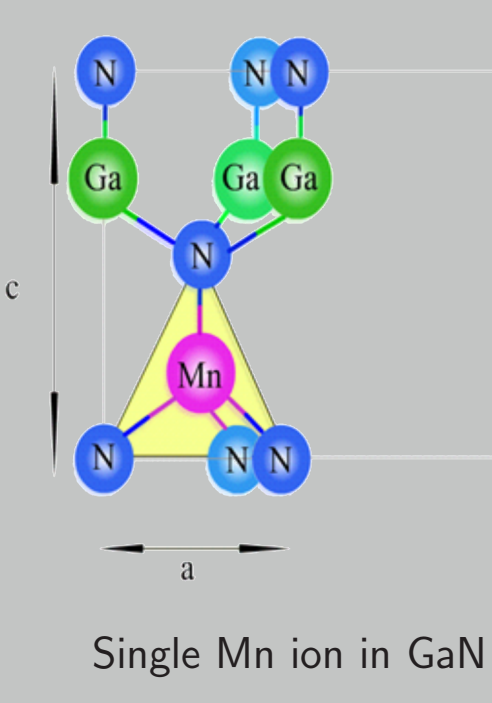


Motivation



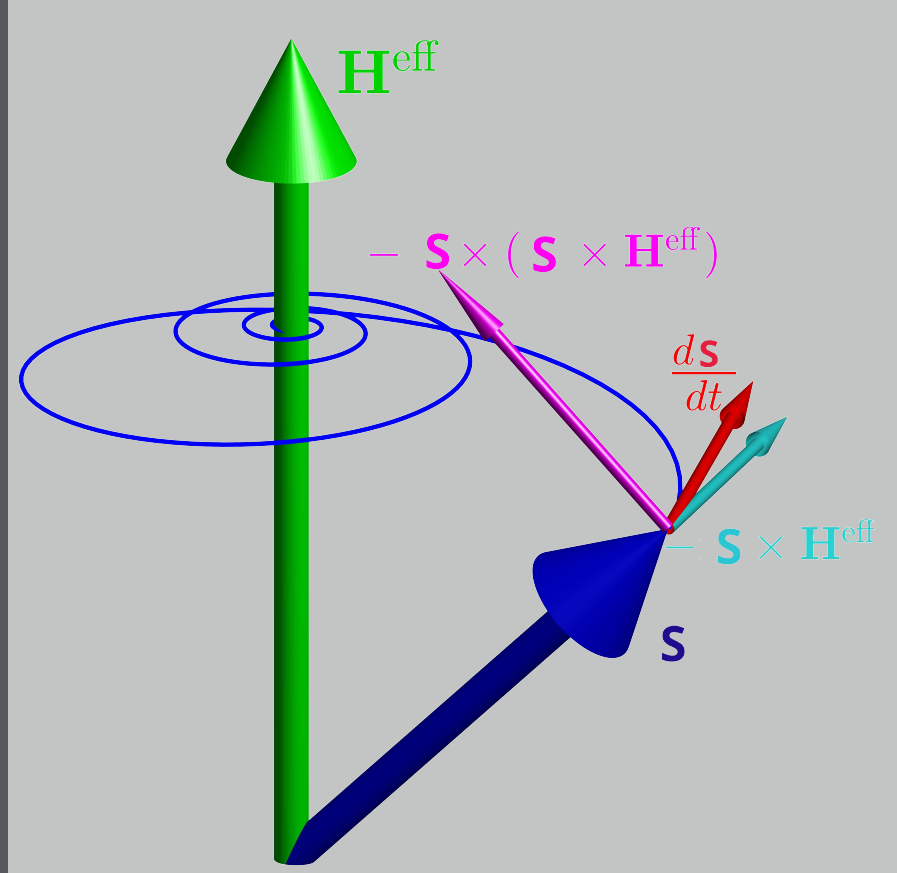
Here we investigate both experimentally and theoretically the magnetic properties of GaN doped with Mn. The MBE grown ferromagnetic $\text{Ga}_{1-x}\text{Mn}_x\text{N}$ layers, with $x = 6\%$, are studied by a superconducting quantum interference device (SQUID) and ferromagnetic resonance (FMR). The experimental data is analysed using a newly developed atomistic spin model on few thousand Mn ion coupled by superexchange. The magnetic moment M and the microwave power absorbed during a ferromagnetic resonance[1] is calculated after the system has reached a steady state. Preliminary numerical results on small systems verifies the correctness of the applied model. This is the first ever simulation effort aimed at calculation of both magnetization and FMR in dilute magnetic semiconductor using atomistic approach.

Numerical Model

The magnetic moment of i^{th} Mn^{3+} ion is \mathbf{S}_i . The classical Heisenberg Hamiltonian[2] is

$$\mathcal{H} = \underbrace{-J_{ij} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j}_{\text{Exchange}} - \underbrace{\frac{1}{4} K^{TR} \sum_i [S_{iz}^2 - (S_{ix}^2 + S_{iy}^2)]}_{\text{Trigonal}} - \underbrace{\frac{1}{2} K^{JT} \sum_i \sum_{j=A,B,C} (\mathbf{S}_i \cdot \mathbf{e}_j)^4}_{\text{Jahn-Teller}} - \underbrace{\sum_i \mathbf{S}_i \cdot \mathbf{H}^{ze}}_{\text{Zeeman}}$$

The stochastic Landau-Lifshitz-Gilbert (sLLG) equation



$$\frac{\partial \mathbf{S}_i}{\partial t} = -\frac{\gamma}{(1 + \alpha^2)} \mathbf{S}_i \times (\mathbf{H}_i^{\text{eff}} + \alpha \mathbf{S}_i \times \mathbf{H}_i^{\text{eff}})$$

$$P_{\text{FMR}} = -\frac{M}{N t_0} \sum_i \int_t^{t+t_0} \mathbf{S}_i(t) \cdot \frac{\partial \mathbf{H}^{\text{ac}}(t)}{\partial t} dt$$

- ▶ $\mathbf{H}_i^{\text{eff}} = -\frac{1}{M} (\partial \mathcal{H} / \partial \mathbf{S}_i) + \mathbf{H}^{\text{ac}} + \boldsymbol{\xi}_i(t) \sqrt{\frac{2\alpha k_B T}{\gamma M \delta t}}$
- ▶ $\boldsymbol{\xi}(t)$ is Gaussian distribution in 3D with mean 0.

