FEW-LAYER VDW MULTIFERROICS · SP-STM + SPIN MODEL + SPINGNN++

Tuning Spin Spirals in Few-Layer NiI_2 by Thickness and Curvature

Thickness drives a dimensional crossover of the spin-spiral wavevector *q*, while **curvature** locally deflects *q* through magneto-elastic coupling — two complementary knobs for engineering helical magnetism.

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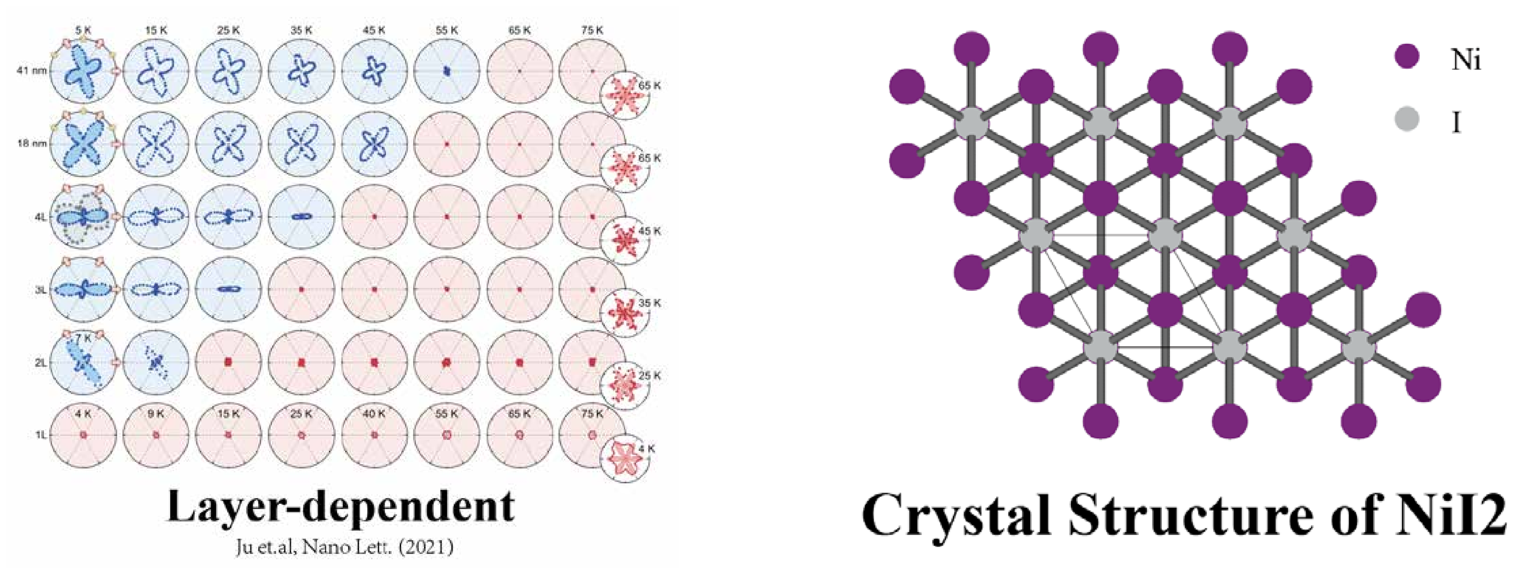
01 Thickness tunes *q* globally

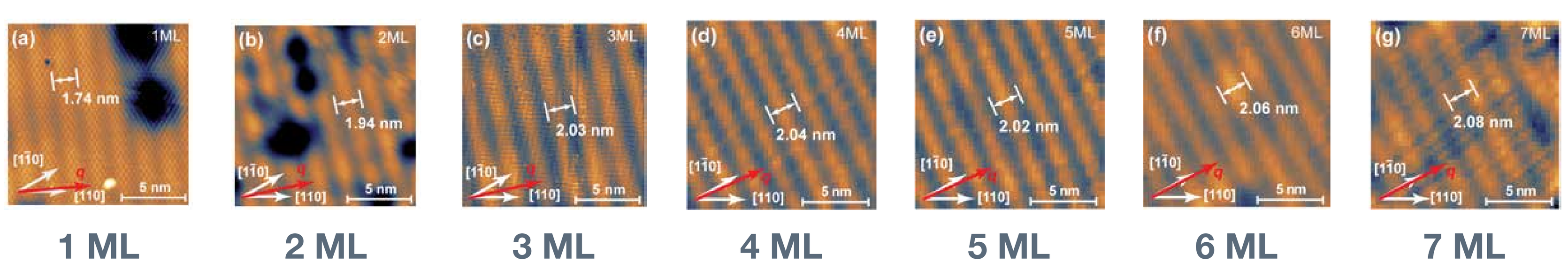
DIMENSIONAL CROSSOVER OF THE SPIN-SPIRAL WAVEVECTOR

