

# **harmonic measurement of NiPS3**

# outline

- why harmonic measurement
- theoretical work review
- others data
- guess for NiPS3

**Why harmonic measurement**

$$R(I) = R(0) + \frac{\partial R}{\partial I} I + \frac{1}{2} \frac{\partial^2 R}{\partial I^2} I^2$$

plug in  $I = I_0 \cos \omega t$  into  $V = IR$

$$V = IR$$

$$= R(0)I_0 \cos \omega t + \frac{\partial R}{\partial I} I_0^2 \cos^2 \omega t + \frac{1}{2} \frac{\partial^2 R}{\partial I^2} I_0^3 \cos^3 \omega t + \dots \quad V_{2\omega} = \frac{1}{2} \frac{\partial R}{\partial I} I_0^2$$

$$\approx R(0)I_0 \cos \omega t + \frac{1}{2} \frac{\partial R}{\partial I} I_0^2 \cos 2\omega t + \frac{1}{8} \frac{\partial^2 R}{\partial I^2} I_0^3 \cos 3\omega t + \dots \quad V_{3\omega} = \frac{1}{8} \frac{\partial^2 R}{\partial I^2} I_0^3$$

**theoretical review**



## Theory of spin Hall magnetoresistance

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We present a theory of the spin Hall magnetoresistance (SMR) in multilayers made from an insulating ferromagnet F, such as yttrium iron garnet (YIG), and a normal metal N with spin-orbit interactions, such as platinum (Pt). The SMR is induced by the simultaneous action of spin Hall and inverse spin Hall effects and therefore a nonequilibrium proximity phenomenon. We compute the SMR in F|N and F|N|F layered systems, treating N by spin-diffusion theory with quantum mechanical boundary conditions at the interfaces in terms of the spin-mixing conductance. Our results explain the experimentally observed spin Hall magnetoresistance in N|F bilayers. For F|N|F spin valves we predict an enhanced SMR amplitude when magnetizations are collinear. The SMR and the spin-transfer torques in these trilayers can be controlled by the magnetic configuration.

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$$\rho_{\text{long}} = \sigma_{\text{long}}^{-1} = \left( \frac{\overline{j_{c,\text{long}}}}{E_x} \right)^{-1} \approx \rho + \Delta\rho_0 + \Delta\rho_1 (1 - m_y^2), \quad (19)$$

$$\rho_{\text{trans}} = -\frac{\sigma_{\text{trans}}}{\sigma_{\text{long}}^2} \approx -\frac{\overline{j_{c,\text{trans}}/E_x}}{\sigma^2} = \Delta\rho_1 m_x m_y + \Delta\rho_2 m_z, \quad (20)$$



## Research article

## Theory of harmonic Hall responses of spin-torque driven antiferromagnets

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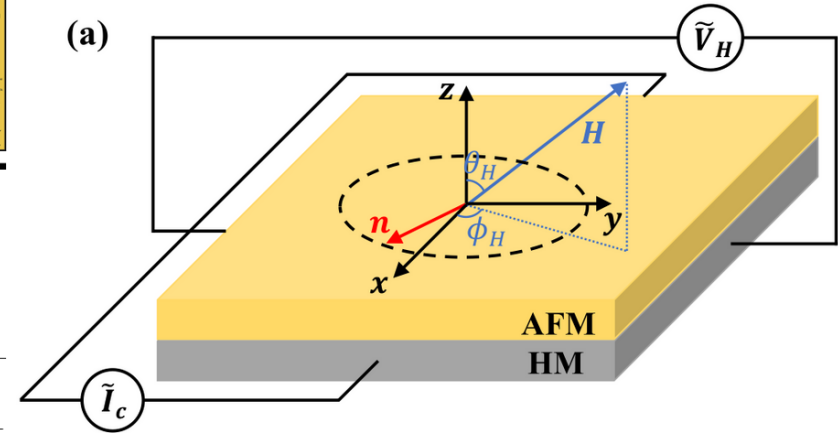
## ARTICLE INFO