Funkmich008, CC BY-SA 4.0 via Wikimedia

Analytical Model

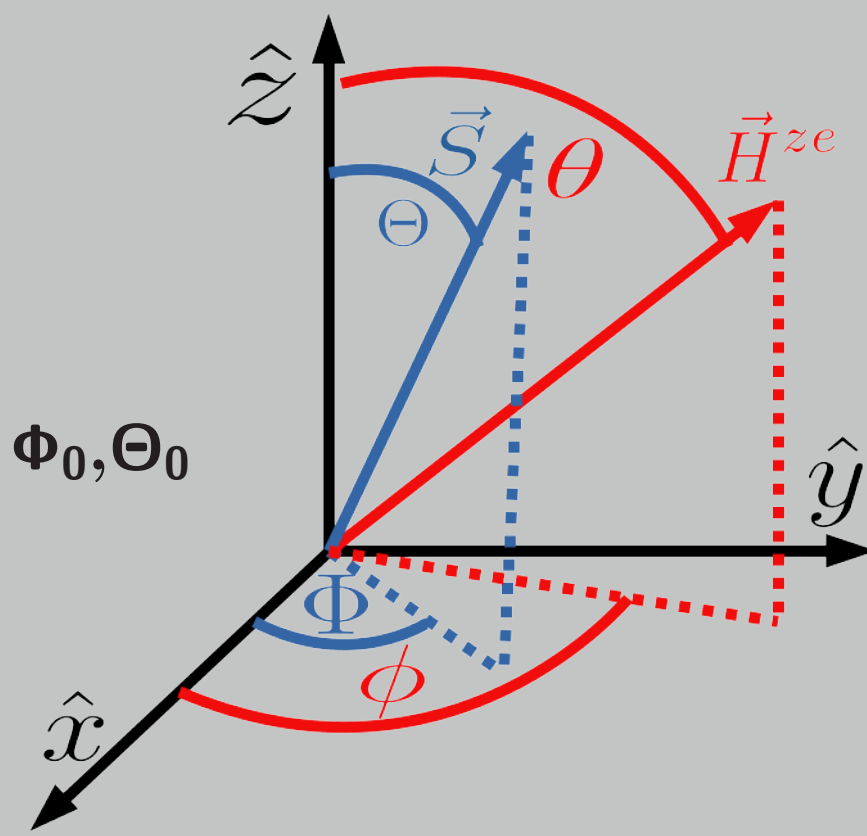
In spherical polar coordinate

$$\mathcal{H} = -M H^{ze} \{ \sin \Theta \sin \theta \cos(\Phi - \phi) + \cos \Theta \cos \theta \} - \frac{K^{TR}}{2} \cos 2\Theta - \frac{K^{JT}}{2} \sum_{j=A,B,C} (e_j^x \sin \Theta \cos \Phi + e_j^y \sin \Theta \sin \Phi + e_j^z \cos \Theta)^4$$