Thickness tunes *q* globally

- **SP(Spin Polarized)-STM** resolves **spin spirals** in **1–7 ML** NiI_2.
- The **wavelength** increases from **1.7 → 2.1 nm.**
- The **wavevector angle** rotates from **7° → 26°.**



NiI_2 layered structure and the helical (spin-spiral) ground state that gives rise to ferroelectricity.



SP-STM maps from 1 to 7 monolayers show a continuous evolution of stripe periodicity and orientation.

WAVELENGTH λ	q ANGLE α
1.7 → 2.1 nm	**7° → 26°**

Interlayer exchange drives dimensional crossover

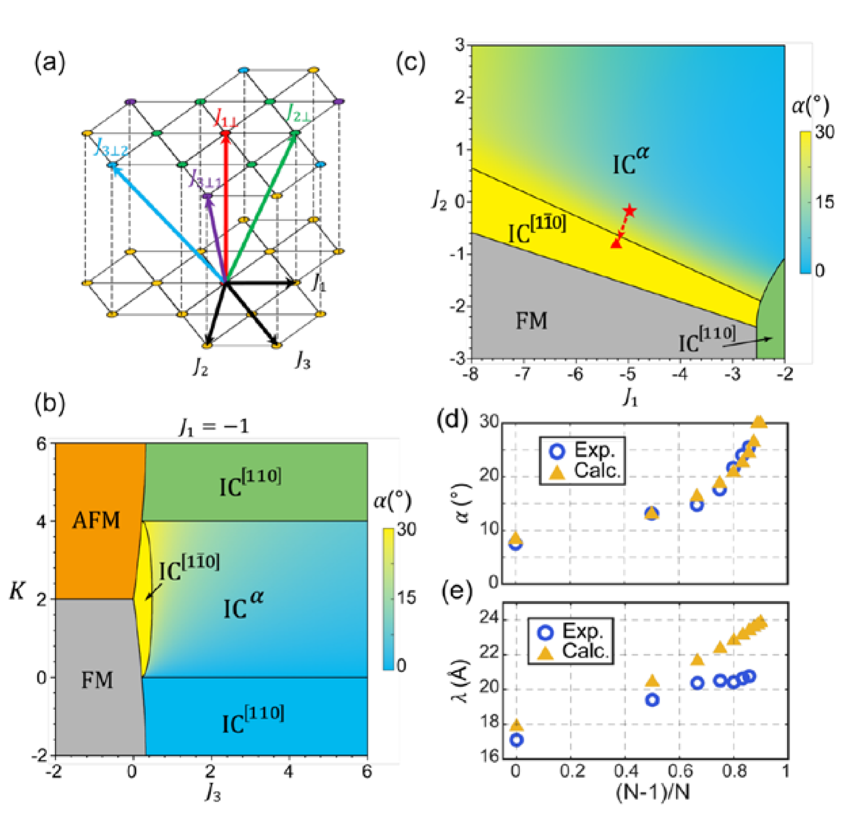
- Spin spirals arise from **frustrated J_1–J_3–K interactions.**
- Increasing thickness restores **AFM-like interlayer coupling.**
- This **renormalizes the effective exchange balance** and drives $q(N)$.