## Keywords:

Spin-orbit torque  
Antiferromagnetic spintronics  
Harmonic Hall analysis

## ABSTRACT

Harmonic analysis is a powerful tool to characterize and quantify current-induced torques acting on magnetic materials, but so far it remains an open question in studying antiferromagnets. Here we formulate a general theory of harmonic Hall responses of collinear antiferromagnets driven by current-induced torques including both field-like and damping-like components. By scanning a magnetic field of variable strength in three orthogonal planes, we are able to distinguish the contributions from field-like torque, damping-like torque, and concomitant thermal effects by analyzing the second harmonic signals in the Hall voltage. The analytical expressions of the first and second harmonics as functions of the magnetic field direction and strength are confirmed by numerical simulations with good agreement. We demonstrate our predictions in two prototype antiferromagnets,  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and NiO, providing direct and general guidance to current and future experiments.



$$R_H = R_0 n_x n_y$$

$$n_x = \sin \phi_H + \Delta \phi \cos \phi_H,$$

$$n_y = -\cos \phi_H + \Delta \phi \sin \phi_H$$

$$n_z = -\Delta \theta_H,$$



$$V_{1\omega} = -\frac{1}{2} I_0 R_0 \sin(2\phi_H),$$


$$V_{2\omega} = -\frac{1}{2} I_0 R_0 \left[ \frac{H_F \cos(2\phi_H) \cos \phi_H}{H \sin \theta_H} - \frac{H_D H_E H \cos \theta_H \cos(2\phi_H) \sin \phi_H}{(D^2 + 2H_E H_\perp) H \sin \theta_H + D(H^2 + 4H_E H_\perp + D^2)/2} \right]$$

$$\frac{E}{\hbar\gamma} = H_E \mathbf{S}_1 \cdot \mathbf{S}_2 + H_{\perp} \sum_{i=1}^2 (\mathbf{S}_i \cdot \hat{\mathbf{z}})^2 - H_{\parallel} \sum_{i=1}^2 (\mathbf{S}_i \cdot \hat{\mathbf{x}})^2 \\ - D\hat{\mathbf{z}} \cdot (\mathbf{S}_1 \times \mathbf{S}_2) - \mathbf{H}_t \cdot (\mathbf{S}_1 + \mathbf{S}_2),$$

The AFM dynamics can be described by the Landau–Lifshitz–Gilbert–Slonczewski (LLGS) equation

$$\frac{d\mathbf{S}_i}{\gamma dt} = \mathbf{H}_{\text{eff},i} \times \mathbf{S}_i + (\mathbf{H}_D \times \mathbf{S}_i) \times \mathbf{S}_i, \quad \mathbf{H}_{\text{eff},i} = -(1/\hbar\gamma)\delta E/\delta \mathbf{S}_i$$

$$\mathbf{n} \times \left\{ \frac{1}{2H_E} \left[ -\frac{\partial^2 \mathbf{n}}{\partial t^2} - \frac{\partial \mathbf{n}}{\partial t} \times \mathbf{H}_t + \frac{\partial}{\partial t} (\mathbf{H}_t \times \mathbf{n}) \right. \right. \\ \left. \left. - D\hat{\mathbf{z}}(D\hat{\mathbf{z}} \cdot \mathbf{n}) - D\hat{\mathbf{z}} \times \mathbf{H}_t - (\mathbf{n} \cdot \mathbf{H}_t)\mathbf{H}_t \right] \right. \\ \left. - 2H_{\perp}(\mathbf{n} \cdot \hat{\mathbf{z}})\hat{\mathbf{z}} + 2H_{\parallel}(\mathbf{n} \cdot \hat{\mathbf{x}})\hat{\mathbf{x}} \right\} = \mathbf{n} \times (\mathbf{n} \times \mathbf{H}_D).$$

 **E.O.M of Neel vector**



# Magnetic anisotropy and exchange interactions of two-dimensional FePS<sub>3</sub>, NiPS<sub>3</sub> and MnPS<sub>3</sub> from first principles calculations