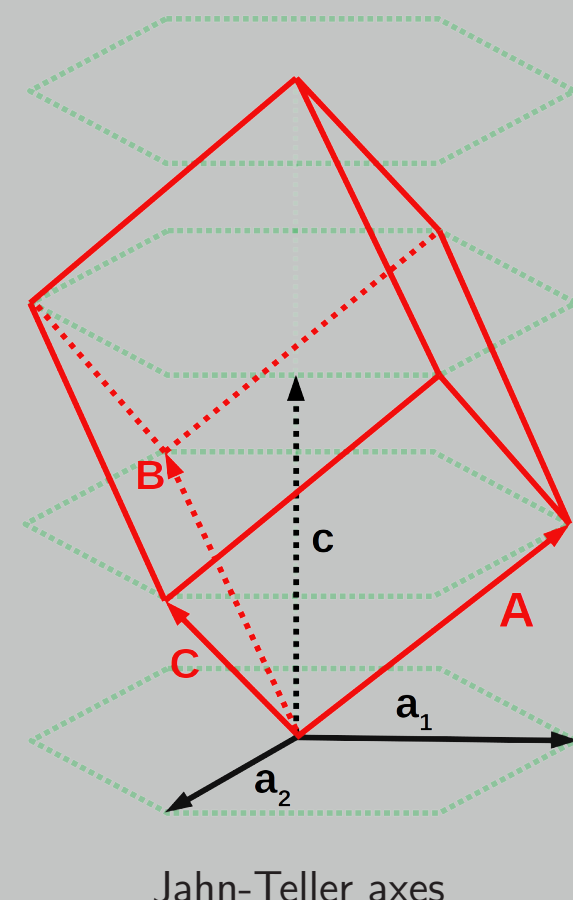
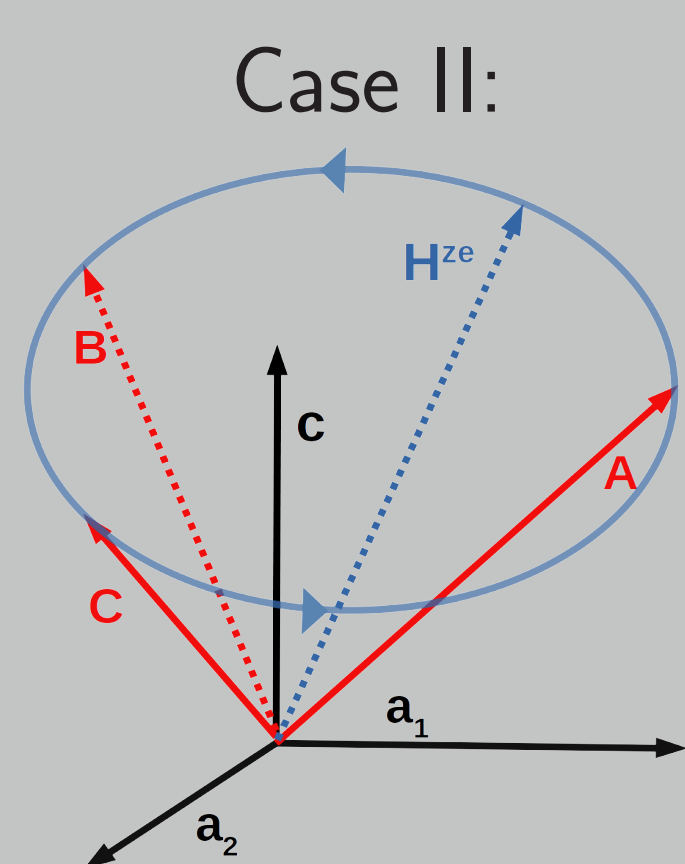
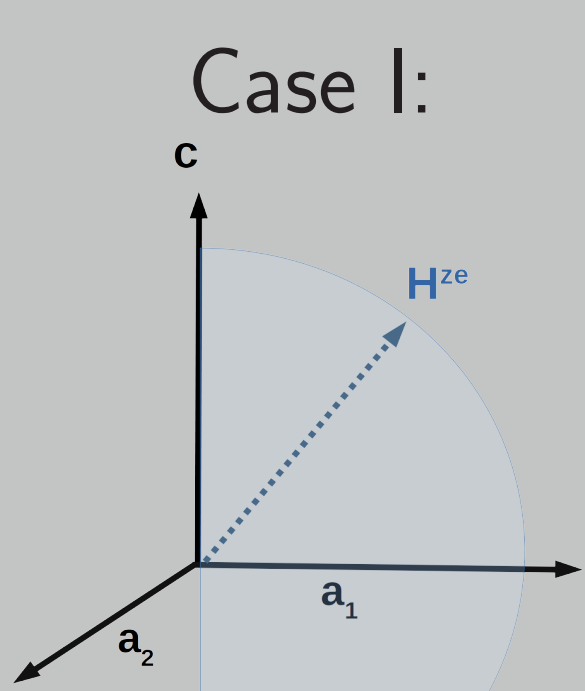
$$\omega = \frac{\gamma}{M \sin \Theta} \left[\sqrt{\left(\frac{\partial^2 \mathcal{H}}{\partial \Phi^2} \right) \left(\frac{\partial^2 \mathcal{H}}{\partial \Theta^2} \right) - \left(\frac{\partial^2 \mathcal{H}}{\partial \Phi \partial \Theta} \right)^2} \right]_{\Phi_0, \Theta_0}$$

The saturation magnetization

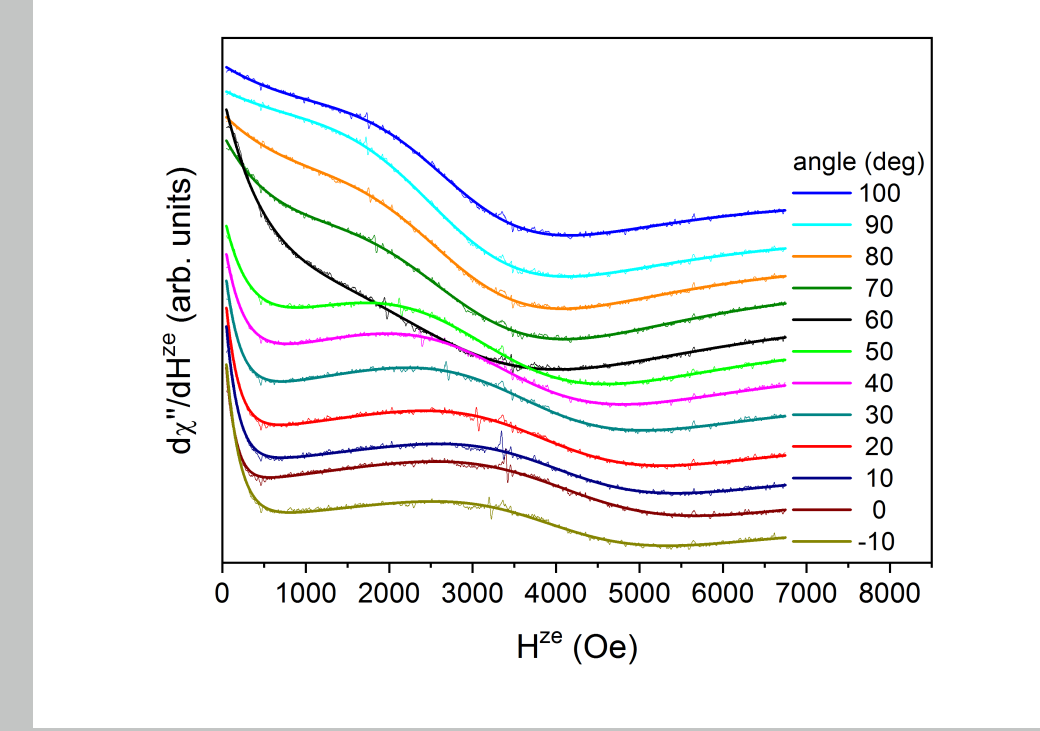
$$\frac{\partial \mathcal{H}}{\partial \Phi} \Big|_{\Phi=\Phi_0} = \frac{\partial \mathcal{H}}{\partial \Theta} \Big|_{\Theta=\Theta_0}$$