MINIMAL SPIN MODEL

$$\mathcal{H} = \mathcal{H}_{intra}(J_1, J_2, J_3, K, B) + \mathcal{H}_{inter}(J_\perp)$$

$$N \rightarrow J_\perp \rightarrow J_{eff}(N) \rightarrow q(N)$$

$$H = \sum_{n=1}^{3} J_n \sum_{\langle i,j \rangle_n} S_i \cdot S_j + K \sum_{\langle i,j \rangle_1} S_i^\gamma S_j^\gamma + B \sum_{\langle i \rangle} (S_i \cdot S_j)^2 + \sum J_\perp S_{i,l} \cdot S_{j,l+1}$$



Spin model and phase diagram reproduce the experimentally observed wavevector evolution.

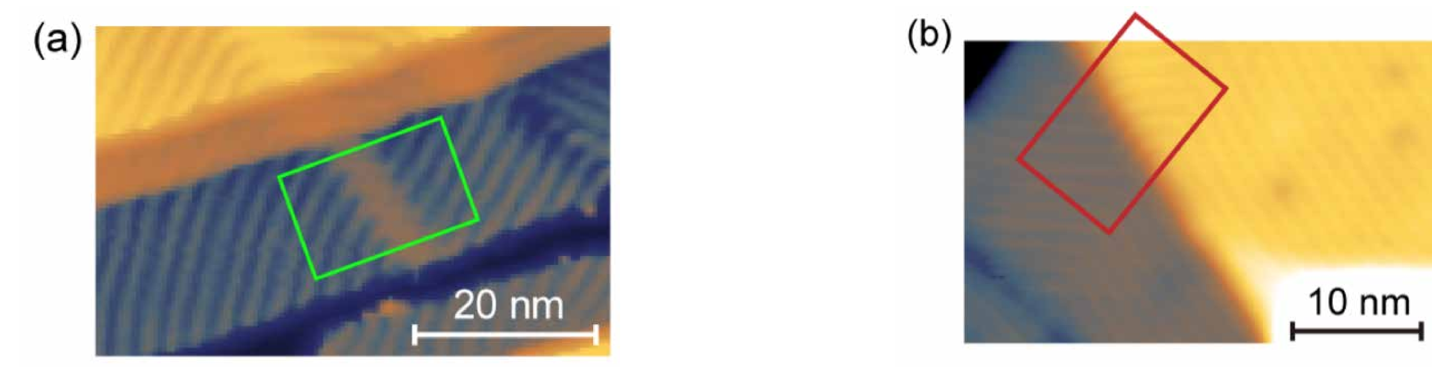
Thickness is a *global* tuning knob.

02 Curvature deflects *q* locally

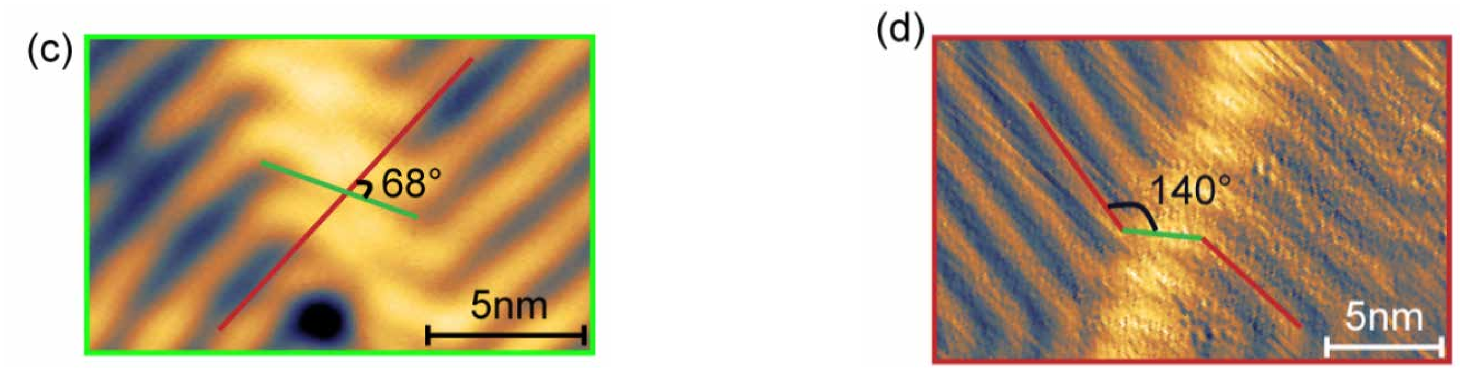
MAGNETO-ELASTIC COUPLING RESHAPES THE SPIRAL

Curvature deflects *q* locally

- **Wrinkles** and substrate steps create **local curvature** in NiI_2 films.
- Spin spirals ***bend*** when crossing curved regions.
- The deflected stripes **recover** away from the wrinkle.



