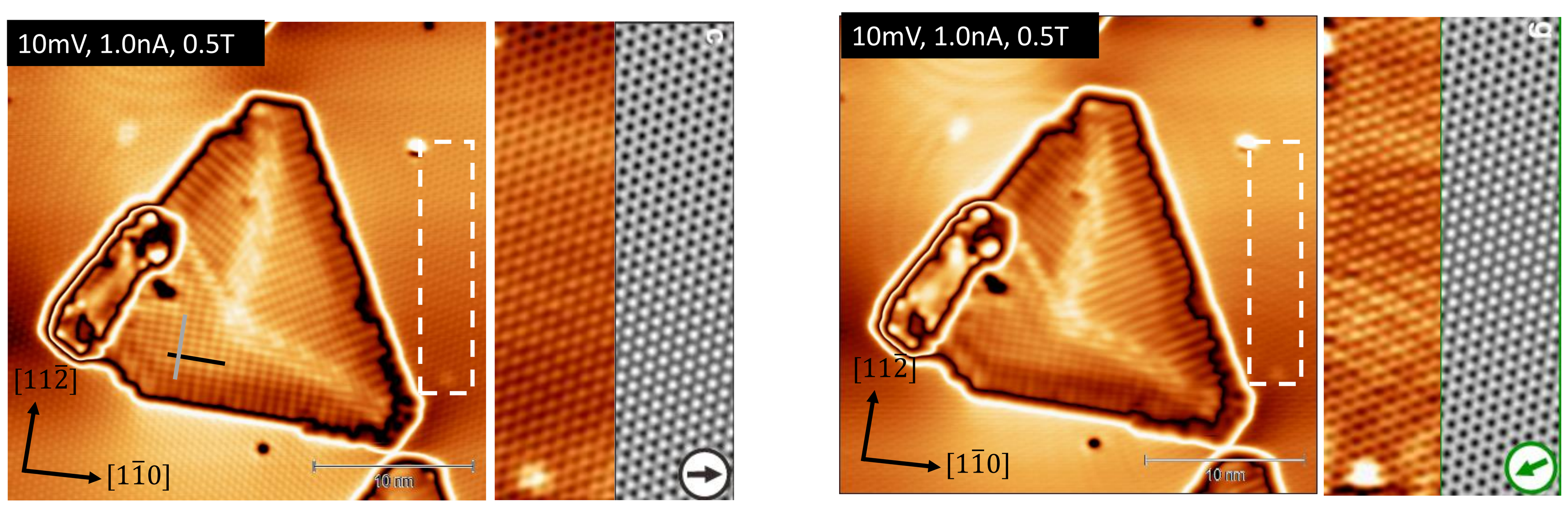


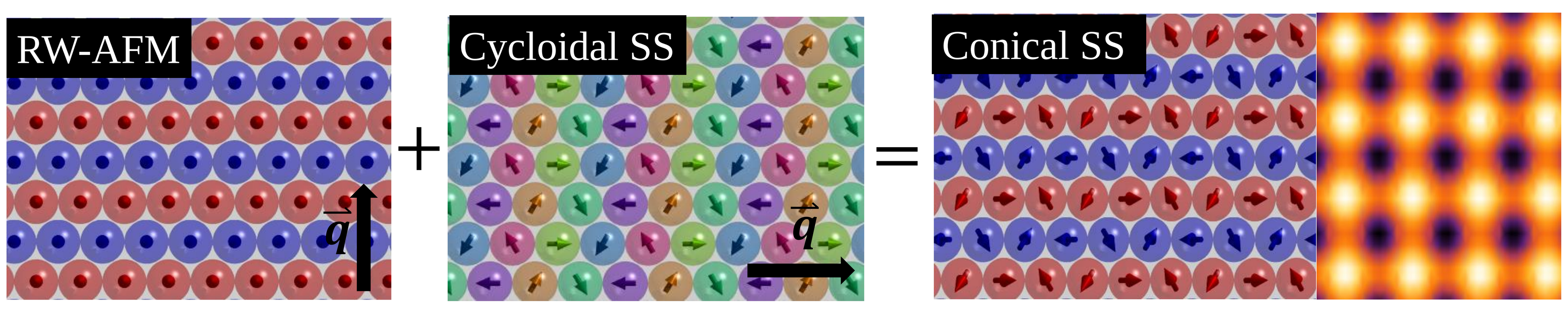
Experimental result

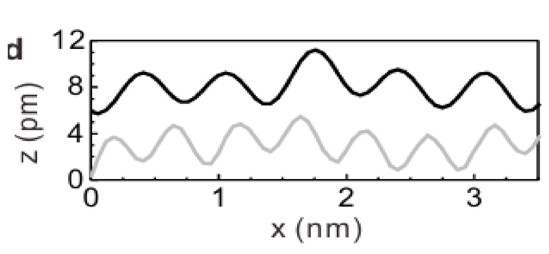
- **Topographic overview**



- **DL Mn/Ag(111) – Psudomorphic phase (DL_s Mn)**