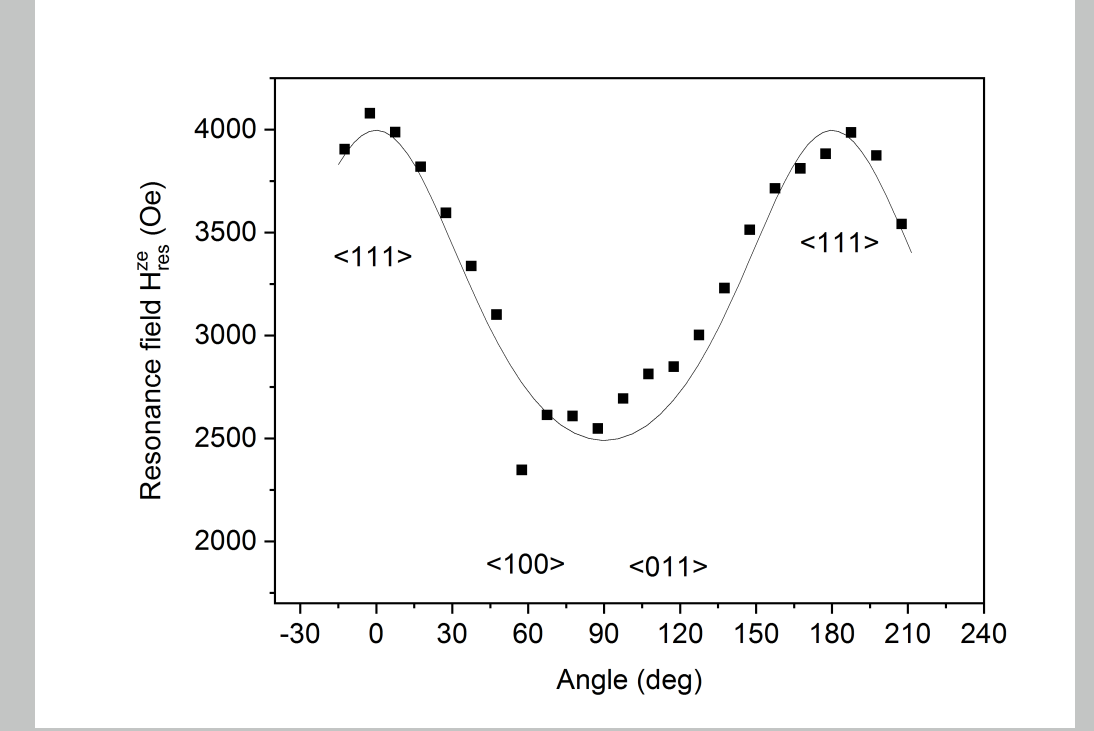
Conditions



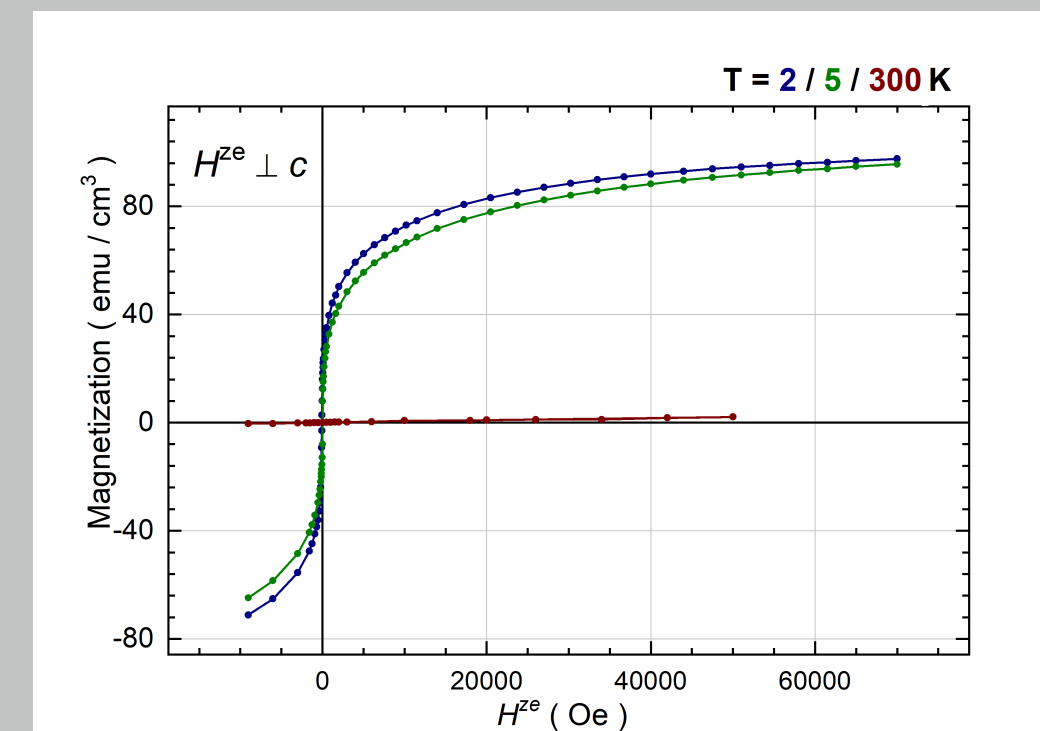
Experimental Results



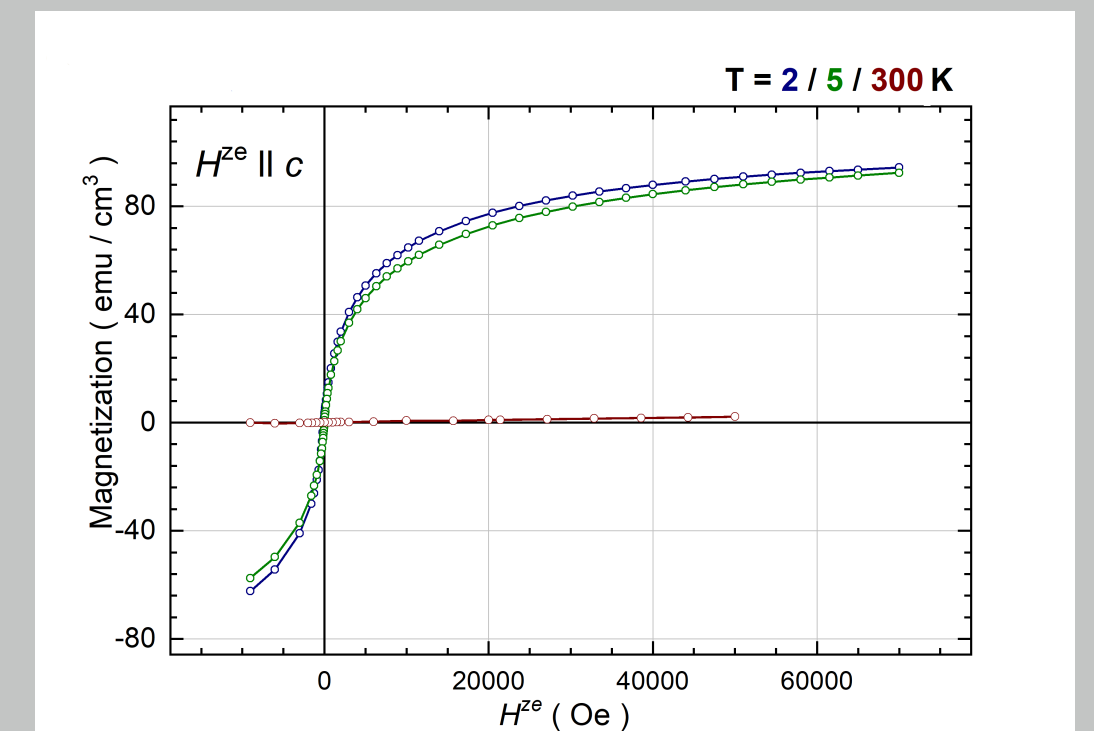
