Local defect properties and their signatures in electrical probes of GaN defect spin dynamics

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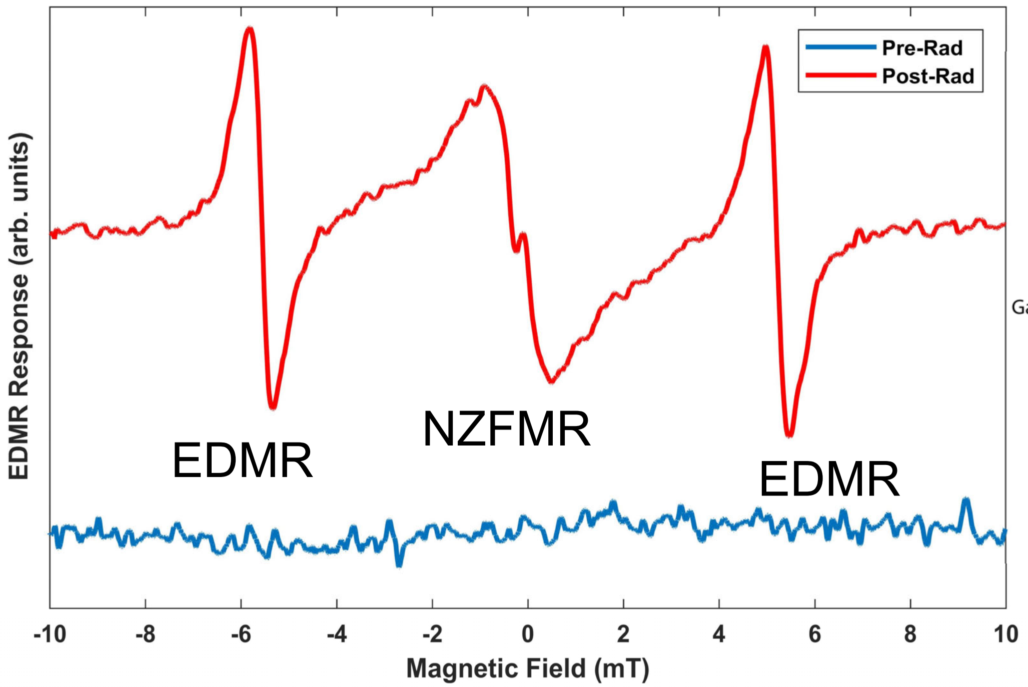
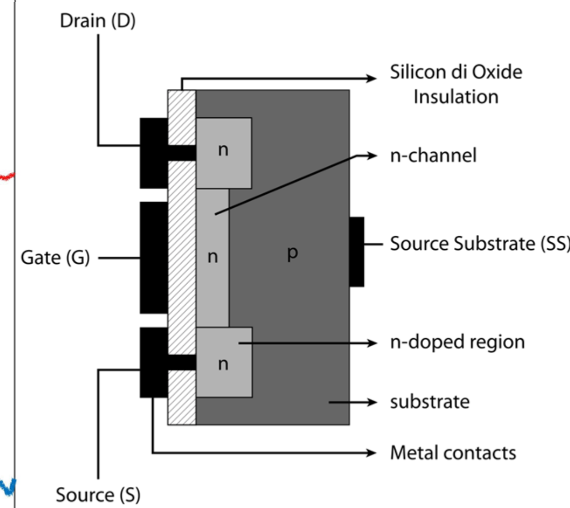
Joseph Sink (here)

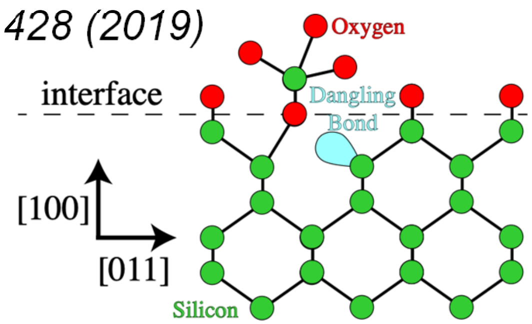
Measurements: Lenahan
Devices: Chu
Additional theoretical discussion: Tuttle

gate leakage through irradiated nonmagnetic Si/SiO_2 junctions



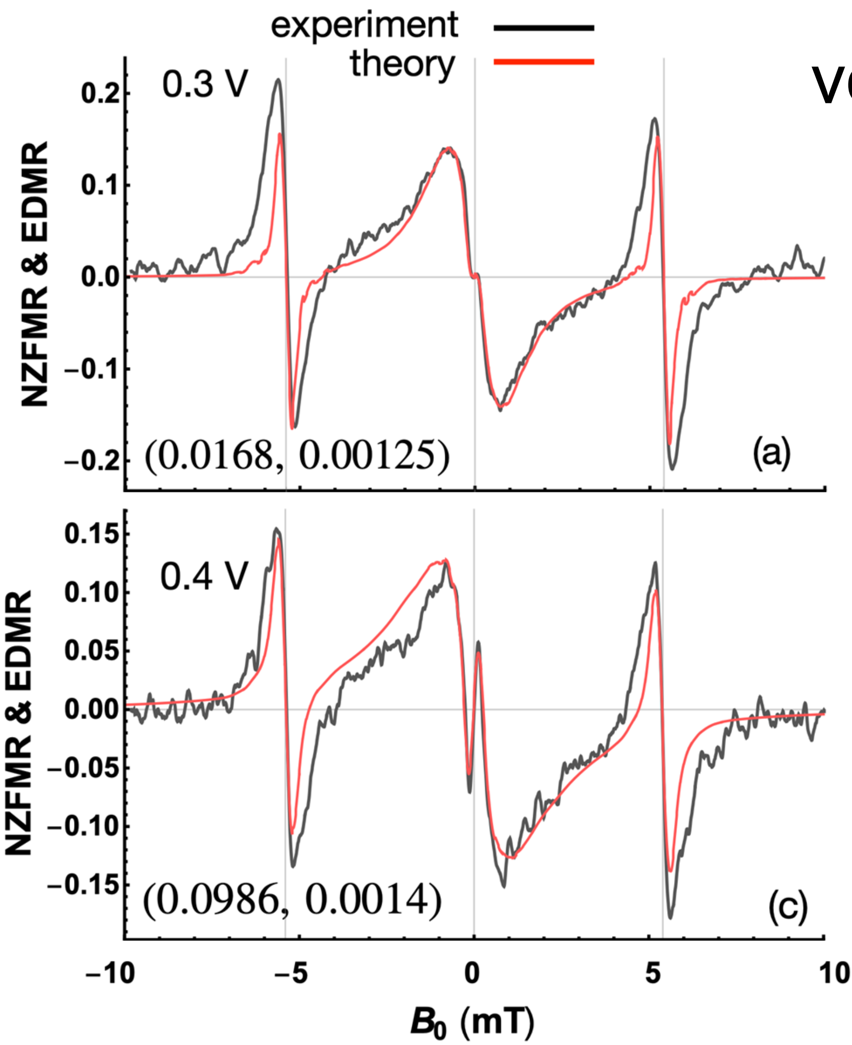


IEEE TNS 66, 428 (2019)



RF frequency 151 MHz, source and drain 0.33 V, gate 0.3 V

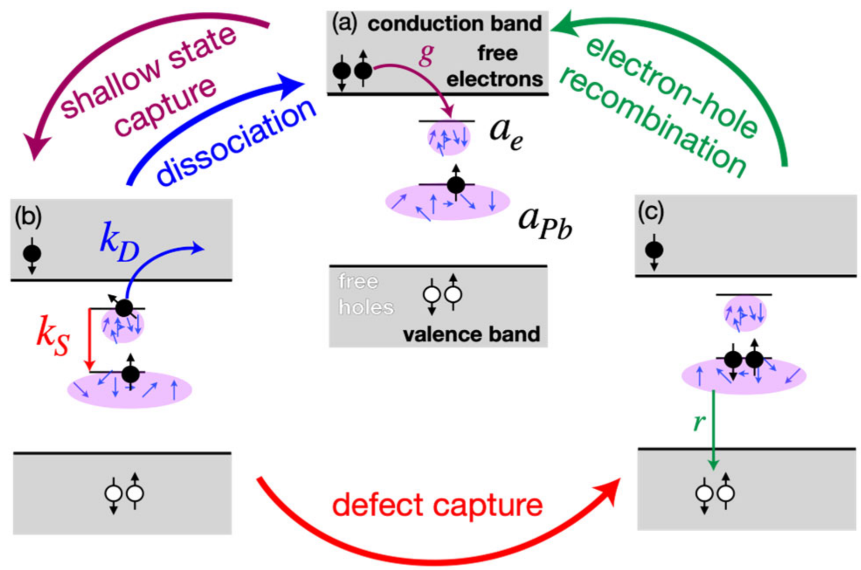
near-interface trap (P_b, which has hyperfine interactions)



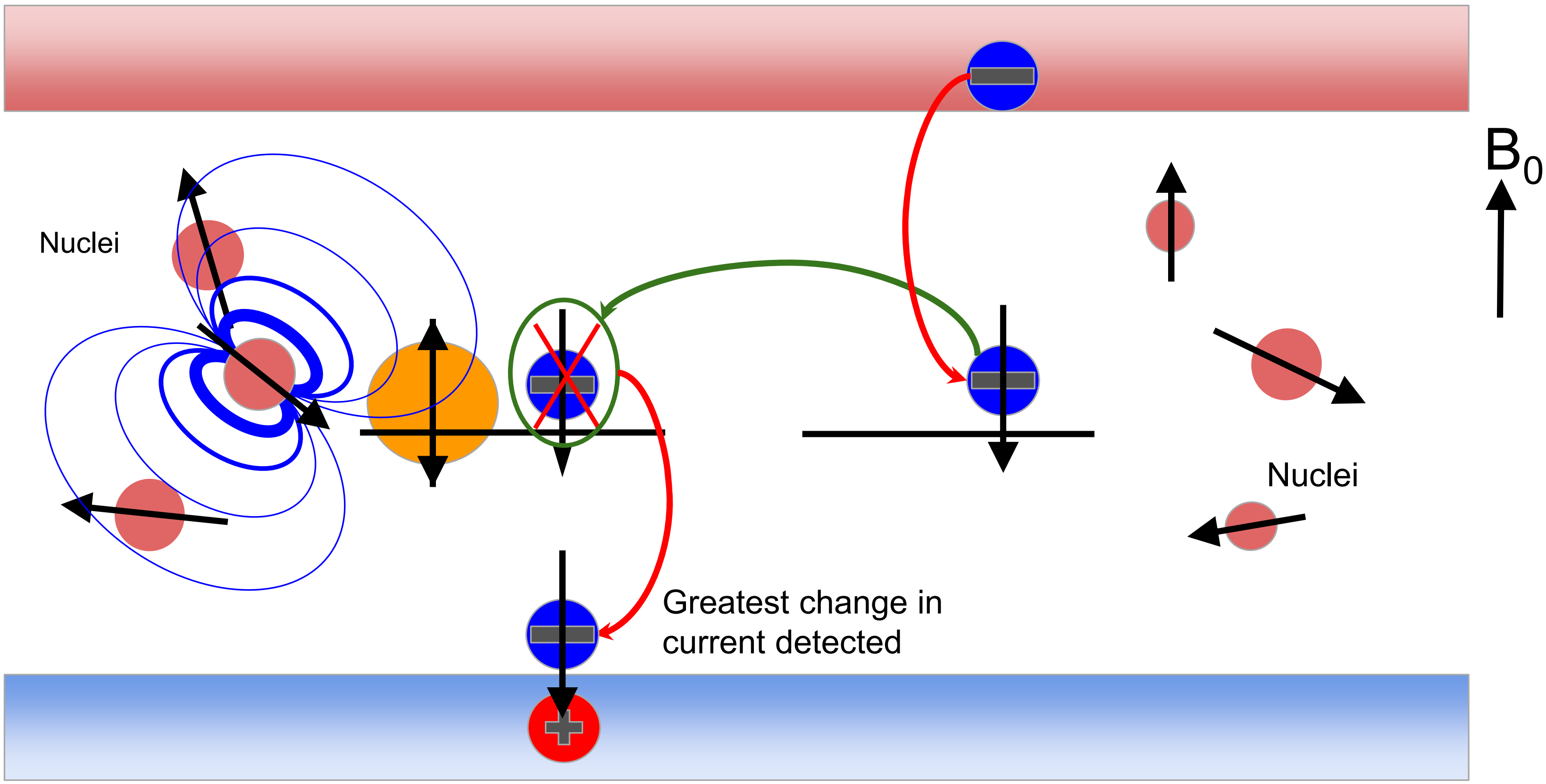
voltage dependence reveals rates

features depend on rates as well as hyperfine fields

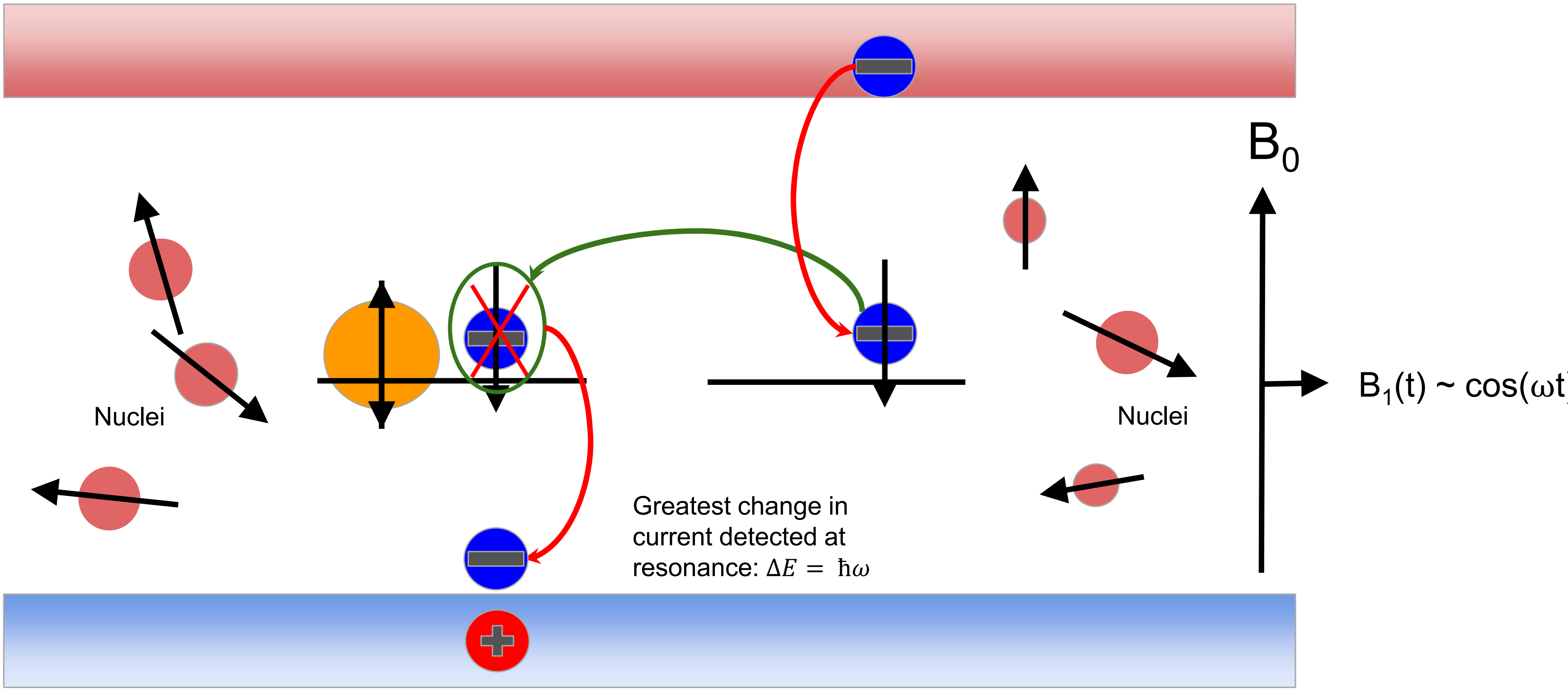
APL 123, 251603 (2023)
arXiv:2008.08121



Near Zero-Field Magnetoresistance (NZFMR)