Topography of NiI_2 films with wrinkles — locally curved regions act as strain templates.

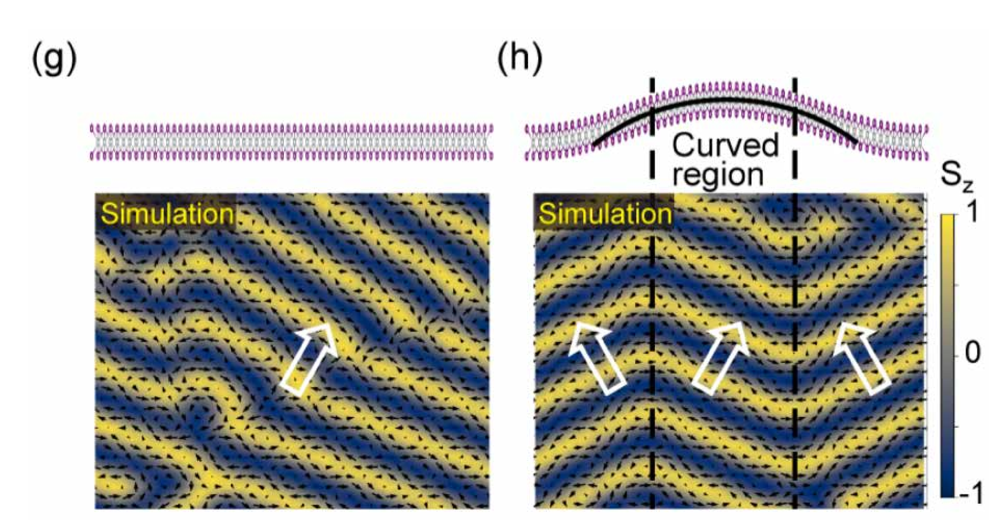


Zoom-in SP-STM images showing the spin-spiral stripes bending as they traverse the curved region.

LOCAL CURVATURE	SPIRAL RESPONSE
~10–20 μm^{-1}	***q* deflected**

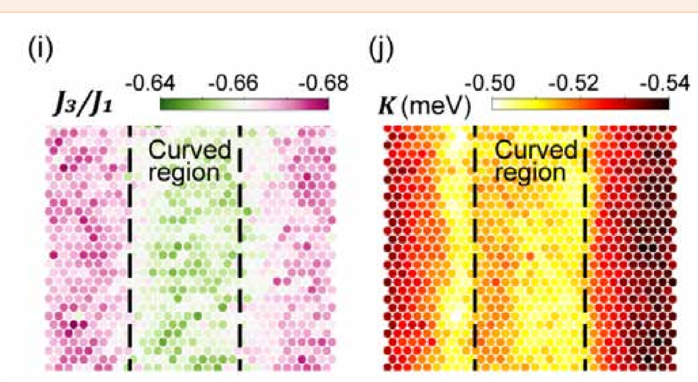
Magneto-elastic coupling modifies exchange interactions

- **Spin-lattice simulations** reproduce the observed stripe deflection.
- Curvature distorts **local bond geometry.**
- The modified ***J* and Kitaev *K*** interactions **shift the local spin-spiral wavevector.**



SpinGNN++ spin-lattice simulations: flat film (left) vs. curved film (right) reproduce the curvature-induced stripe deflection.

κ → bond geometry → J, K → q deflection



Spatial maps of exchange (*J*) and Kitaev (*K*) parameters across the curved region.

Curvature is a *local* tuning knob.

◆ Take-Home Messages

1 — Spin spirals in few-layer NiI_2 evolve **continuously** with thickness.

2 — **Interlayer exchange** drives a **dimensional crossover** of the spin-spiral wavevector *q*.

3 — Local **curvature** deflects *q* via **magneto-elastic coupling.**

Outlook — Thickness *and* **strain** *provide two practical knobs for engineering* **multiferroic spin textures** *and their accompanying electric polarization in van der Waals magnets.*