FMR data obtained from experiments



Resonance field with angle to the (Ga,Mn)N c-axis



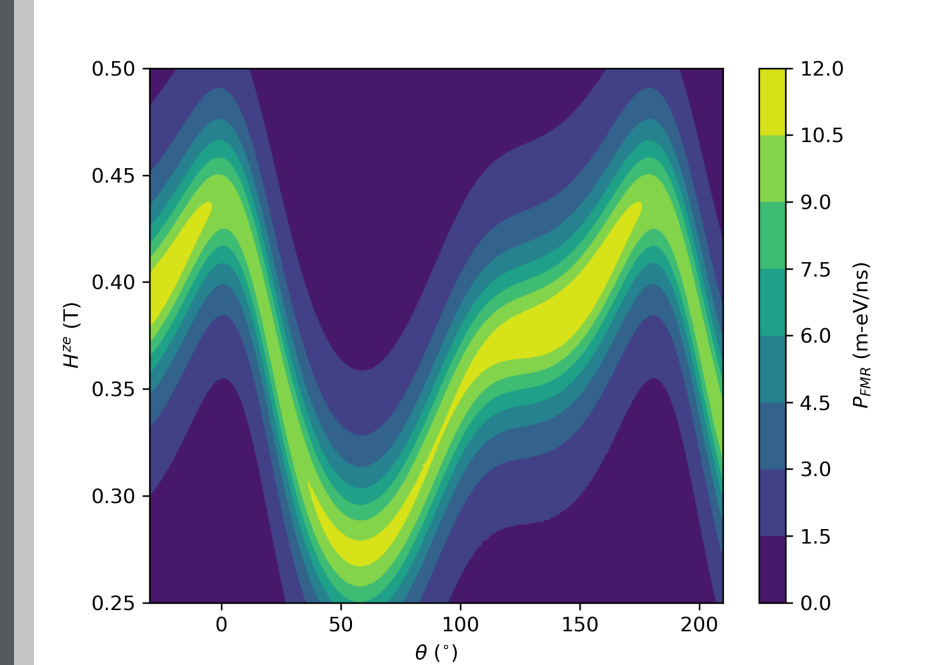
Magnetization along easy axis



Magnetization along hard axis