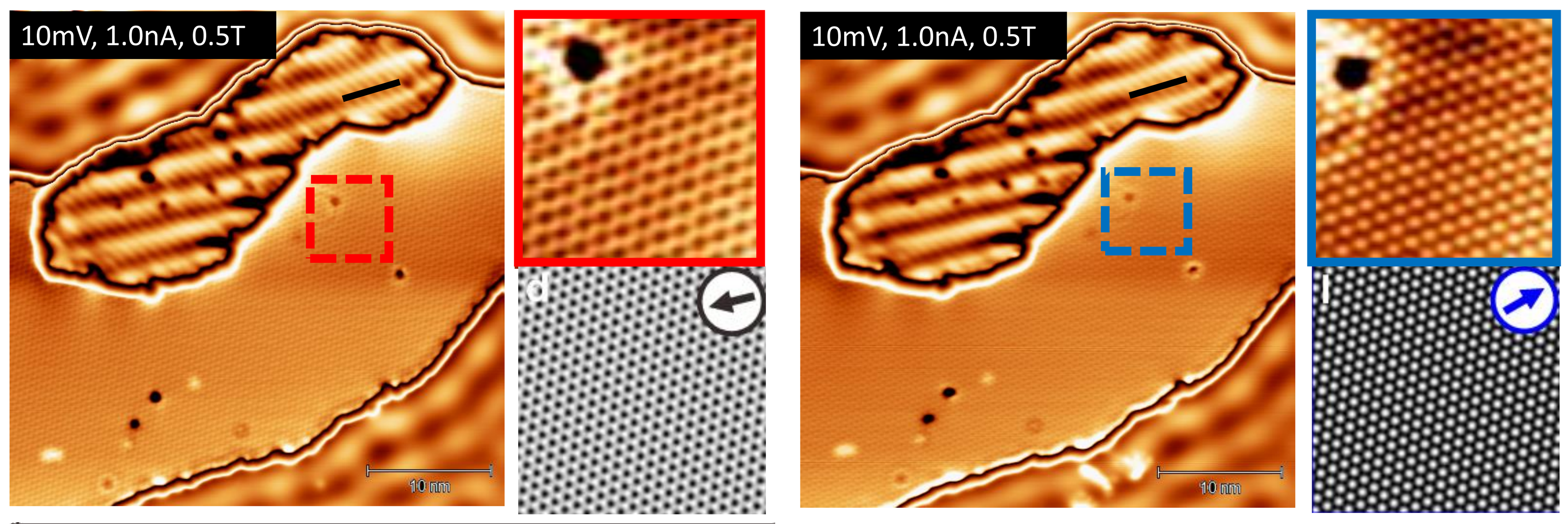


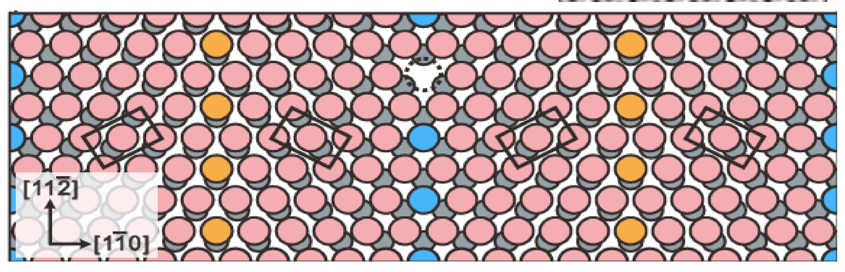


$T_{[1\bar{1}0]} \approx 0.70 \pm 0.05\ nm \rightarrow$ **Spin Spiral**
$T_{[11\bar{2}]} \approx 0.50 \pm 0.05\ nm \rightarrow$ **RW − AFM** $(\sqrt{3}a_{Mn})$