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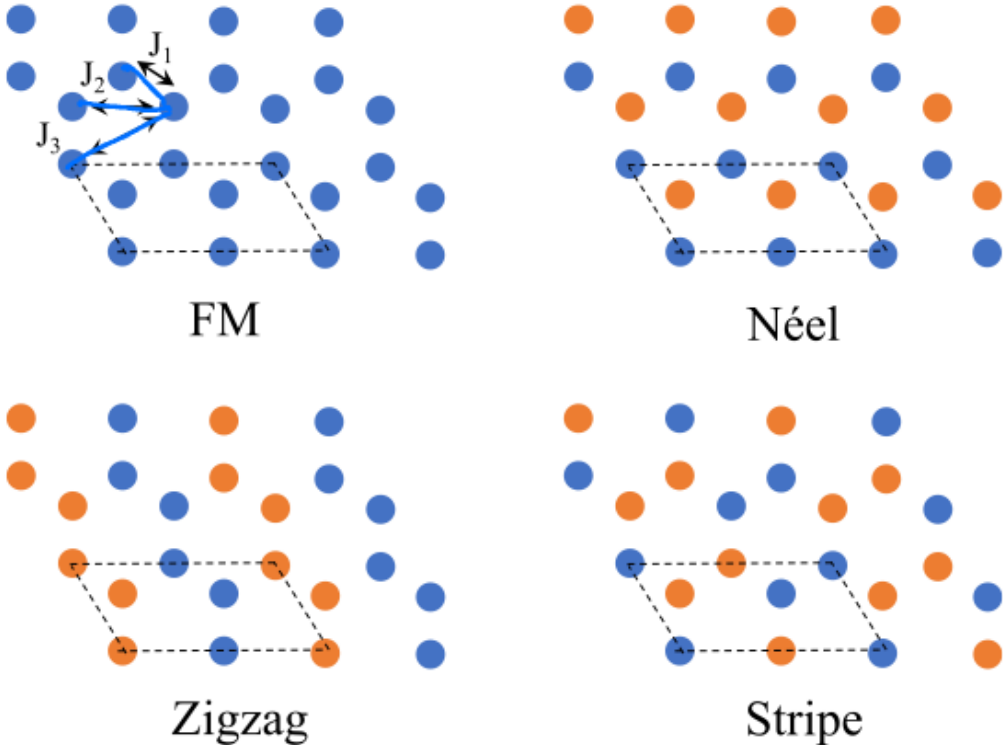
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**Abstract**  
The van der Waals bonded transition metal phosphorous trichalcogenides FePS<sub>3</sub>, NiPS<sub>3</sub> and MnPS<sub>3</sub> have recently attracted renewed attention due to the possibility of exfoliating them into their monolayers. Although the three compounds have similar electronic structure, the magnetic structure differs due to subtle differences in exchange and magnetic anisotropy and the materials thus comprise a unique playground for studying different aspects of magnetism in 2D. Here we calculate the exchange and anisotropy parameters of the three materials from first principles paying special attention to the choice of Hubbard parameter *U*. We find a strong dependence of the choice of *U* and show that the calculated Néel temperature of FePS<sub>3</sub> varies by an order of magnitude over commonly applied values of *U* for the Fe *d*-orbitals. The results are compared with parameters fitted to experimental spin-wave spectra of the bulk materials and we find excellent agreement between the exchange constants when a proper value of *U* is chosen. However, the anisotropy parameters are severely underestimated by density functional theory and we discuss possible origins of this discrepancy.

**Keywords:** magnetism, anti-ferromagnetism, 2D materials, first principles, density functional theory, magnetic order in 2D

(Some figures may appear in colour only in the online journal)



Material	$J_1$	$J_2$	$J_3$	$\lambda_1$	$\lambda_3$	$\lambda_3$	A
FePS <sub>3</sub> ( $U = 2$ eV)	2.1	−0.21	−2.6	$−4.1 \times 10^{-3}$	$1.1 \times 10^{-3}$	$2.5 \times 10^{-3}$	0.101
FePS <sub>3</sub> (experimental) [15]	2.92	−0.08	−1.92	—	—	—	2.66
NiPS <sub>3</sub> ( $U = 3$ eV)	2.6	0.32	−14	$−0.32 \times 10^{-3}$	$−0.51 \times 10^{-3}$	$−0.25 \times 10^{-3}$	−0.018
NiPS <sub>3</sub> (experimental) [16]	3.8	−0.2	−13.8	—	—	—	0.3
MnPS <sub>3</sub> ( $U = 3$ eV)	−1.42	−0.081	−0.52	$−1.2 \times 10^{-3}$	$−0.19 \times 10^{-3}$	$0.37 \times 10^{-3}$	−0.0035
MnPS <sub>3</sub> (experimental) [13]	−1.54	−0.14	−0.36	—	—	—	0.0086