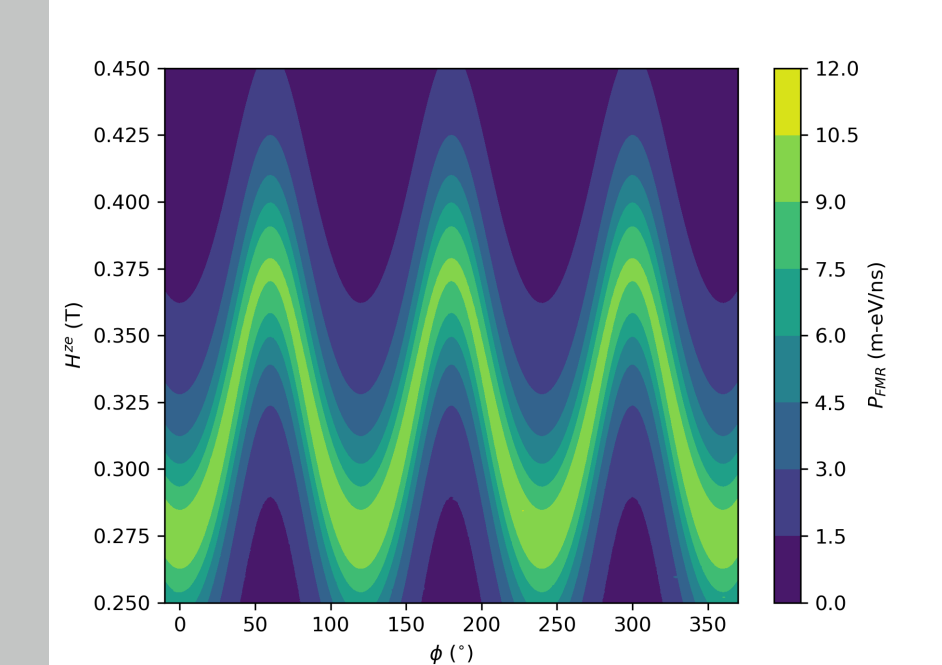
Mono Spin Model Results

Case I



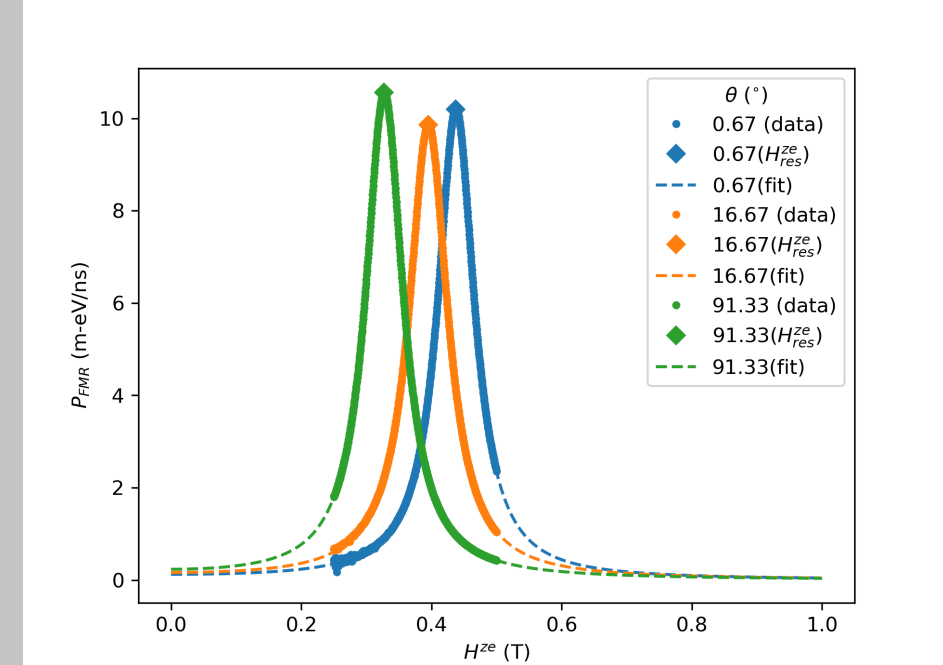
FMR Power using numerical model with mono spin