Electrically Detected Magnetic Resonance (EDMR)



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Simulation of EDMR and NZFMR - Lindblad Equations

$\vec{S}_d = \text{Spin of deep level defect} \qquad \vec{S}_e = \text{Spin of electron at shallow level}$

$$\hat{H} = g\mu_B \underbrace{\left(\vec{B}_0 + \vec{B}_1\right)}_{\substack{\text{Zeeman and} \\ \text{Microwave B Fields}}} \cdot \left(\vec{S}_d + \vec{S}_e\right) + \vec{S}_d \cdot \underbrace{\sum \overleftrightarrow{A}_i \cdot \vec{I}_i}_{\substack{\text{Deep level} \\ \text{nuclear bath}}} + \vec{S}_e \cdot \underbrace{\sum \overleftrightarrow{A}_j \cdot \vec{I}_j}_{\substack{\text{Shallow level} \\ \text{nuclear bath}}}$$

$$\partial_t \hat{\rho}(t) = \underbrace{-\frac{i}{\hbar}\left[\hat{H}(t), \hat{\rho}(t)\right]}_{\substack{\text{Schrödinger Equation} \\ \text{(coherent evolution)}}} + \sum_i \underbrace{k_i \left(\hat{L}_i \hat{\rho}(t) \hat{L}_i^\dagger - \frac{1}{2}\left\{\hat{L}_i^\dagger \hat{L}_i, \hat{\rho}(t)\right\}\right)}_{\substack{\text{Hopping of Transport Electron and} \\ \text{Quantum Noise}}}$$

Comparing Simulation to Experiment (Signal)

$$I(B_0) \propto Tr\left[\hat{P}_S \hat{\rho}_{ss}\right] = \rho_S \qquad \text{Signal}(B_0) \equiv \partial_{B_0} I(B_0)$$

Magnetic field derivative of singlet spin population in the steady-state
is proportional to the experimental signal measured by Lenahan group

Computational Difficulties of Nuclear Baths in GaN

^{69}Ga (60% n.a.), ^{71}Ga (40% n.a.) have 4 states/nuclei (I=3/2)

Nitrogen vacancy nuclear bath involves ≥ 4^4 = **256 quantum states**

^{14}N (100% n.a.) have 3 states/nuclei (I=1)

Gallium Vacancy nuclear bath involves ≥ 3^4 = **81 quantum states**

Number of matrix equations scales with nuclear bath - **approximations needed**

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V(N) NZFMR Fit to Commercial Device Data

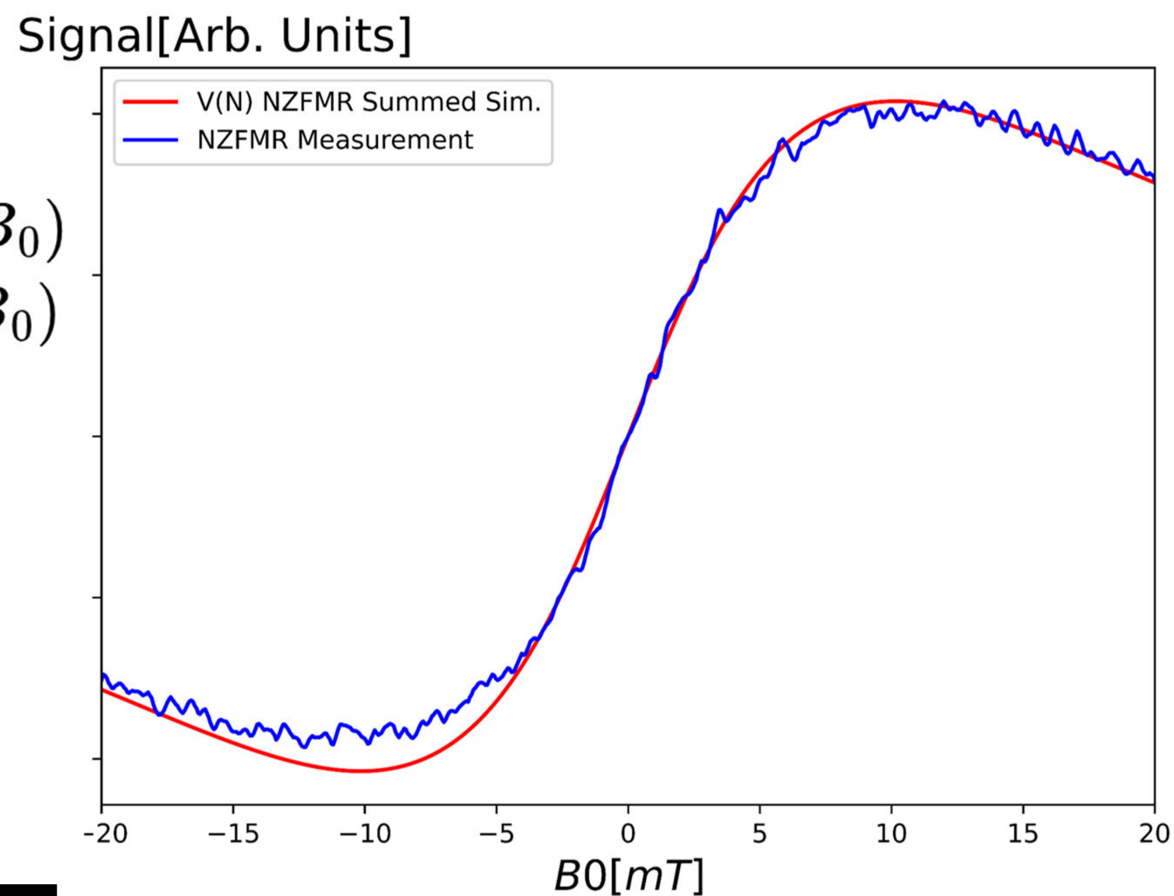
Classical nuclear hyperfine averaging theory for both isotopes of Gallium:

$$\text{Signal}(B_0) = 0.6 \times \text{Signal}_{69Ga}(B_0) + 0.4 \times \text{Signal}_{71Ga}(B_0)$$

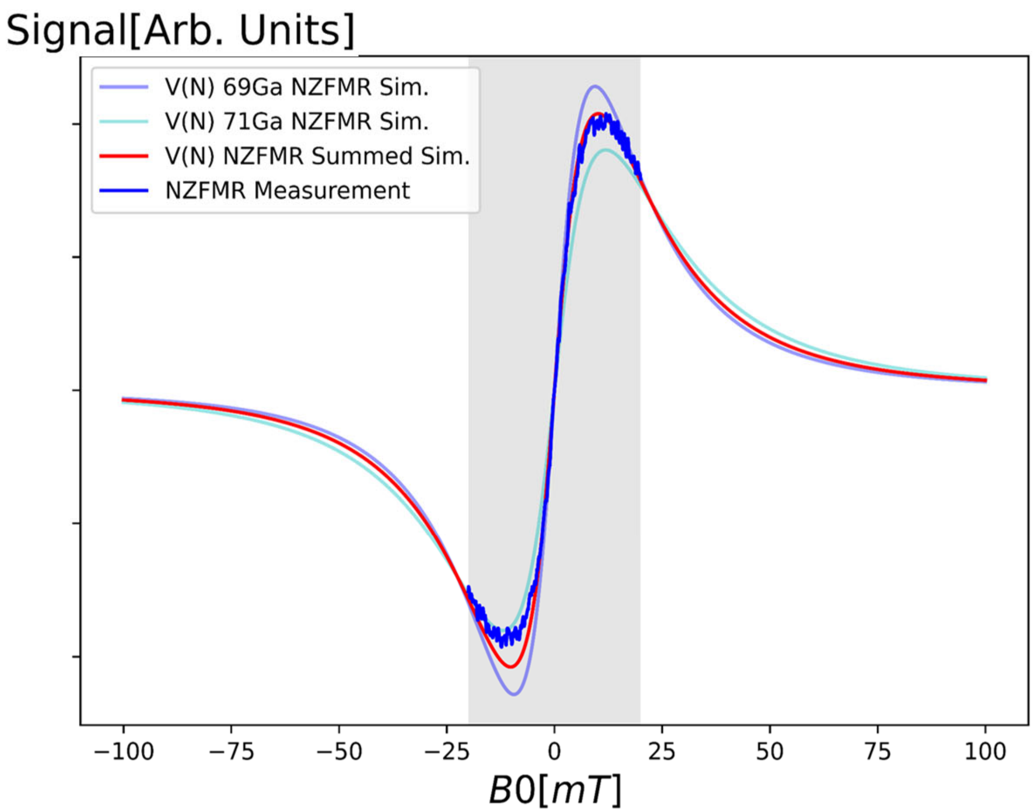
$$A_{\perp,eff} = A_{zz,eff} = 28 \text{ MHz}$$

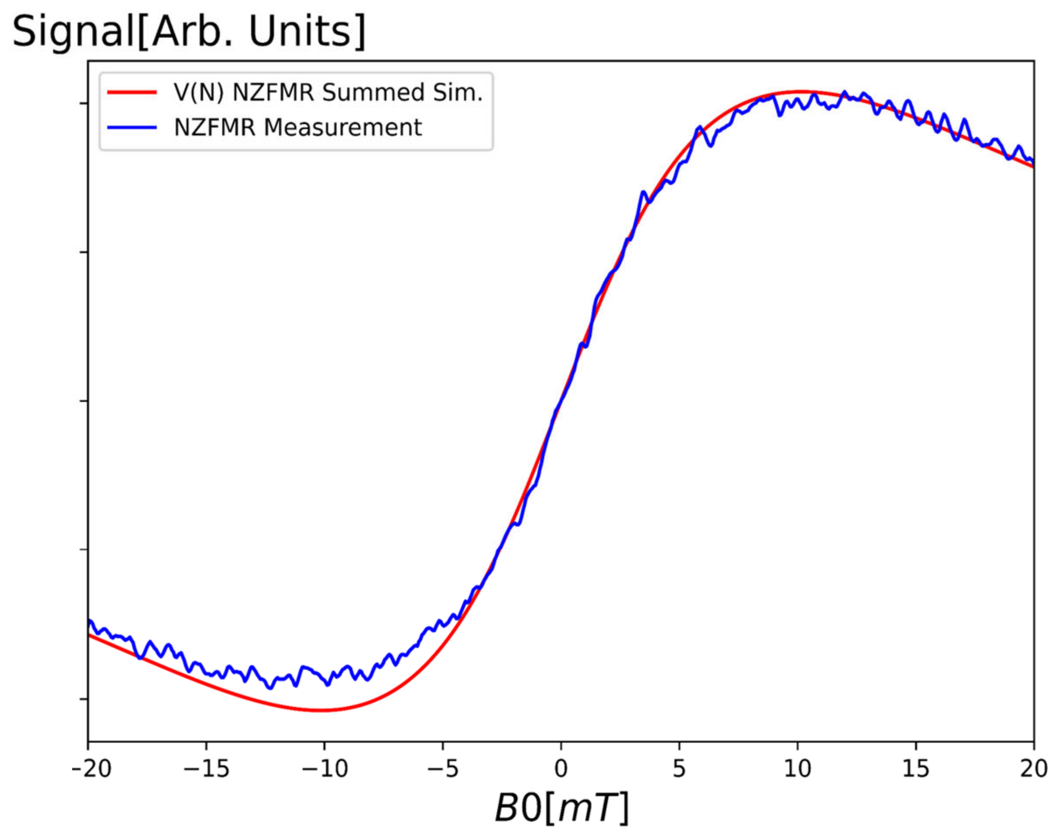
Hyperfine coupling calculations will be described towards end of presentation

Defect coherence time: T2 = 20 ns (fit)