**others data**

**key word:**

**antiferromagnetic, second harmonic, Hall effect**

# Quantifying Spin-Orbit Torques in Antiferromagnet–Heavy-Metal Heterostructures

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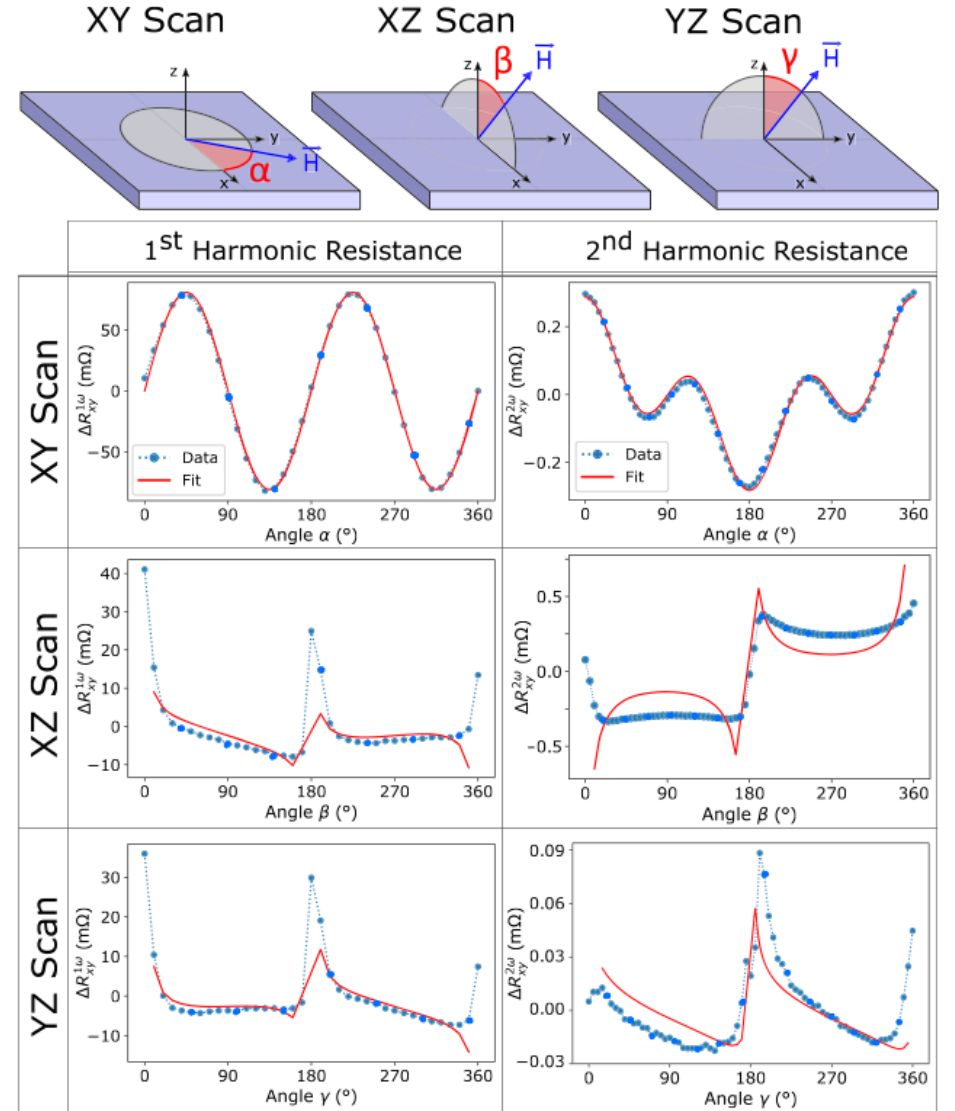
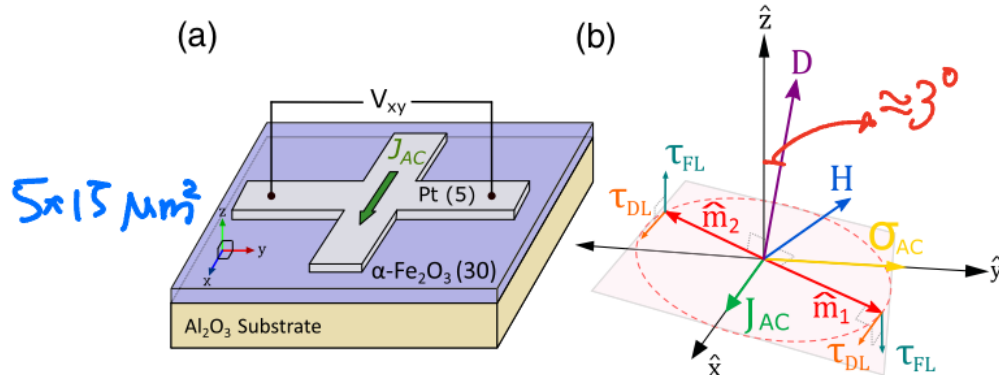
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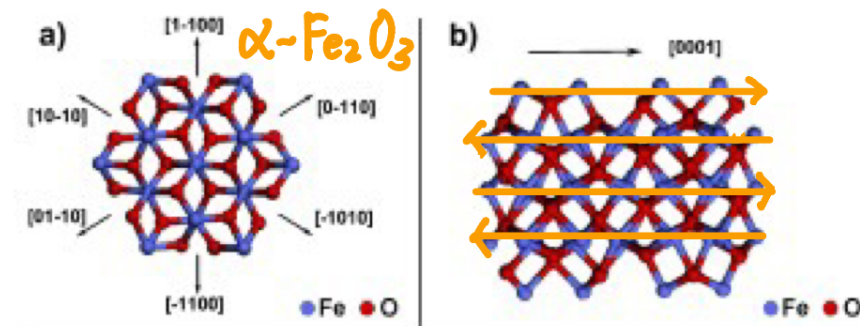
The effect of spin currents on the magnetic order of insulating antiferromagnets (AFMs) is of fundamental interest and can enable new applications. Toward this goal, characterizing the spin-orbit torques (SOTs) associated with AFM–heavy-metal (HM) interfaces is important. Here we report the full angular dependence of the harmonic Hall voltages in a predominantly easy-plane AFM, epitaxial  $c$ -axis oriented  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> films, with an interface to Pt. By modeling the harmonic Hall signals together with the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> magnetic parameters, we determine the amplitudes of fieldlike and dampinglike SOTs. Out-of-plane field scans are shown to be essential to determining the dampinglike component of the torques. In contrast to ferromagnetic–heavy-metal heterostructures, our results demonstrate that the fieldlike torques are significantly larger than the dampinglike torques, which we correlate with the presence of a large imaginary component of the interface spin-mixing conductance. Our work demonstrates a direct way of characterizing SOTs in AFM–HM heterostructures.