Case II

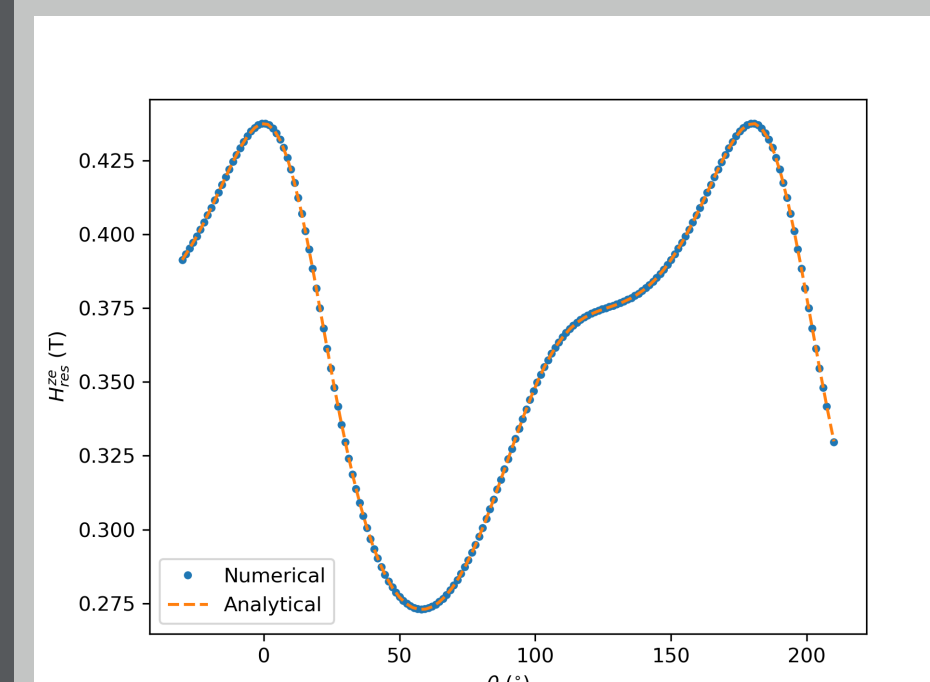


FMR Power using numerical model with mono spin

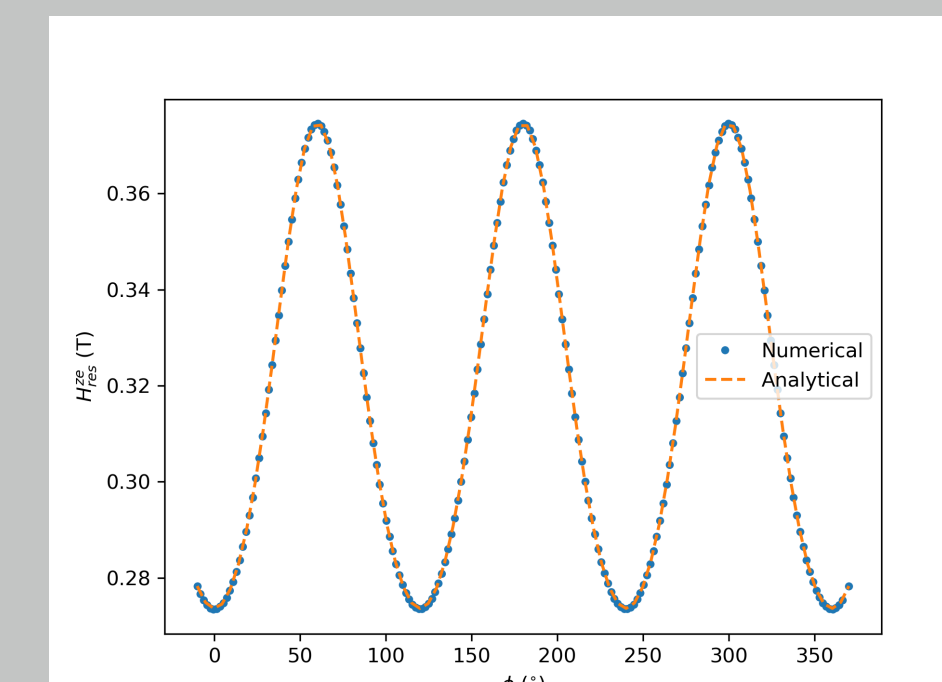
Case I



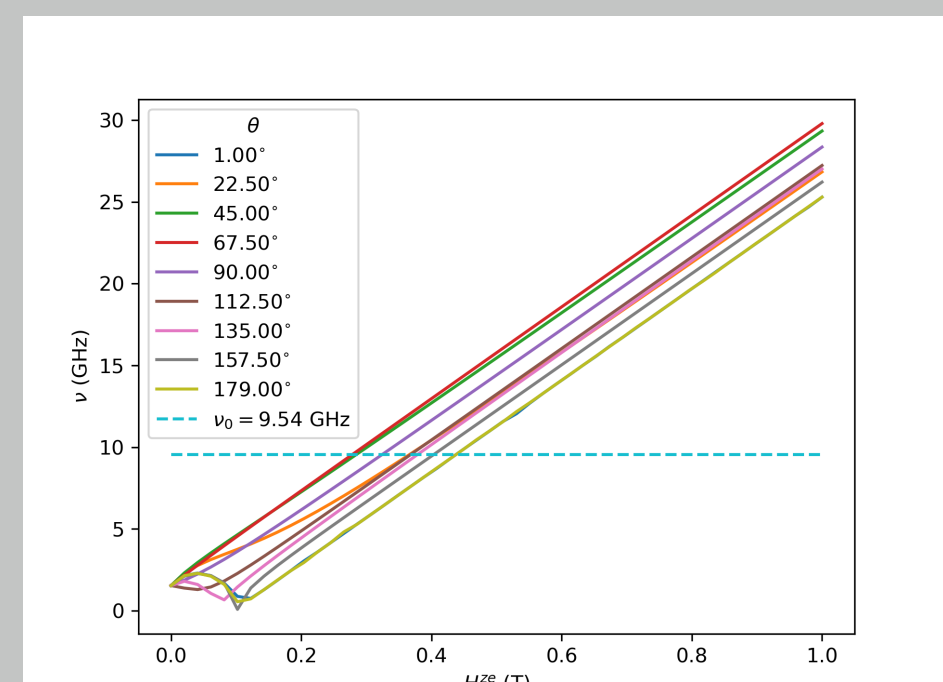
Finding $H_{\text{res}}^{\text{ze}}$ from numerical simulation data