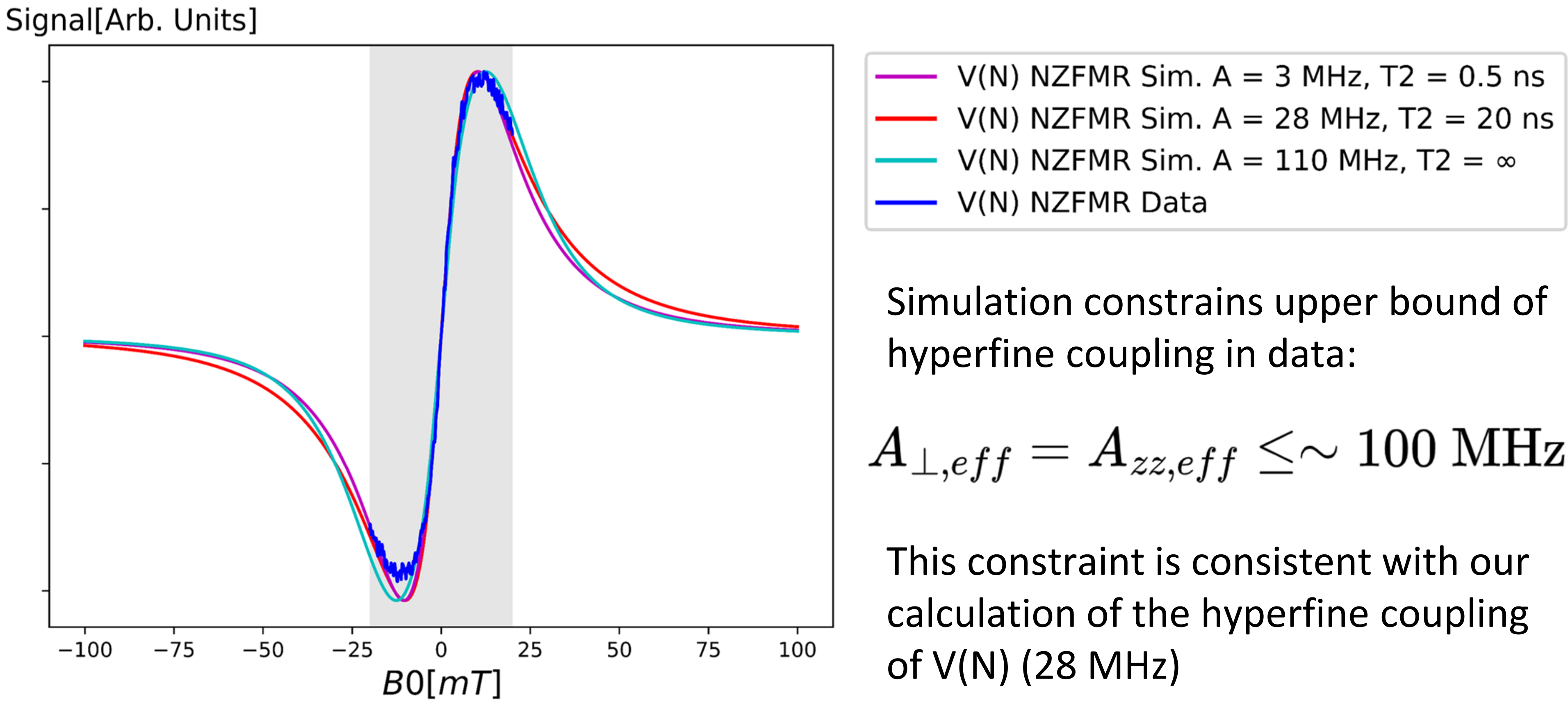


V(N) NZFMR Fit to Commercial Device Data





V(N) NZFMR Fit - Constraining Hyperfine Values



Simulation constrains upper bound of hyperfine coupling in data:

$$A_{\perp,eff} = A_{zz,eff} \leq\sim 100\ \text{MHz}$$

This constraint is consistent with our calculation of the hyperfine coupling of V(N) (28 MHz)

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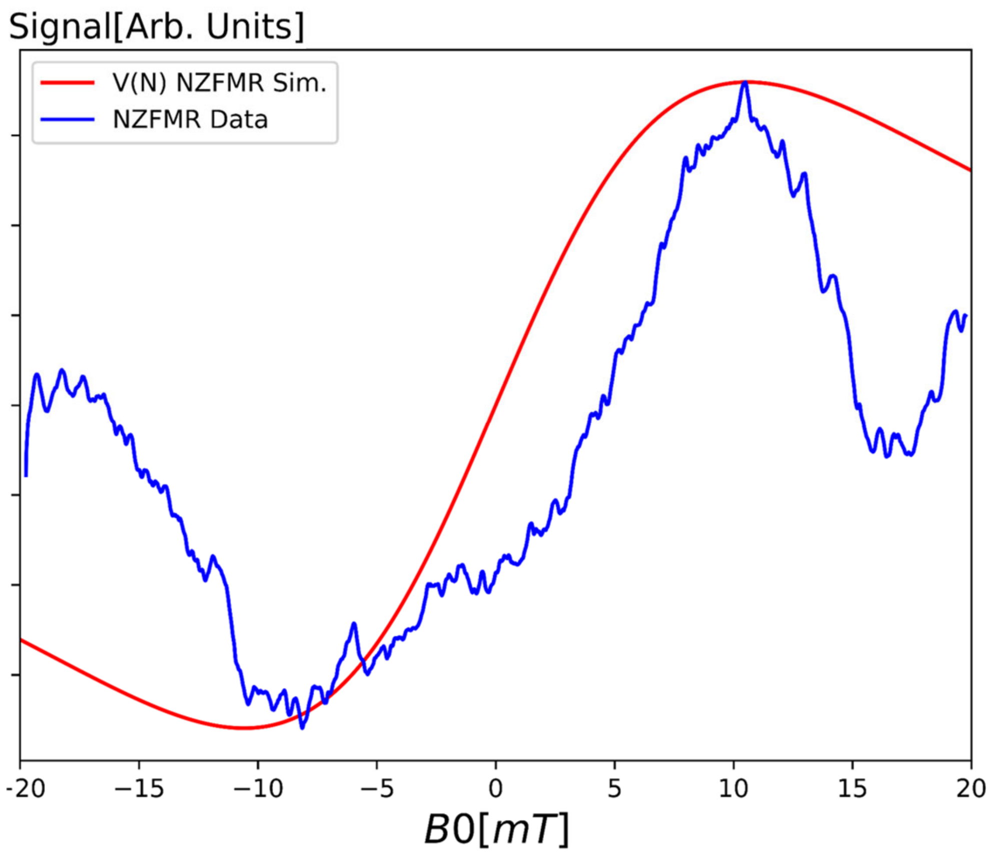
V(N) NZFMR Fit to Penn State Device Data



NZFMR simulation based on V(N) is not consistent with the NZFMR measurement on this device.

Other defects playing a role?

V(Ga) EDMR Fit to Penn State Device Data

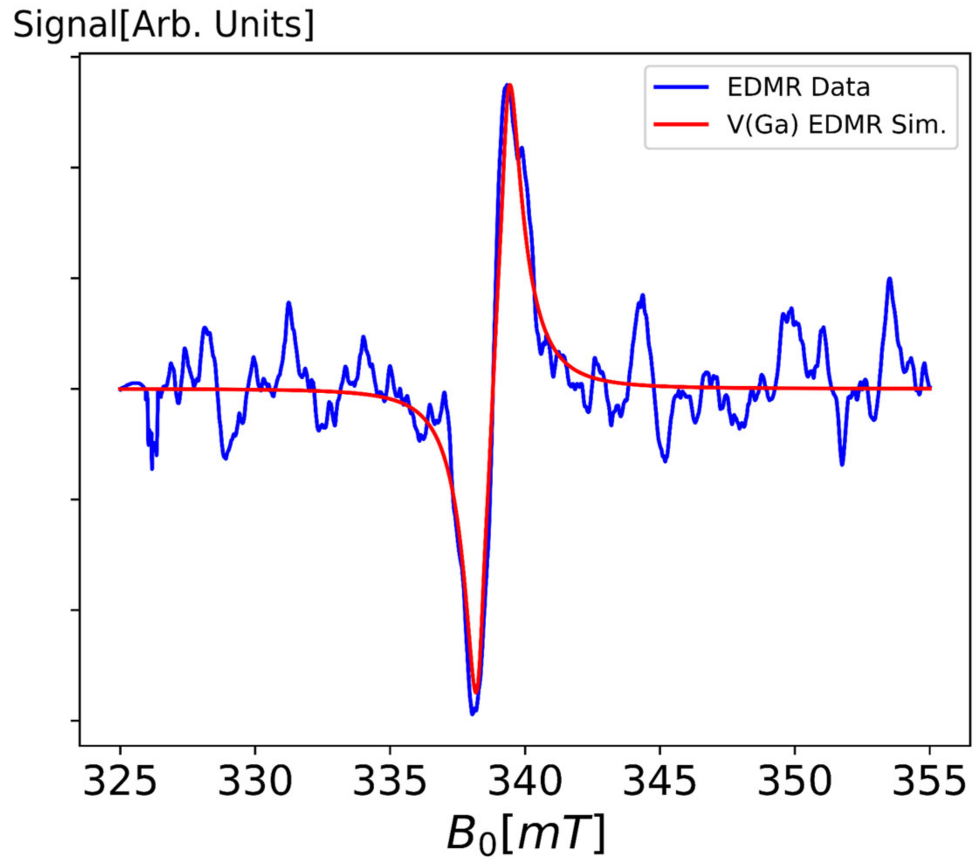
EDMR signal is dominated by the Azz component of nitrogen on axial site:

$$A^a_{zz} = -10.7\ \mathrm{MHz}$$

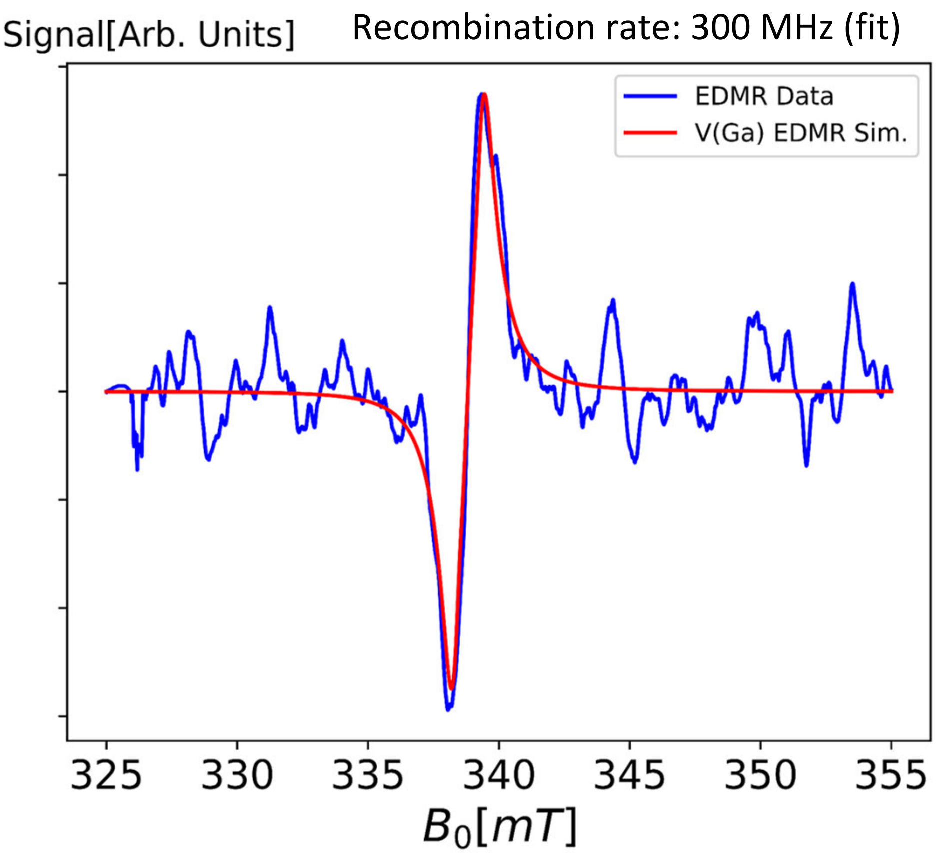
Contribution from basal nitrogens is negligible: $A^b_{zz} = 0.17\ \mathrm{MHz}$

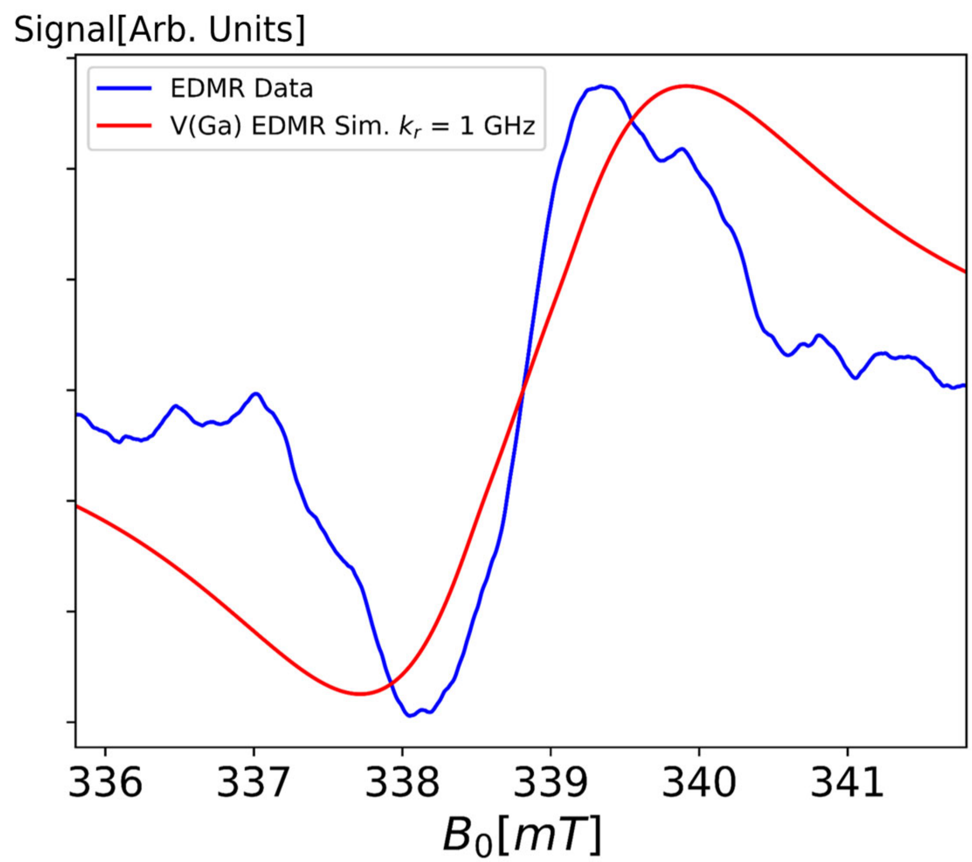
Hyperfine couplings calculated using tight-binding Green's functions as described later