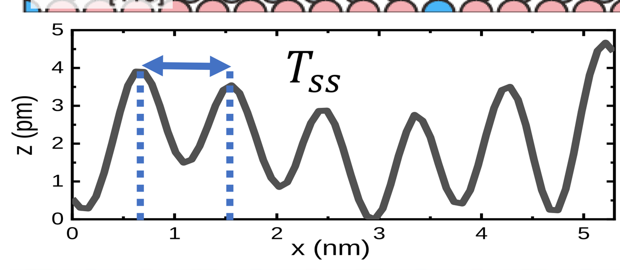
Experimental result

- **DL Mn/Ag(111) – Reconstructed phase (DL_R Mn)**

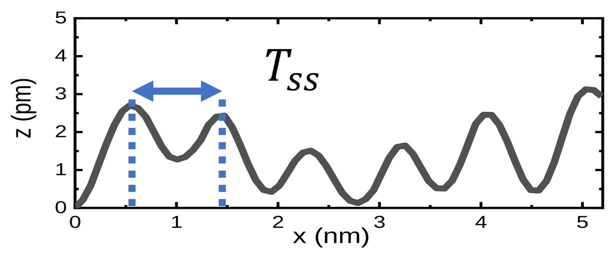


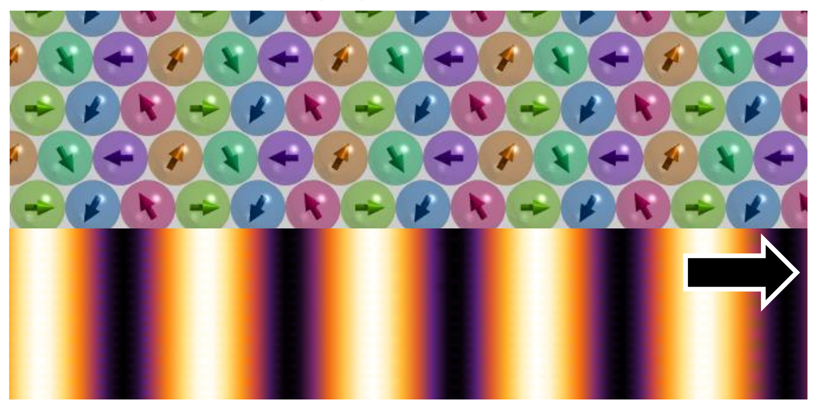


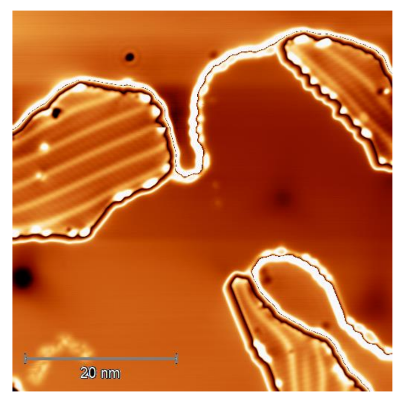
Compressed about **9 %** along $[1\bar{1}0]$
🔵: Hollow site → dark
🟡: Top site → bright