Comparison between numerical & analytical model using mono spin



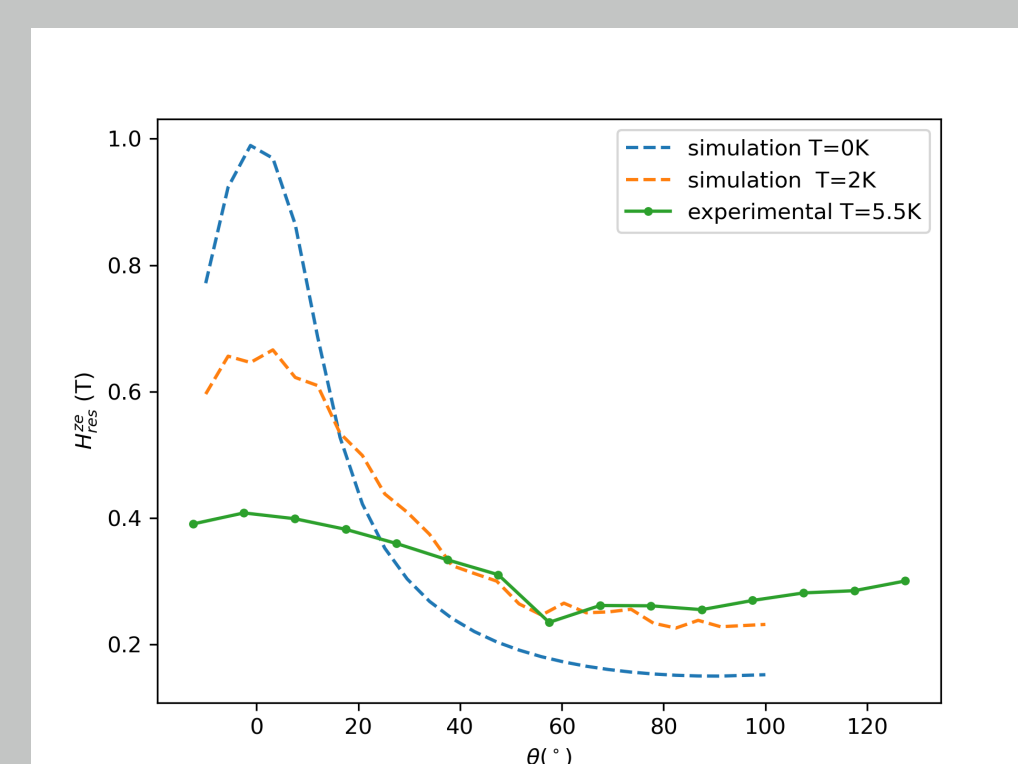
Comparison between numerical & analytical model using mono spin



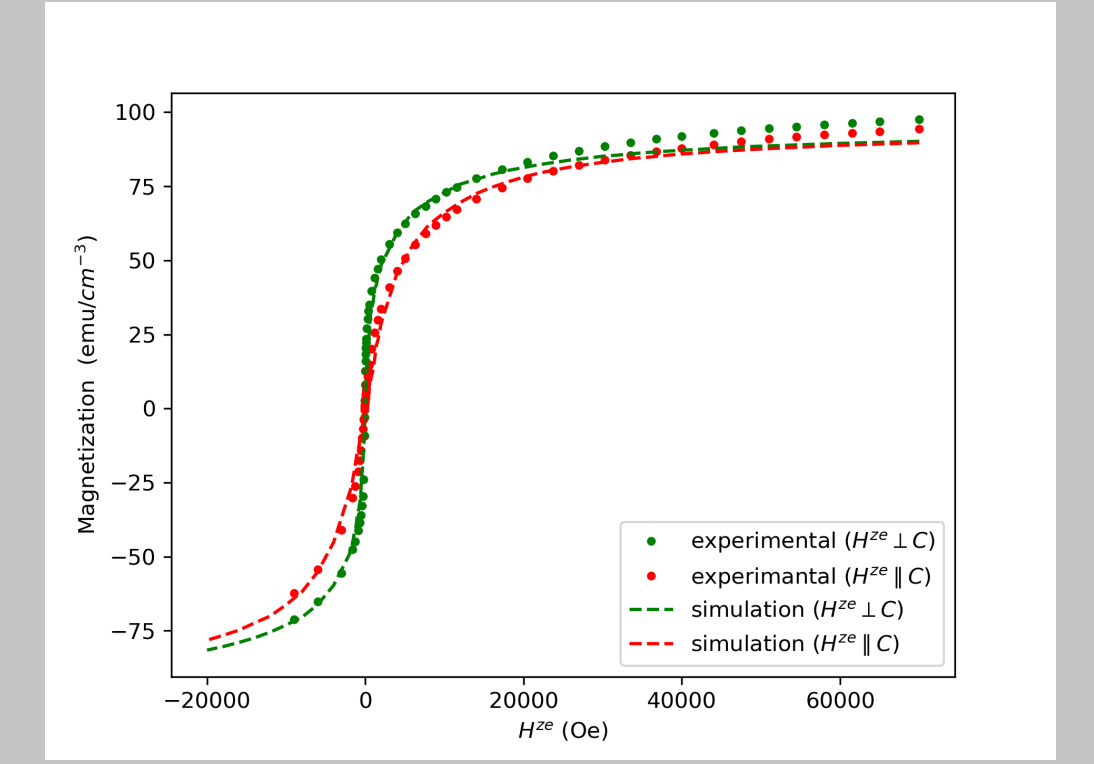
Finding $H_{\text{res}}^{\text{ze}}$ from analytical data; ν_0 is frequency of H^{ac}

At $T = 0 \text{ K}$

Atomistic Simulation Results



Comparison of experimental and numerical FMR data



Comparison of magnetization curves between experimental and simulation at $T=2 \text{ K}$

Case I $J_0 = 8 \text{ m-eV}$

Conclusion

- ▶ We observe both uniaxial (trigonal) & cubic (Jahn-Teller) anisotropy in FMR curves.
- ▶ A noise free FMR simulation data at higher T not only demands more computational time but also requires a larger simulation box. To this end, to produce a proper simulated FMR curve that agrees with our experimental data at $T=5.5 \text{ K}$, requires huge simulation box and higher computational time.

Reference & Acknowledgment

- ▶ 1. K. D. Usadel, Phys. Rev. B 73, 212405 (2006).
- ▶ 2. Y. K. Edathumkandy and D. Sztenkiel, arXiv :2108.01474
- ▶ The work is supported by the National Science Centre, Poland, through projects DEC-2018/31/B/ST3/03438 and by the Interdisciplinary Centre for Mathematical and Computational Modelling at the University of Warsaw through the access to the computing facilities.