Recombination rate: 300 MHz (fit)

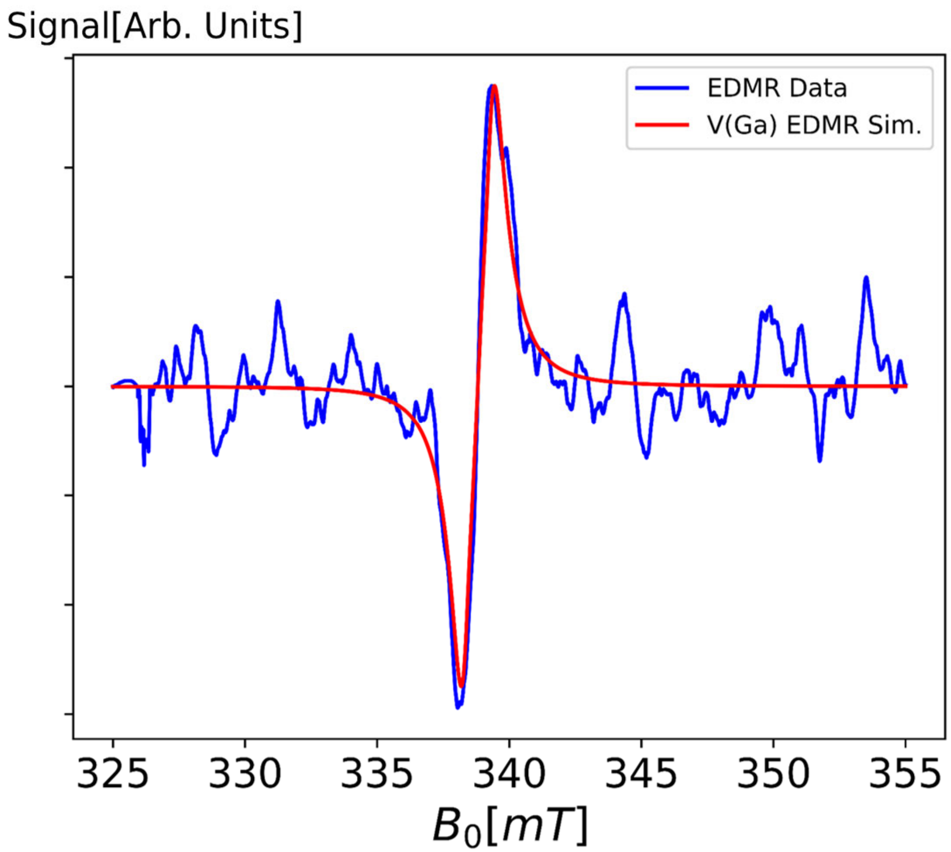


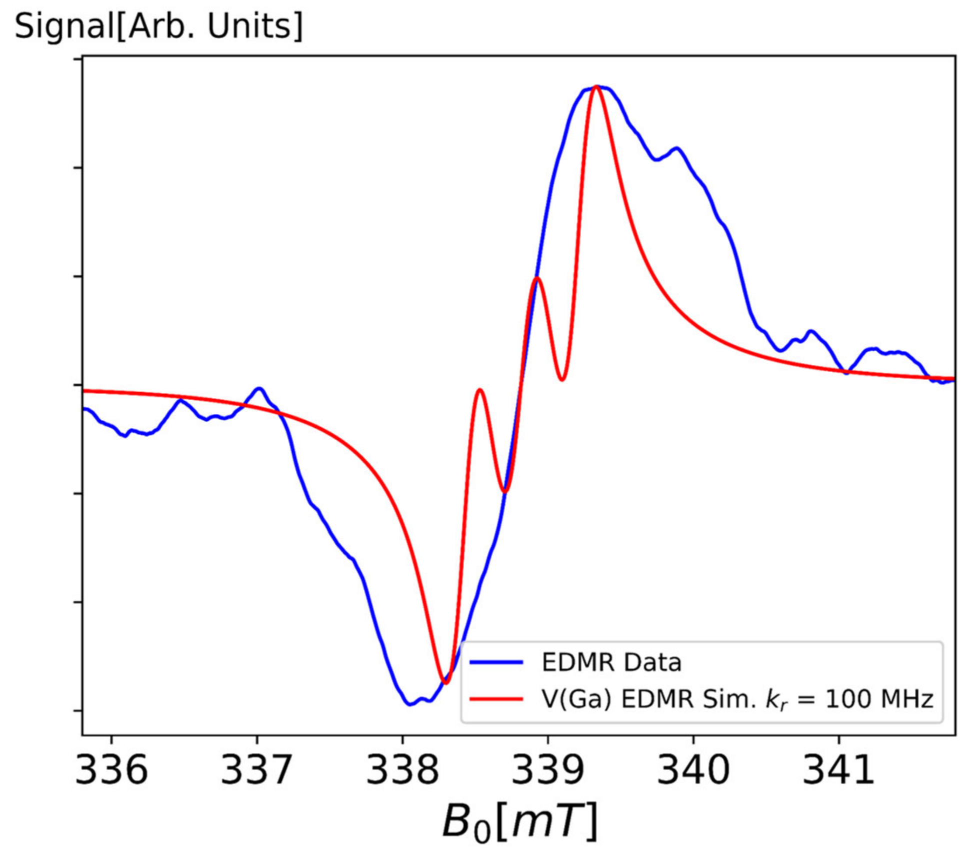
V(Ga) EDMR Fit – Vary Recombination Rate



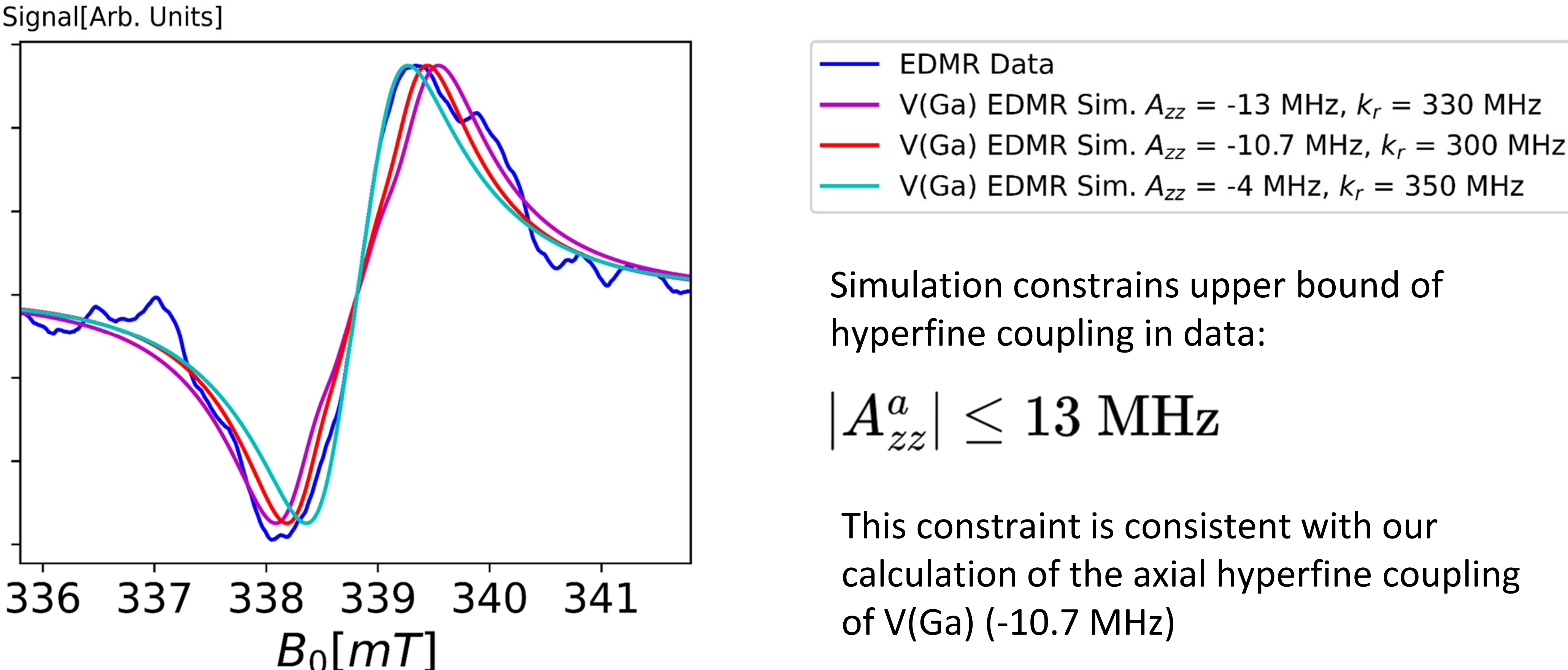


V(Ga) EDMR Fit – Vary Recombination Rate





V(Ga) EDMR Fit – Vary Axial Hyperfine



Simulation constrains upper bound of hyperfine coupling in data:

$$|A^a_{zz}| \leq \mathbf{13\ MHz}$$

This constraint is consistent with our calculation of the axial hyperfine coupling of V(Ga) (-10.7 MHz)

Tight-Binding Green's Functions

Defects in bulk can be efficiently solved via the Dyson Eqn[1,2,3],

$$\hat{G} = \left(1 - \hat{g}\hat{V}'\right)^{-1}\hat{g}$$

1) <u>Homogeneous</u>

$$\hat{g}(\delta\boldsymbol{R};\omega) = \int_{BZ} d^3k\left[\omega - \hat{H}(\boldsymbol{k})\right]^{-1} e^{i\boldsymbol{k}\cdot\delta\boldsymbol{R}}$$

2) <u>Inhomogeneous</u>

$$\hat{M}_{nn} = \left(1 - \hat{g}_{nn}\hat{V}'_{nn}\right)^{-1}$$
$$\hat{G}_{nn} = \hat{M}_{nn}\hat{g}_{nn}$$
$$\hat{G}_{ff} = \hat{g}_{ff} + \hat{g}_{fn}\hat{V}'_{nn}\hat{M}_{nn}\hat{g}_{nf}$$

with,

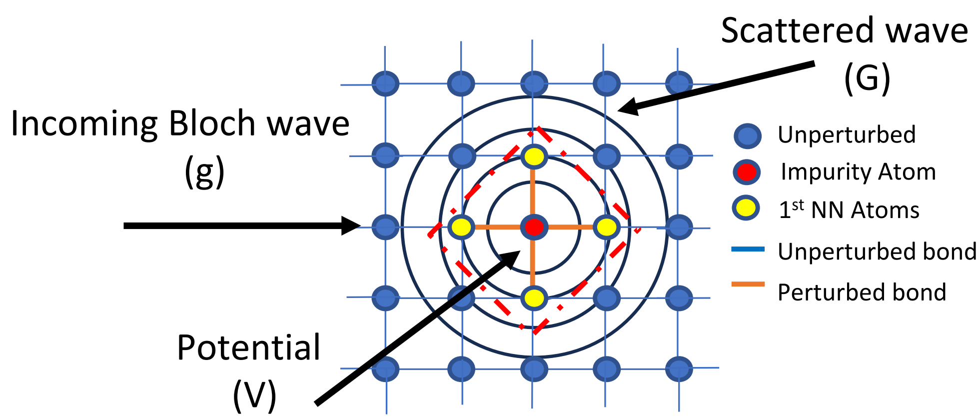
$$\hat{V}' = \begin{pmatrix} \hat{V}'_{nn} & 0 \\ 0 & 0 \end{pmatrix}$$

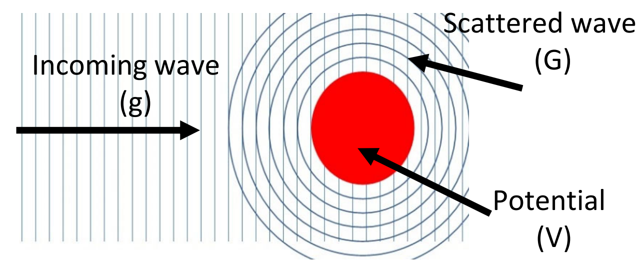
3 <u>Observables</u>

$$\eta(\boldsymbol{R},\omega) = \frac{-1}{\pi} Im\left[Tr\left[\hat{G}(\boldsymbol{R},\boldsymbol{R};\omega)\right]\right]$$
$$\left\langle \hat{A}_{iso}\right\rangle_{\omega} = \frac{-1}{\pi}\frac{8\pi}{3}A_0|\psi_s(0)|^2\hat{G}_{s,s}(\omega)$$
$$\langle \hat{A}_{ij}\rangle_{\omega} = \frac{-1}{\pi} Im\left[Tr\left[\hat{G}(\omega)A_0\hat{r}^{-3}\hat{Q}_{ij}\right]\right]$$

with,

$$\hat{Q}_{ij} = 3\hat{r}_i\hat{r}_j - \delta_{ij}$$
$$A_0 = \frac{g_S g_N \mu_0 \mu_B}{4\pi\langle S_z\rangle}$$





[1]Koster/Slater PR 95, 1167 1954
[2]Hjalmarson et al. PRL. 44, 810 1980
[3]Tang/Flatté PRL 92, 047201 2004
[4]A. Koh and D. Miller, Atom. and Nuc. Data 33, 235 (1985)