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We fit the experimental results with three free parameters: the direction of the hard axis ( $e_h$ ) and the amplitudes of the spin-orbit torques ( $H_{\text{FL}}$  and  $H_{\text{DL}}$ ). For every scan, first we fit the first harmonic response, where we extract the current-independent constant  $R_0$  [Eq. (4)]. Then together with the  $R_0$ , we use material parameters from the literature  $H_D = 2$  T,  $H_K = 0.01$  T, and  $H_{\text{ex}} = 900$  T [36–38], to fit the responses with our model. These fits allow us to extract the amplitudes of effective fields associated with the spin-orbit torques per current density which are  $H_{\text{FL}}/J_{\text{ac}} \approx 7.5 \times 10^{-2}$  T/( $10^{12}$  A/m<sup>2</sup>) and  $H_{\text{DL}}/J_{\text{ac}} \approx 4.2 \times 10^{-4}$  T/( $10^{12}$  A/m<sup>2</sup>).

A slight tilting ( $\sim 3^\circ$ ) of the hard-axis  $e_h$  f








# Enhanced second harmonic Hall resistance in in-plane synthetic antiferromagnets

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## AFFILIATIONS

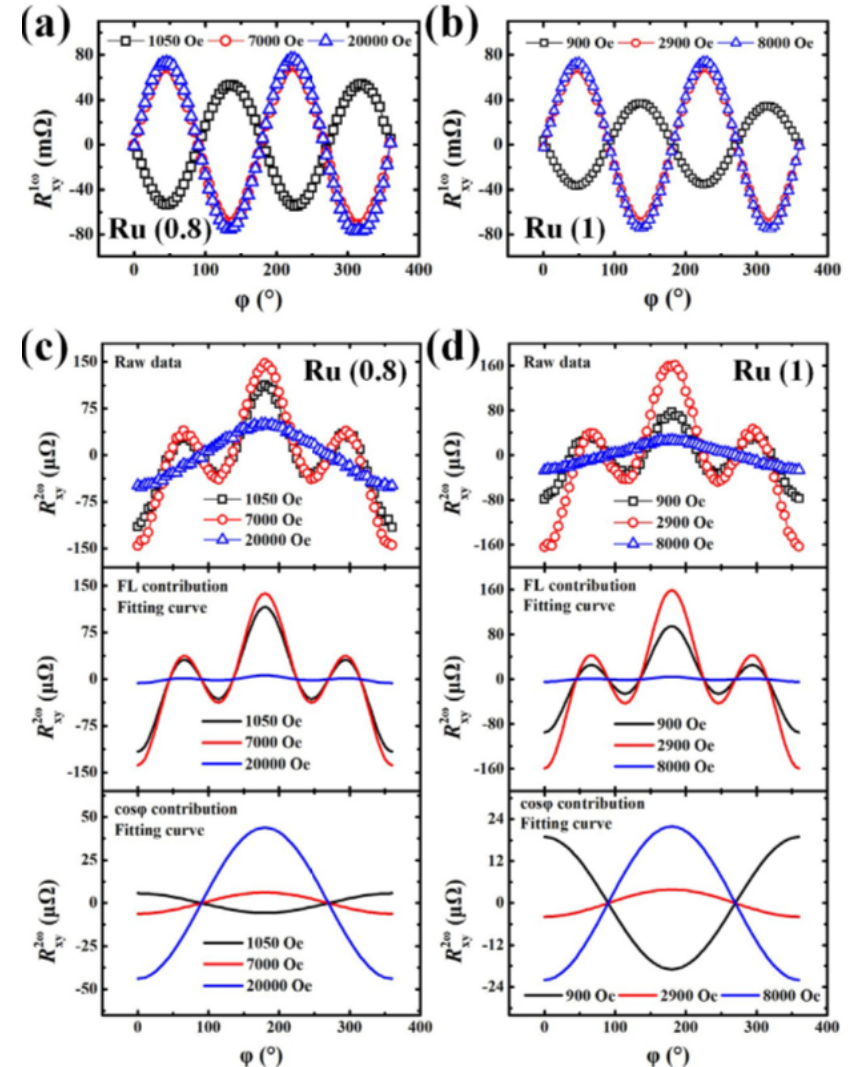
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## ABSTRACT

Synthetic antiferromagnet (SyAF) has been demonstrated to be an ideal candidate for spin-orbit torque (SOT) based spintronic devices. However, the detailed mechanism needs to be clarified due to the coexistence of multiple effects. This paper studies SOT and the thermoelectric effect in SyAF of Pt/Co/Ru/Co/Pt by harmonic Hall resistance measurements. Different from the traditional Co/Pt bilayers, the second harmonic Hall resistance signals of the SyAF-based devices are obviously enhanced under a large external magnetic field ( $B_{\text{ext}}$ ), which is caused by the antiferromagnetic exchange coupling fields weakening the influence of  $B_{\text{ext}}$ . By fitting the Hall resistance curves, the field-like torque is demonstrated to be the main contribution to the Hall resistance. Interestingly, both the SOT effective fields are greatly enhanced for antiparallel alignment. This study separates the contributions of SOT and the thermoelectric effect in the SyAF structures and enables the design of the spintronic devices with stability under a large magnetic field.