$T_{ss} \approx 0.85 \pm 0.10\ nm$

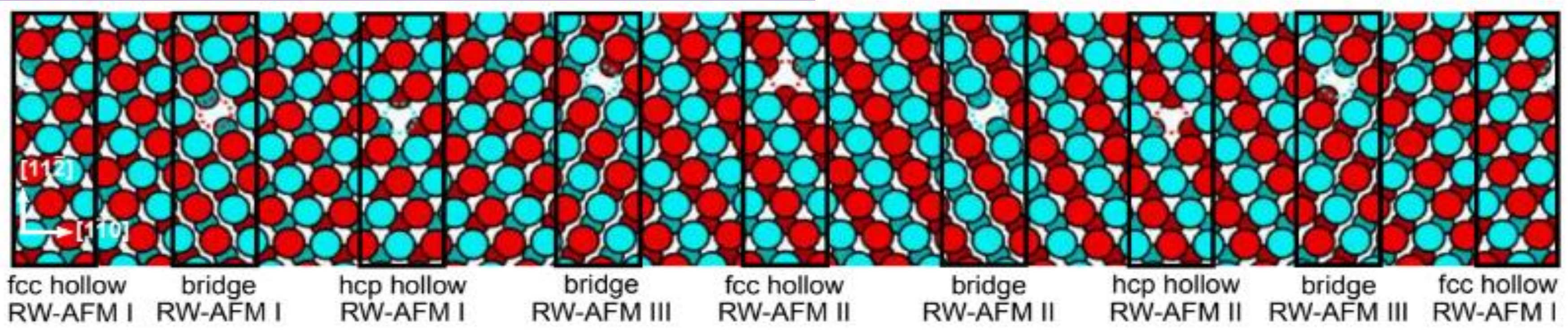






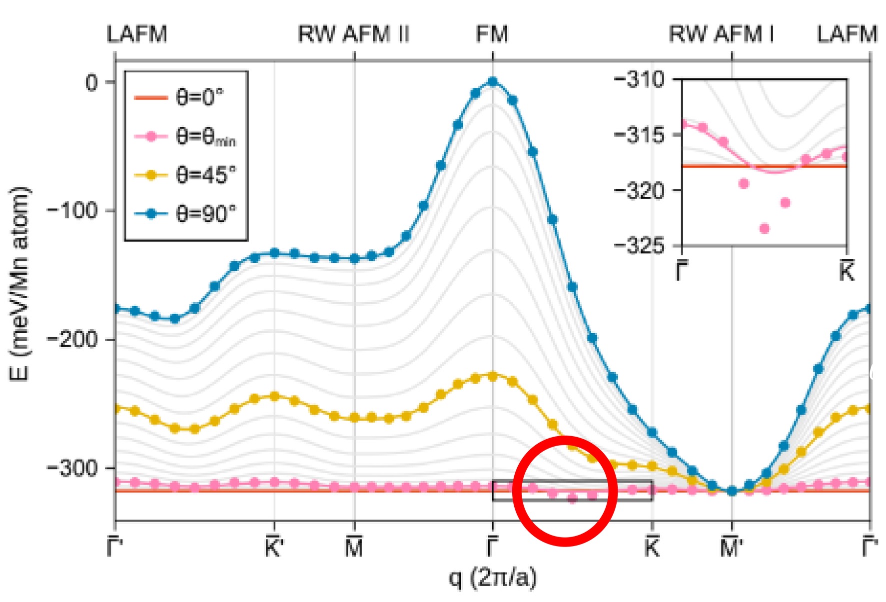
- Three rotationally symmetry domain

DFT calculation result



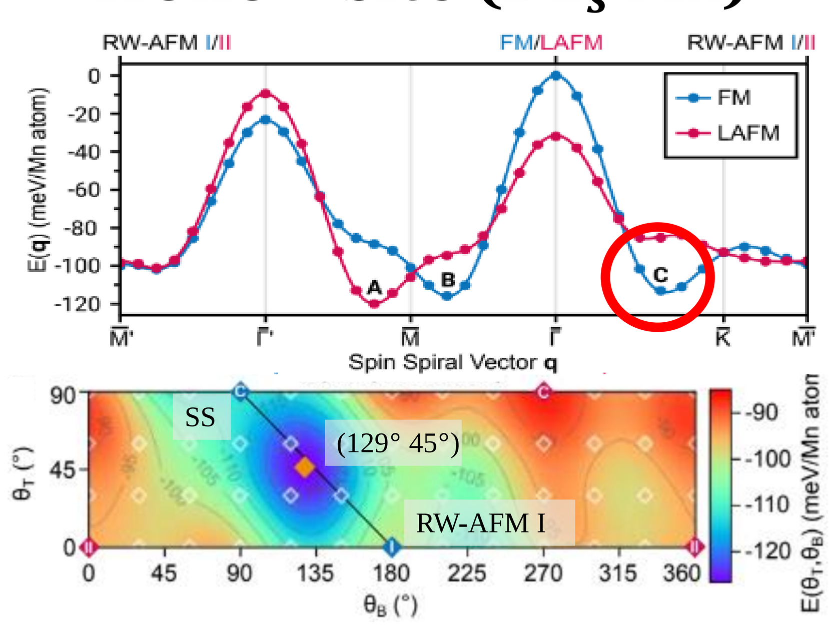
- **Bridge site (DL_R Mn)**

$\vec{S}_{super} = \cos(\theta)\,\vec{S}_{\mathrm{AFM\,I}} + \sin(\theta)\vec{S}_{SS}$