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Nitrogen Vacancy

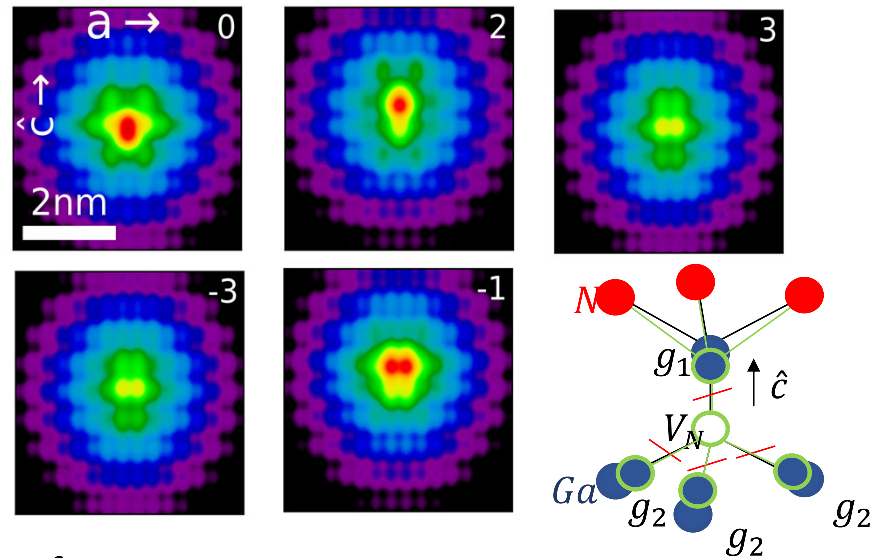
The V_N donor (31meV) is modelled using a (C_{3v} symmetric) potential,

$$\hat{V}' = \hat{E}_{Onsite} + \hat{V}_{NN}^{Strain} - \hat{V}_{NN}^{Bulk}$$

Where,

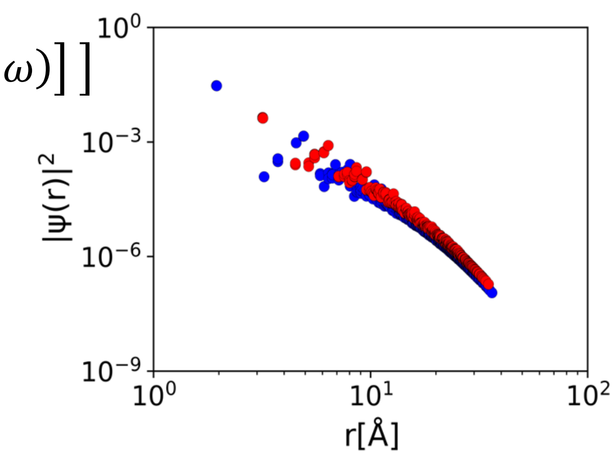
- $-\hat{V}_{NN}^{Bulk}$ creates four dangling Ga bonds as well as a non-interacting atomic nitrogen
- $\hat{E}_{Onsite}$ pushes the atomic nitrogen states up in energy, making them inaccessible
- $\hat{V}_{NN}^{Strain}$ allows the Ga to relax inward

The Nitrogen Vacancy wave function is highly isotropic and spread out over many atoms



Local Density of States

$$\eta(\boldsymbol{R}, \omega) = \frac{-1}{\pi} Im\left[Tr\left[\hat{G}(\boldsymbol{R}, \boldsymbol{R}; \omega)\right]\right]$$



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Nitrogen Vacancy Hyperfine

The V_N (C_{3v} symmetric) donor we model has s-like orbital character

We compute the strain dependent isotropic (Fermi Contact) hyperfine at $\boldsymbol{R_i}$ as,

$$\langle \hat{A}_{iso} \rangle^{i}_{\omega} = \frac{-1}{\pi}\frac{8\pi}{3} A_0 |\psi_s(0)|^2 G_{ss}(\boldsymbol{R_i}, \boldsymbol{R_i}, \omega)$$

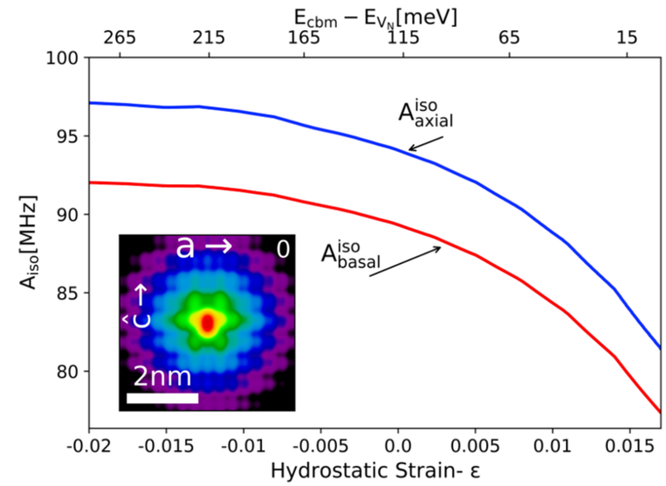
Defect Calculation

$G_{ss}(\boldsymbol{R_i}, \boldsymbol{R_i}, \omega) \Rightarrow \psi_s$ of wave function to LDOS for atom i

Atomic Constants[1]

$$\mathrm{A}_0 = \frac{g_S g_N \mu_0 \mu_B}{4\pi\langle S_z \rangle}$$

$|\psi_s(0)|^2 \Rightarrow$ Fermi Contact Amp. from ψ_s at nucleus



[I,J,K,L]	r_0[Å]	A_{iso}[MHz]
1NN Axial - Gallium		
$[0,0,0,1]$	1.9540	80.6125
1NN Basal - Gallium		
$[0,\bar{1},\bar{1},3]$, $[\bar{1},0,\bar{1},3]$, $[0,0,\bar{1},3]$	1.9487	84.8936
2NN - Nitrogen		
$[\bar{1},0,0,2]$, $[0,0,\bar{1},2]$, $[0,\bar{1},0,2]$ $[\bar{1},0,\bar{1},2]$, $[0,0,0,2]$, $[0,\bar{1},\bar{1},2]$	3.1798	2.1615
$[0,\bar{1},0,0]$, $[\bar{1},0,0,0]$, $[\bar{1},1,0,0]$ $[0,1,0,0]$, $[1,0,0,0]$, $[1,\bar{1},0,0]$	3.1890	2.1684

[1]A. Koh and D. Miller, Atom. and Nuc. Data 33, 235 (1985)

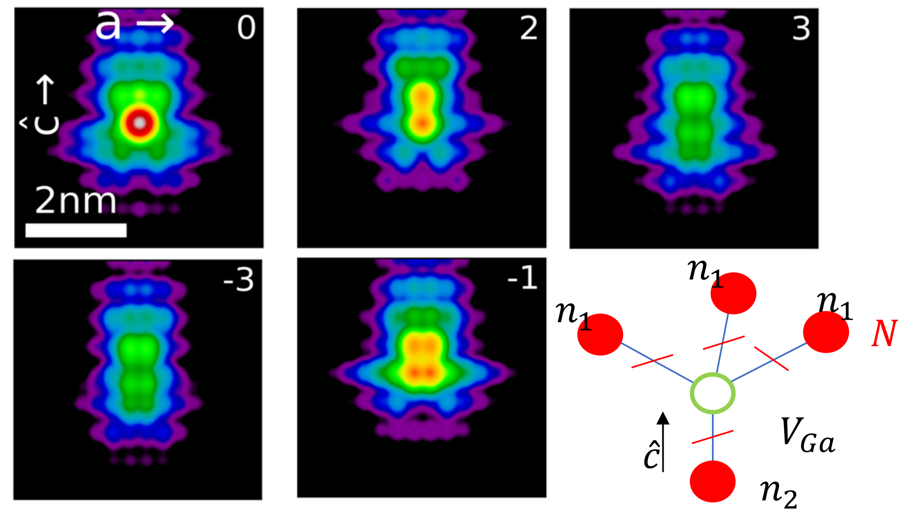
Gallium Vacancy

The V_{Ga} Acceptor (238meV) is modelled using the (C_{3v} symmetric) potential,

$$\hat{V}' = \hat{E}_{Onsite} - \hat{V}_{NN}^{Bulk}$$

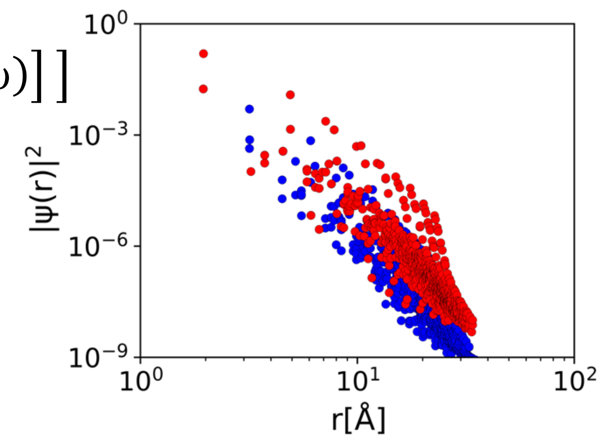
Where,

- $-\hat{V}_{NN}^{Bulk}$ creates four dangling N bonds and one free atomic gallium
- $\hat{E}_{Onsite}$ pushes the atomic nitrogen states up in energy, making them inaccessible



Local Density of States

$$\eta(\boldsymbol{R},\omega) = \frac{-1}{\pi} Im\left[Tr\left[\hat{G}(\boldsymbol{R},\boldsymbol{R};\omega)\right]\right]$$



The gallium vacancy wave function is highly anisotropic with a spatial decay with a much shorter range than the nitrogen vacancy.

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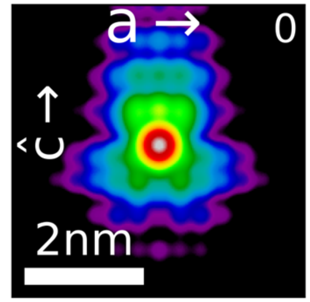
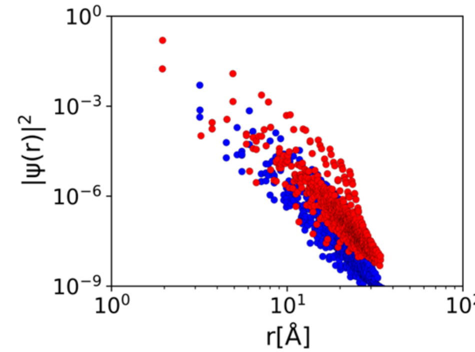
Gallium Vacancy Hyperfine





The V_{Ga} (C_{3v} symmetric) acceptor we model has p-like orbital character.

We compute the anisotropic orbital hyperfine at $\boldsymbol{R_i}$ as,

$$\langle \hat{A}_{ij} \rangle_{\omega}^{q} = \frac{-1}{\pi} Im\left[\sum_{\beta\beta'} G_{\beta\beta'}(\boldsymbol{R_q}, \boldsymbol{R_q}, \omega) A_0^{\beta} \langle r^{-3} \rangle_{\beta} Q_{\beta\beta'}\right]$$

Defect Calculation

$G_{\beta\beta'}(\boldsymbol{R_q}, \boldsymbol{R_q}, \omega) \Rightarrow \psi_s$ of wave function to LDOS for atom q

Tabulated Constants

$\hat{Q}_{ij} = 3\hat{r}_i\hat{r}_j - \delta_{ij} \Rightarrow$ Quadrupole moment tensor

$\mathrm{A}_0 = \frac{g_s g_N \mu_0 \mu_B}{4\pi \langle S_z \rangle}$[1]

$\langle r^{-3} \rangle_{\beta} \Rightarrow$ Expectation of radial decay of orbital-β[1]

[I,J,K,L]	r_0[Å]	A_{qq}[MHz]	$[u_x, u_y, u_z]_q$
1NN Axial - Nitrogen			
[0, 0, 0, 0]	1.9540	-6.4265	[0.8610, 0.5086, 0.0000]
		-6.4265	[0.5086, -0.8610, 0.0000]
		23.7987	[-0.0000, -0.0000, 1.0000]
1NN Basal - Nitrogen			
[0, 0, 0, 2]	1.9487	-0.7025	[-1.0000, -0.0002, -0.0005]
		-0.7020	[-0.0006, 0.2956, 0.9553]
		2.6639	[0.0000, -0.9553, 0.2956]
[$\bar{1}$, 0, 0, 2]	1.9487	-0.7012	[-0.5000, 0.8660, 0.0002]
		-0.7007	[-0.2559, -0.1479, 0.9553]
		2.6591	[-0.8273, -0.4777, -0.2956]
[0, $\bar{1}$, 0, 2]	1.9487	-0.7025	[0.5000, 0.8660, -0.0002]
		-0.7020	[0.2561, -0.1477, 0.9553]
		2.6639	[-0.8273, 0.4777, 0.2956]

[1]A. Koh and D. Miller, Atomic and Nucl[illegible]es 33, 235 (1985)

Summary

Magnetic field effects on transport through junctions containing defects with spin provides insight into

(1) hyperfine structure of the defect

(2) electronic spin character of the defect

(3) transport rates including recombination rates, generation, dissociation

Correlations between EDMR and NZFMR provides insight into any radiation-induced defects

- NZFMR and EDMR simulations validated for GaN devices, including those from Penn State
- Microscopic wave function extent and hyperfine fields for vacancies calculated
- Width and mixing features are fingerprints for recombination pathways

Next steps

- Analyze more device measurements, including those from radiation damage
- Complete hyperfine simulations with simulations of N and Ga antisites and interstitials

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Theory of Classical Nuclear Hyperfine Averaging

1. Nuclear bath approximations

$$\overleftrightarrow{A} = \begin{pmatrix} A_{xx} & A_{xy} & A_{xz} \\ A_{xy} & A_{yy} & A_{yz} \\ A_{xz} & A_{yz} & A_{zz} \end{pmatrix} \approx \begin{pmatrix} A_{\perp} & 0 & 0 \\ 0 & A_{\perp} & 0 \\ 0 & 0 & A_{zz} \end{pmatrix} \qquad \overleftrightarrow{A}_i = \overleftrightarrow{A}_{i'} = \overleftrightarrow{A}_{eff}$$

1. Replace the nuclear bath with a discrete set of classical B-fields and respective weights calculated from $\overleftrightarrow{A}_{eff}$

$$\sum \overleftrightarrow{A}_i \cdot \vec{I}_i \rightarrow \left\{ \vec{B}_i \left(A_{\perp}, A_{zz} \right), w_i \right\} \qquad \hat{H} \rightarrow \left\{ \hat{H}_i \left(\vec{B}_i \right) \right\}$$

1. Calculate a weighted signal:

$$\mathrm{Signal}(B_0) = \sum w_i \times \mathrm{Signal}(B_0, \vec{B}_i)_i$$

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Calculation of Classical Magnetic Fields