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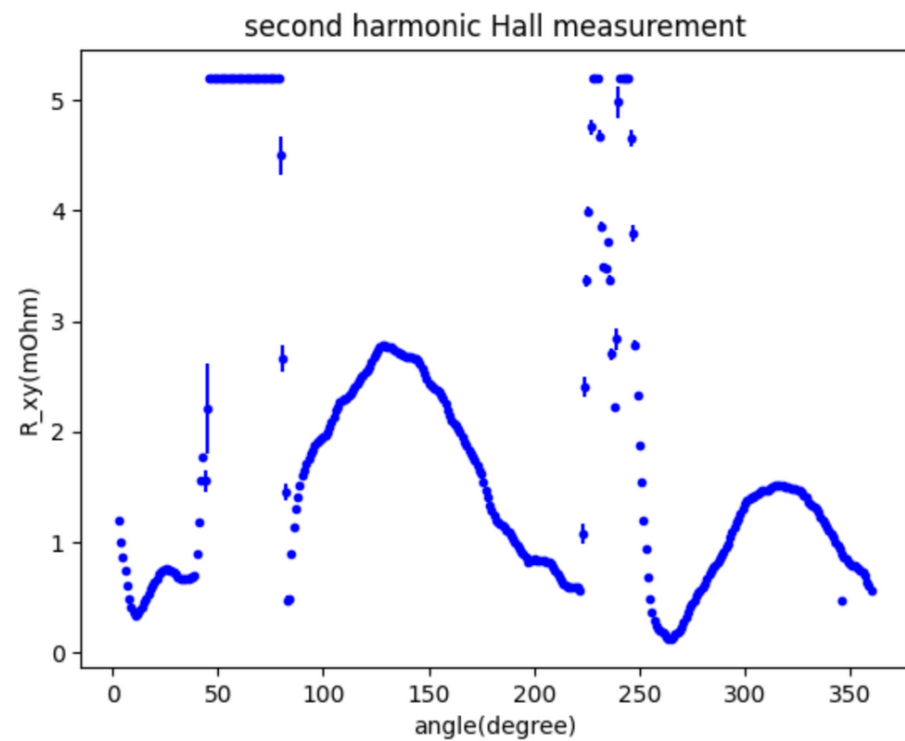
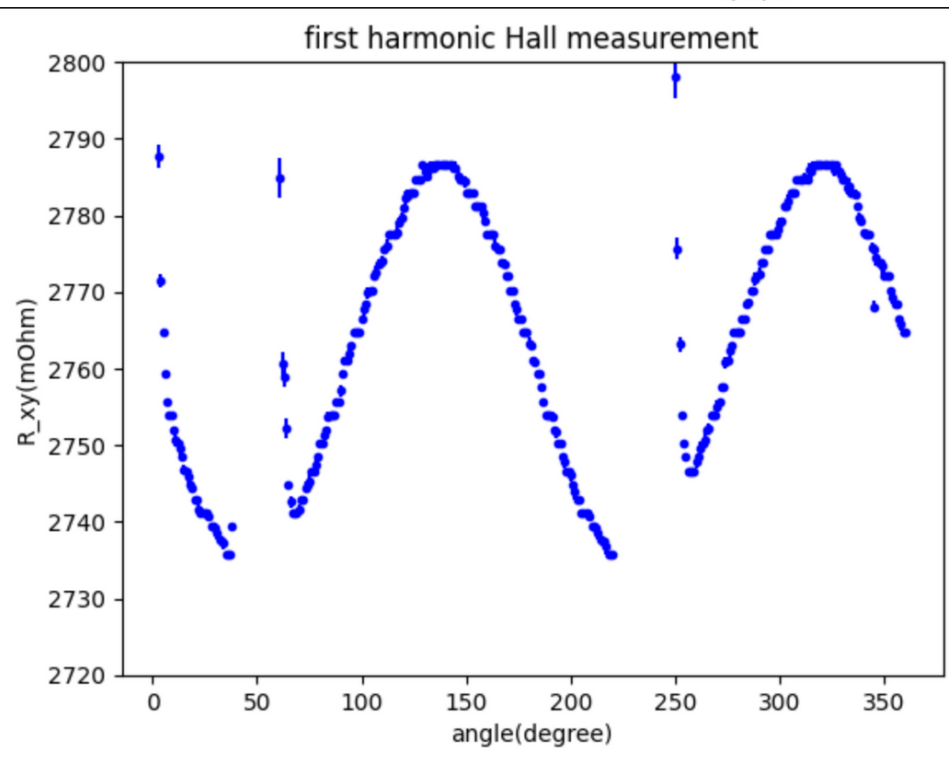
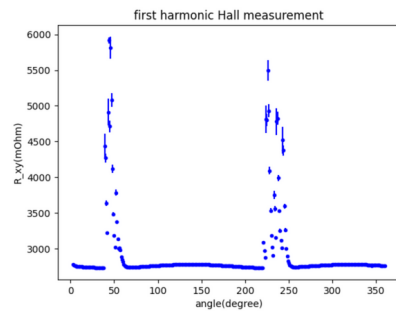
**guess for NiPS3**