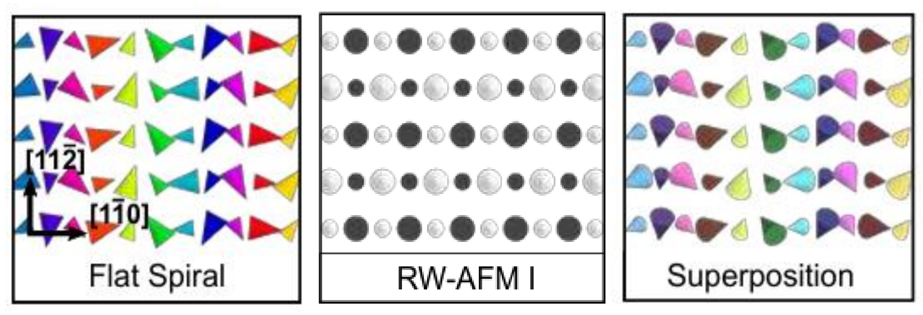
$\theta_{min} = 14°, T_{ss} = \boldsymbol{0.857\ nm}$

- **Hollow site (DL_s Mn)**



θ_T: θ for top Mn θ_B: θ for bottom Mn

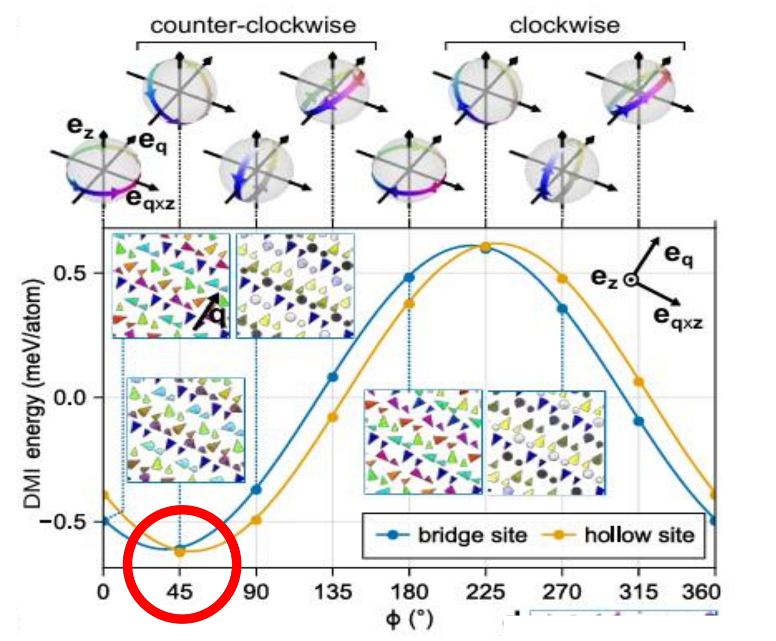
$T_{AFM} = \boldsymbol{0.495\ nm}, T_{ss} = \boldsymbol{0.686\ nm}$



$\theta = 90°$ $\theta = 0°$

∵ RW-AFM I couples to the lattice.
SS doesn't couple to the lattice.
∴**Only SS can occur in DL_R Mn**

- **Influence of SOC**



Summary

1. In DL Mn/Ag(111) system, we found two crystalline structure with different spin texture. The first one is **psudomorphic phase** with a **conical spin spiral state**, the second one is **reconstructed phase** with a **cycloidal spin spiral state**.
2. In the DFT calculations, it provide further detailed theoretical insights on how these complex magnetic orders affected by a **uniaxial strain relief**. Most importantly, the calculation result aligned well to the experimental result