Simplified hyperfine tensor allows Hamiltonian to be written in block-diagonal form:

$$\hat{H} = \begin{pmatrix} \hat{H}_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \hat{H}_N \end{pmatrix}$$

$$\overleftrightarrow{A}_{eff} = \begin{pmatrix} A_\perp & 0 & 0 \\ 0 & A_\perp & 0 \\ 0 & 0 & A_{zz} \end{pmatrix}$$

The hyperfine interaction in each sub-block is mapped onto a classical field:

$$\hat{H}_i = \vec{I} \cdot \overleftrightarrow{A}_{eff} \cdot \vec{S} \equiv g\mu_B \vec{B}_i \cdot \vec{S}$$

$$\vec{B}_i = \frac{1}{g\mu_B} \langle \propto A_\perp, 0, \propto A_{zz} \rangle$$

Proportionality constants depend on nuclear spin value

Calculation of Classical Magnetic Fields (Many Nuclei)

Identical hyperfine tensors allow for nuclear spin angular momenta to be added:

$$\overleftrightarrow{A}_i = \overleftrightarrow{A}_{i'} = \overleftrightarrow{A}_{eff} \qquad \sum \overleftrightarrow{A}_i \cdot \vec{I}_i = \overleftrightarrow{A}_{eff} \cdot \vec{I}_{total}$$

For four nearest-neighbor nuclei, I_{total} takes a range of values with multiplicities Ω

Gallium vacancy:

I_{total}	4	3	2	1	0
Ω	1	3	6	6	3

Nitrogen Vacancy:

I_{total}	6	5	4	3	2	1	0
Ω	1	3	6	10	11	9	4

Calculation of Classical Magnetic Fields (Many Nuclei)

Each possibility of I_{total} corresponds to $2 \times I_{total}$ classical magnetic fields

Distribution of classical field components is a function of I_{total}

$$B_x(I_{total}) = \frac{2A_\perp}{g\mu_B} \times \left\{ \text{matrix elements of } \hat{I}_{total,x} \right\}$$

$$B_y(I_{total}) = 0$$

$$B_z(I_{total}) = \frac{A_{zz}}{g\mu_B} \times \left\{ \text{matrix elements of } \hat{I}_{total-1/2,z} \right\}$$

$$w_i = \frac{\Omega_i}{Total\ \#\ of\ \ Fields} \qquad \text{Signal}(B_0) = \sum w_i \times \text{Signal}(B_0, \vec{B}_i)_i$$

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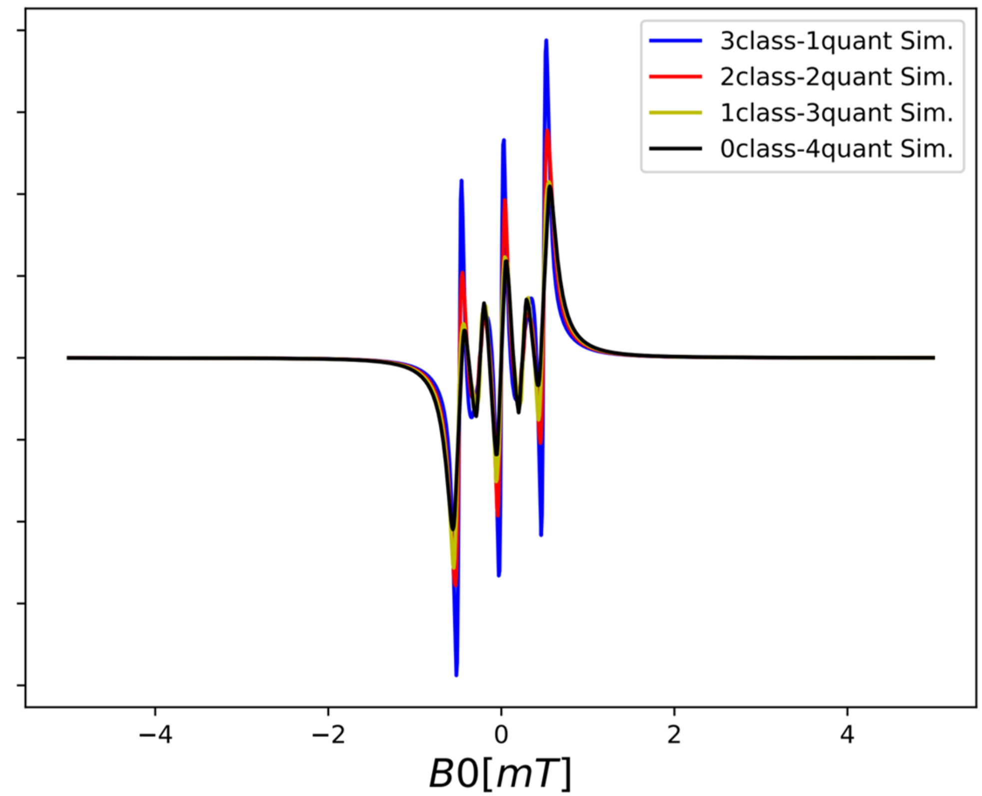
V(Ga) NZFMR - Varying "Quantumness"

Our tight-binding Green's functions hyperfine calculations predict significantly different hyperfine couplings for axial vs. basal nitrogens to V(Ga).

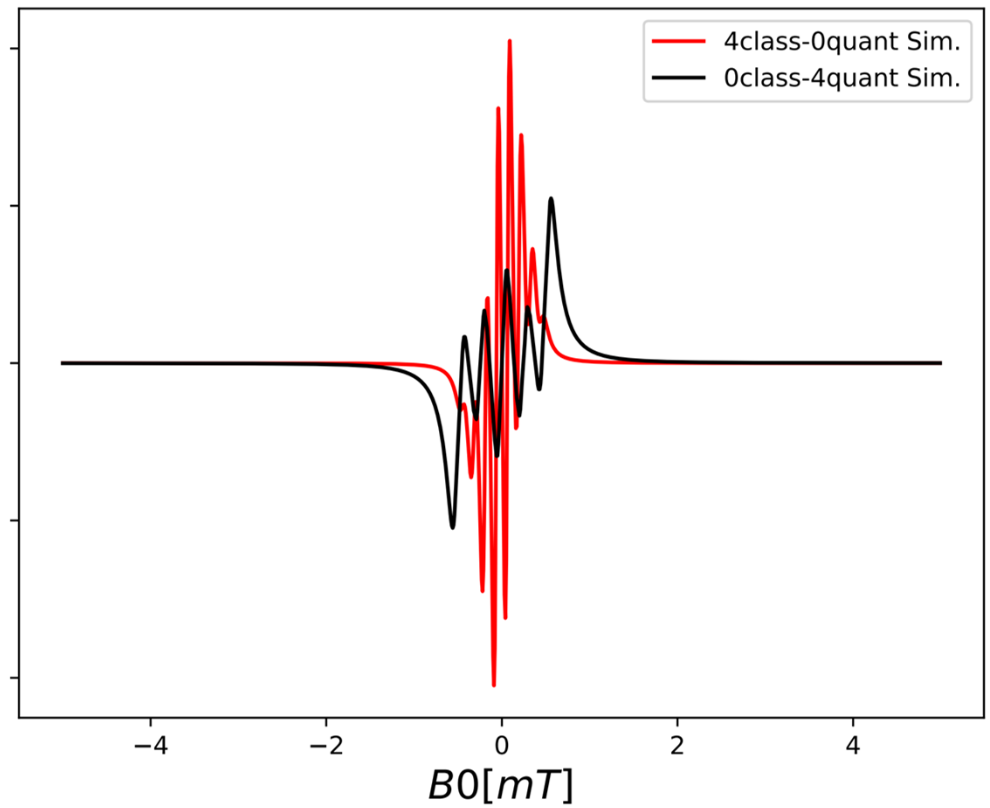
(Right) classical nuclear hyperfine averaging on 0-3 basal nitrogens (**axial nitrogen is left fully quantum for all**):



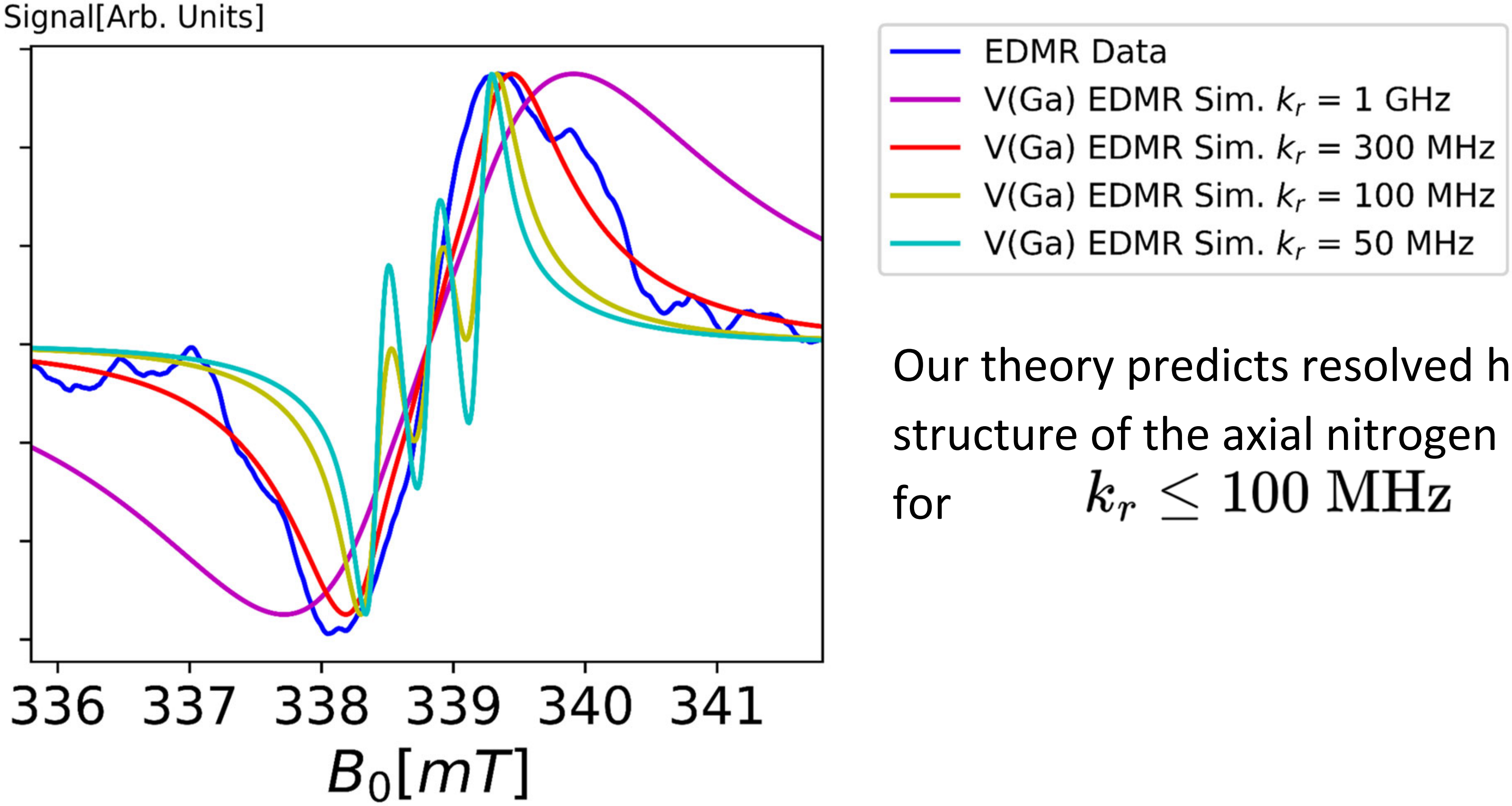
V(Ga) NZFMR - Varying "Quantumness"

Our tight-binding Green's functions hyperfine calculations predict significantly different hyperfine couplings for axial vs. basal nitrogens to V(Ga).

(Right) comparison to fully quantum simulation when the **axial nitrogen nuclear spin is also treated classically**:



V(Ga) EDMR - Varying Recombination Rate



Our theory predicts resolved hyperfine structure of the axial nitrogen nuclear spin for $k_r \leq 100\ \mathrm{MHz}$