$$I_0 = 2.97mA$$

$$f = 953Hz$$

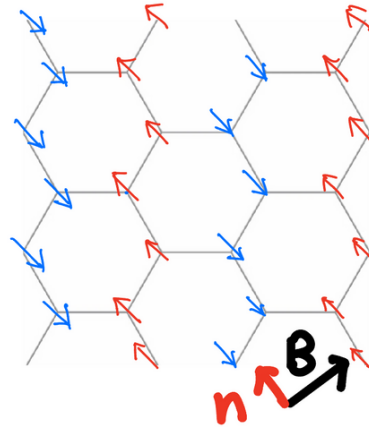
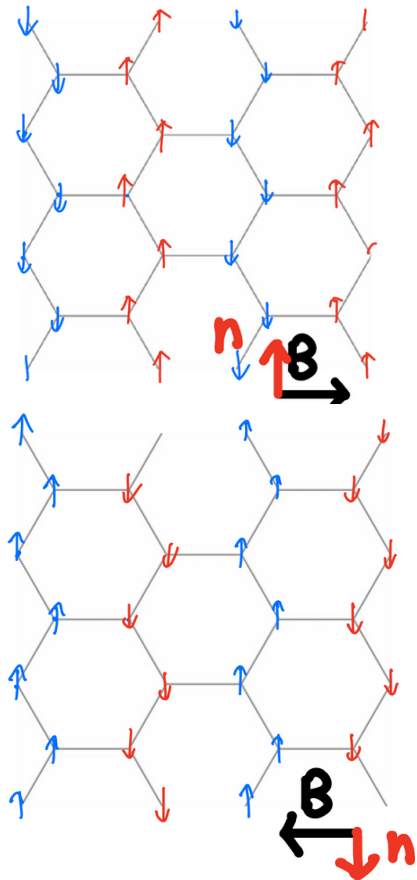
$$H = 5T$$

$$t_{Pt} = 10nm$$





# 1st harmonic shows Neel vector can point at any direction



$S_i^2$   
 $J_1$  2  $\uparrow\uparrow$  1  $\uparrow\downarrow$   
 $J_2$  2  $\uparrow\uparrow$  4  $\uparrow\downarrow$   
 $J_3$  3  $\uparrow\downarrow$

$S_1$   $S_2$   $S_1$

Interaction  
 $J_1: \frac{3N}{2}$   
 $J_2: \frac{N}{2} \cdot 6 = 3N$   
 $J_3: \frac{N}{2} \cdot 3 = \frac{3N}{2}$

average over  $\frac{N}{2}$   
 $\Rightarrow 3J_1 + 6J_2 + 3J_3$

$\Rightarrow \underbrace{(J_1 + 4J_2 + 3J_3)}_{H_E} S_1 \cdot S_2 + \cancel{(2J_1 + 2J_2) S_i^2}$

hexagon #  
 $6J_2$   
 $3J_3$