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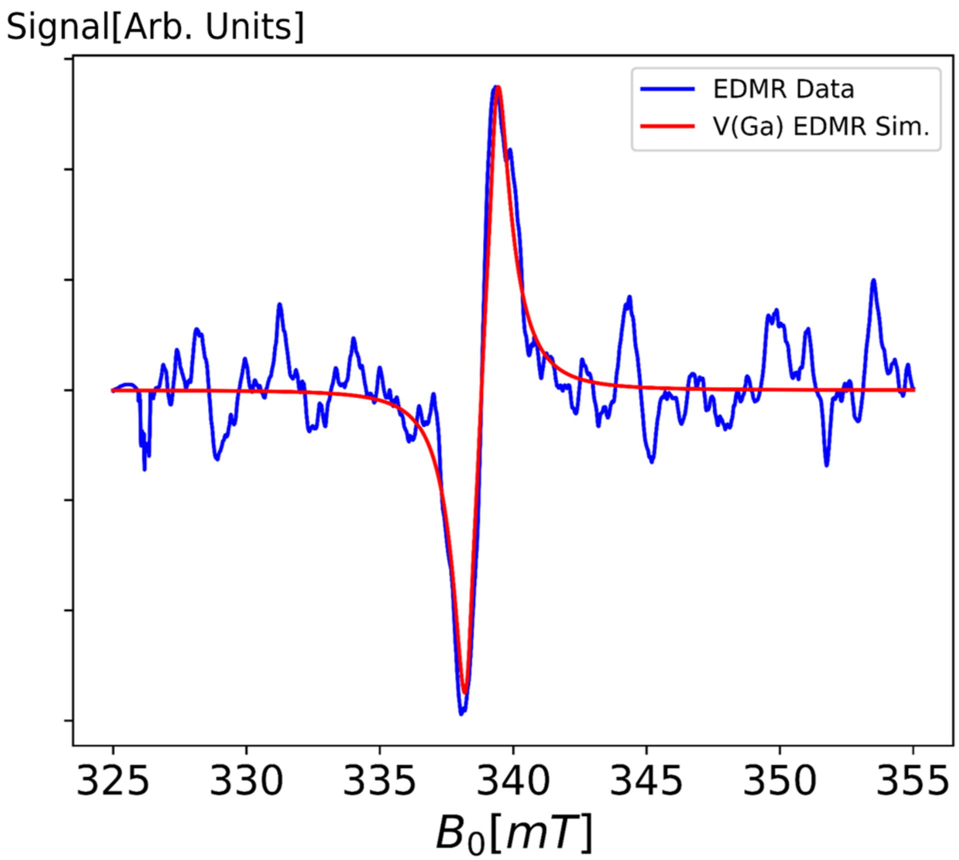
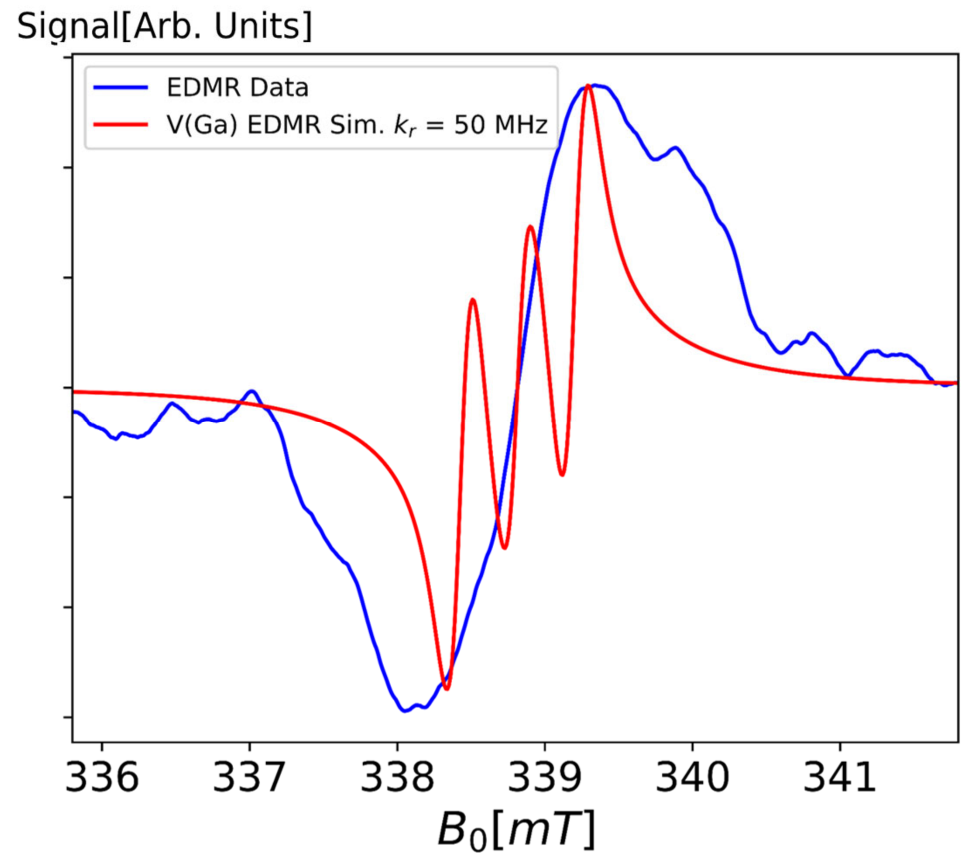
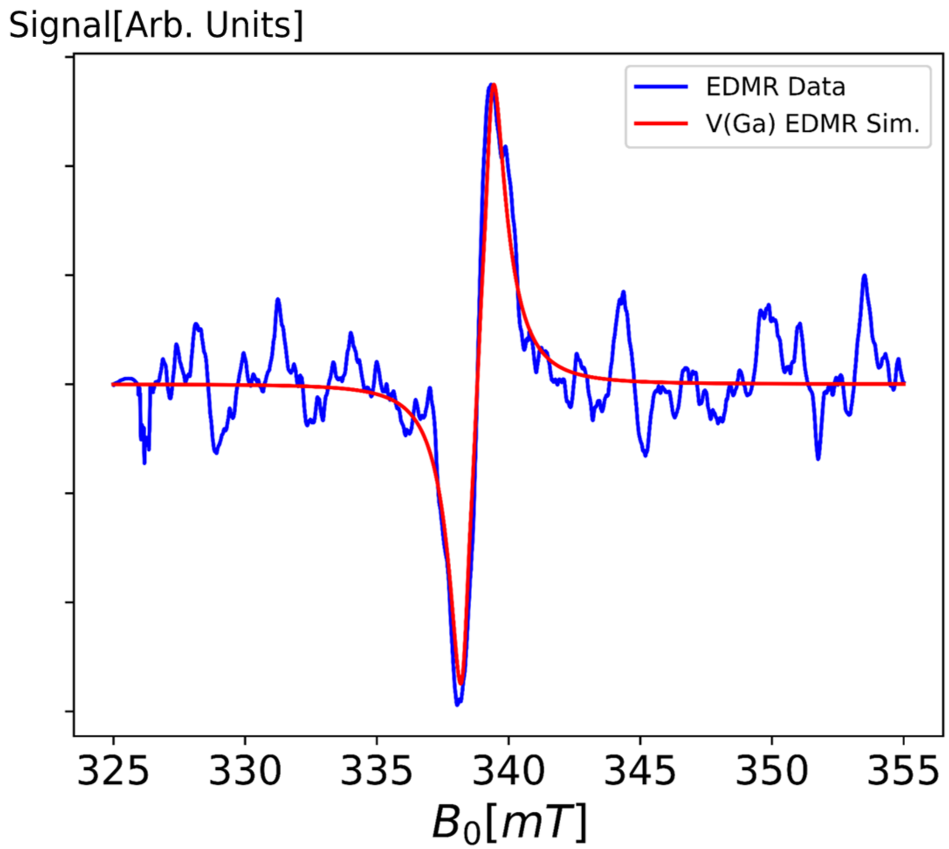
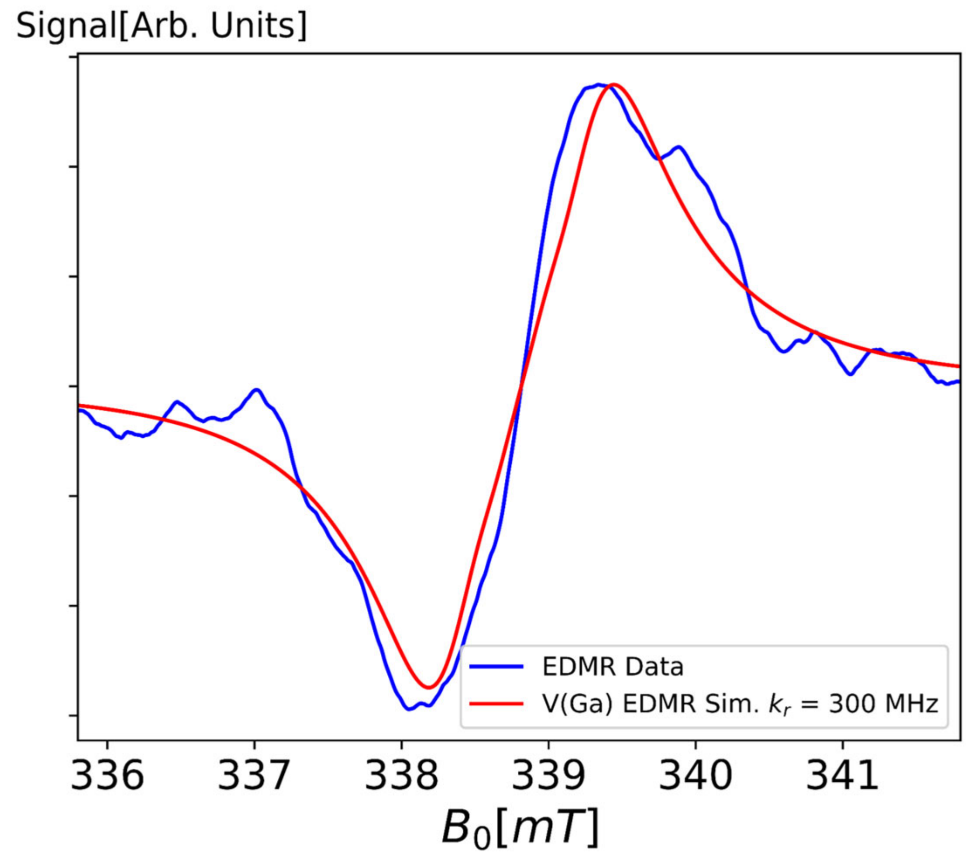
V(Ga) EDMR - Varying Recombination Rate



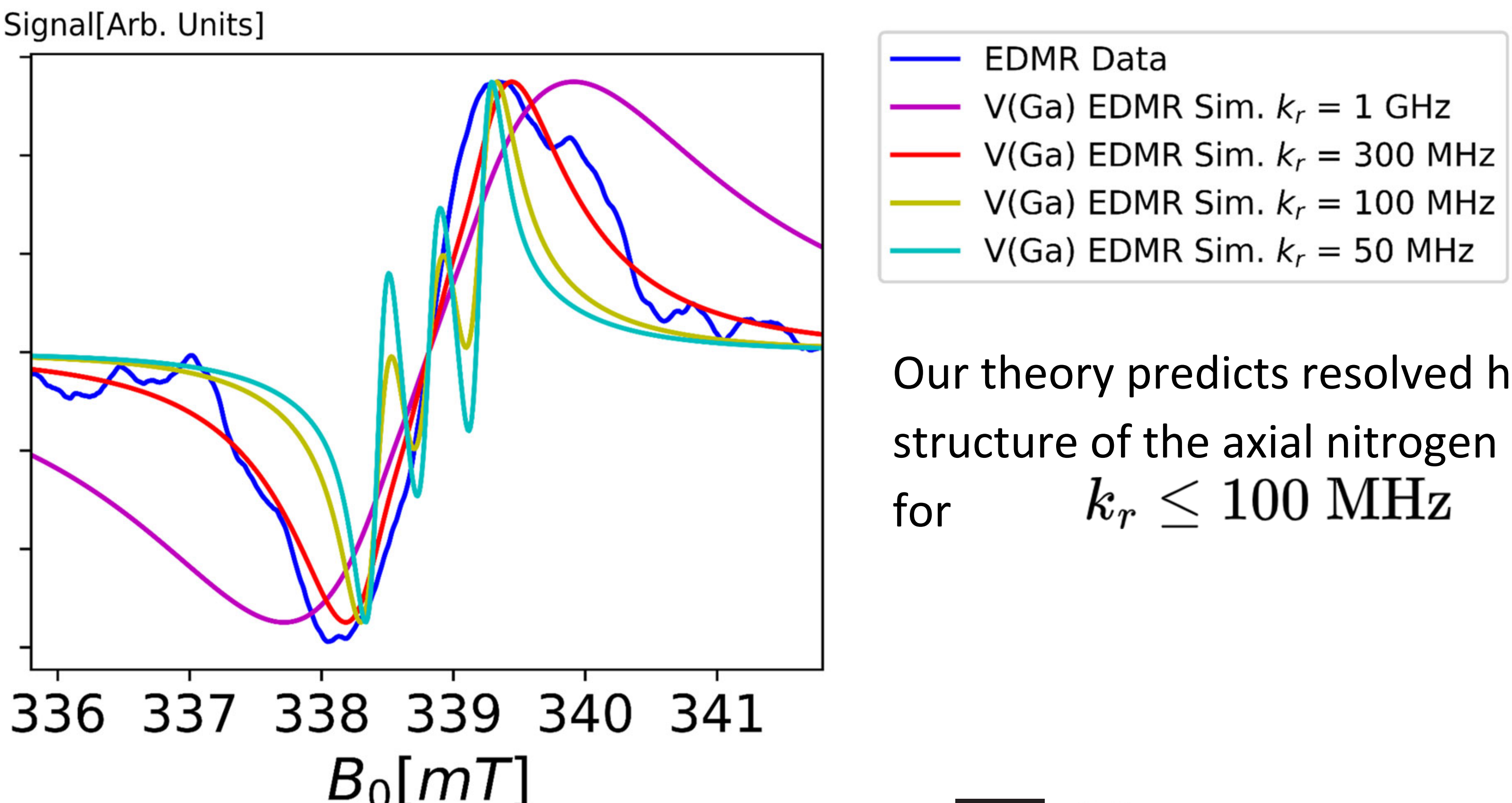


V(Ga) EDMR - Varying Recombination Rate



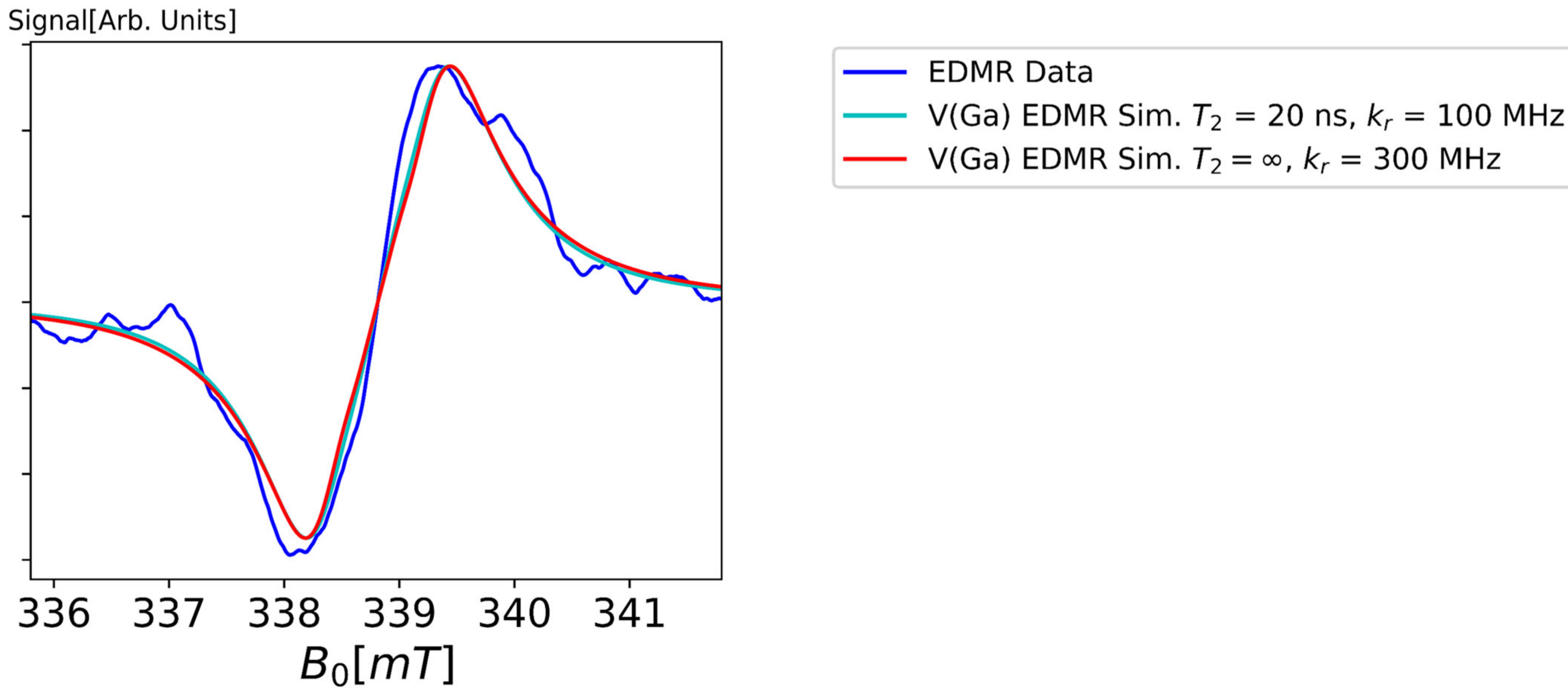


V(Ga) EDMR - Varying Recombination Rate



Our theory predicts resolved hyperfine structure of the axial nitrogen nuclear spin for $k_r \leq 100\ \mathrm{MHz}$

V(Ga) EDMR T_2 versus k_r

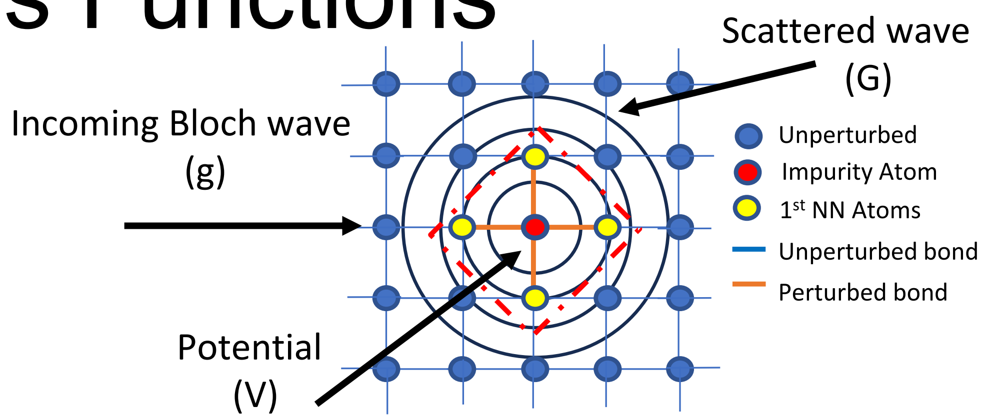


Tight-Binding Green's Functions

Want solution to

$$[\hat{H}_{Bulk}+\hat{V}']\psi = E\psi$$

This can be solved efficiently as a scattering problem[1-3]

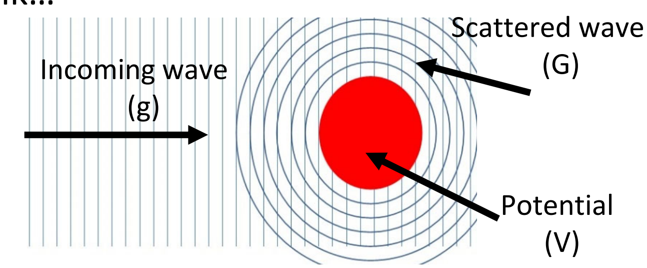


Dyson Eq.: $\hat{G} = \left(1 - \hat{g}\hat{V}'\right)^{-1}\hat{g}$

where,

$$\hat{g}(\delta\boldsymbol{R};\omega) = \int_{BZ} d^3k\,\left[\omega - \hat{H}(\boldsymbol{k})\right]^{-1} e^{i\boldsymbol{k}\cdot\delta\boldsymbol{R}}$$

Think…



Observables

LDOS $\eta(\boldsymbol{R},\omega) = \frac{-1}{\pi} Im\left[Tr\left[\hat{G}(\boldsymbol{R},\boldsymbol{R};\omega)\right]\right]$

Isotropic Hyperfine $\left\langle \hat{A}_{iso}\right\rangle_{\omega} = \frac{-1}{\pi}\frac{8\pi}{3} A_0 |\psi_s(0)|^2 \hat{G}_{s,s}(\omega)$

Anisotropic Hyperfine $\langle \hat{A}_{\,ij}\rangle_{\omega} = \frac{-1}{\pi} Im\left[Tr\left[\hat{G}(\omega) A_0 \hat{r}^{-3}\hat{Q}_{ij}\right]\right]$

[1]Koster/Slater PR 95, 1167 1954
[2]Hjalmarson et al. PRL. 44, 810 1980
[3]Tang/Flatté PRL 92, 047201 2004
[4]A. Koh and D. Miller, Atom. and Nuc. Data 33, 235 (1985)

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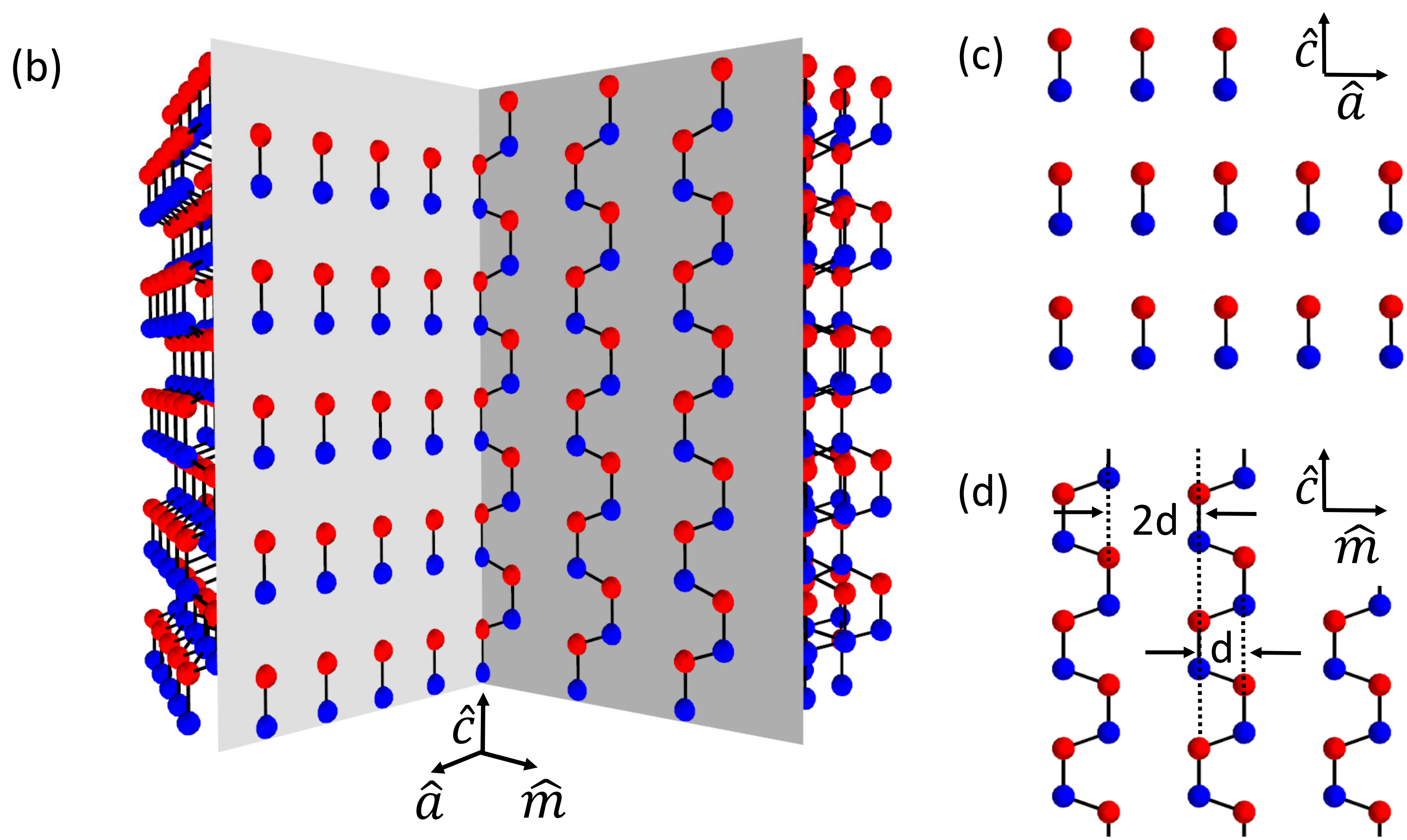

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Observables

$$\langle \hat{O} \rangle_\omega = \frac{-1}{\pi} Im \left[Tr \left[\hat{G}(\omega) \hat{O} \right] \right]$$

$$\hat{A}_{iso} = \frac{8\pi}{3} A_0 \sum_{\beta, \alpha = s} |\beta\rangle\langle\beta| \delta(\mathbf{r} - \mathbf{R}_q)$$

$$\hat{A}_{ij} = A_0 \frac{\hat{Q}_{ij}^{(2)}}{r^3}$$

$$\hat{Q}_{ij}^{(2)} = 3\hat{r}_i \hat{r}_j - \delta_{ij}$$

$$A_0 = g_s g_N \mu_0 \mu_B \mu_N / 4\pi \langle S_z \rangle$$

$$\eta(\mathbf{R}, \omega) = \frac{-1}{\pi} Im[Tr[\hat{G}(\mathbf{R}, \mathbf{R}; \omega)]]$$

$$\langle \hat{A}_{iso} \rangle_\omega = \frac{-8}{3} A_0 \sum_q Im[Tr[G_{s,s}(\mathbf{R}_q, \mathbf{R}_q, \omega)]]$$

$$\langle A_{ij} \rangle_\omega = \frac{-1}{\pi} Im \left[\sum_{\beta, \beta'} A_0^\beta G_{\beta', \beta}(\omega) \langle r^{-3} \rangle_{\beta', \beta} \langle \hat{Q}_{ij} \rangle_{\beta' \beta} \right]$$

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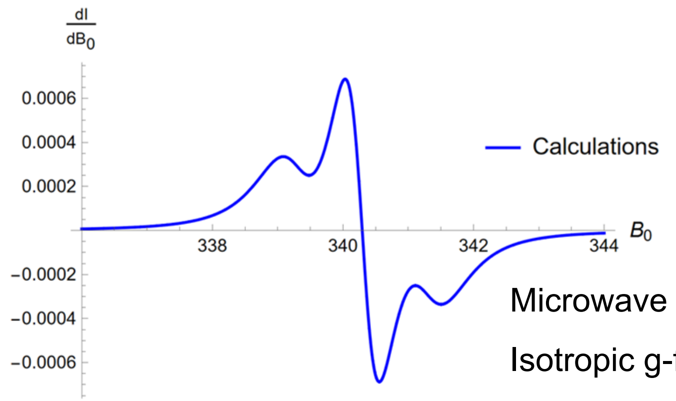
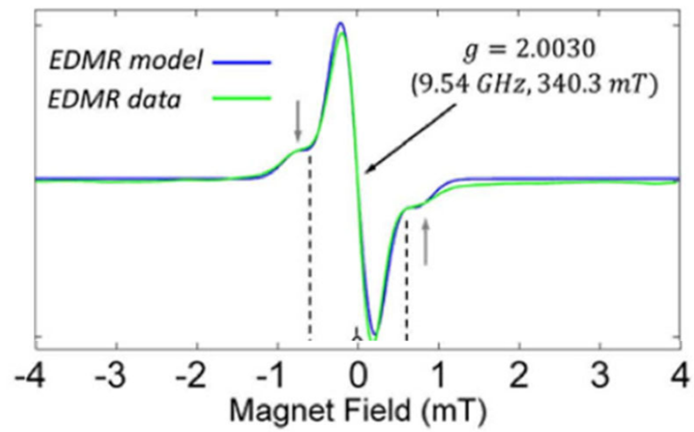
EDMR V_{Si}^{0} (S=1) in 4H-SiC Simulation Results



Microwave Frequency: 9.54 GHz

Isotropic g-factor: 2.003



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Extracted Paramters:

- Axial Zero Field Splitting: $2\mathrm{D} = 57$ MHz
- Microwave B field strength: 0.1 mT
- $T_{2,d}^{*} \sim 25$ ns

Code is validated for these effects

The challenge of EDMR in GaN: large numbers of high-spin magnetic nuclei

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Timeline and Milestones: Year 1

(1) Simulation of nitrogen vacancies in GaN and their effect on EDMR and NZFMR. The nitrogen vacancies are spin ½ shallow donor states with known g tensors, and are likely radiation-induced defects.

(2) Commencement of the AC bias simulations of spin-dependent trap-assisted tunneling (SDTAT) and spin-dependent recombination (SDR) currents. Defect parameters will be taken from the literature, and from Tuttle and Jin as their calculations become available.

Milestone: EDMR and NZFMR magnetic-field-dependent curves for N vacancies a range of device bias for GaN leakage currents.

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Timeline and Milestones: Year 2

(1) Simulation of Ga antisite defects in GaN and their effect on EDMR and NZFMR. These defects have been calculated to have several mid-gap states, but little is known experimentally about these levels and their spin configuration. These are also likely radiation-induced defects.

(2) Completion of AC bias simulation formalism and test calculations of SDTAT and SDR. Inferences on what structures may make devices less sensitive to radiation.

Milestone: EDMR and NZFMR magnetic-field-dependent curves for Ga antisite defects for a range of device bias for GaN leakage currents. Results for AC bias simulations of SDTAT and SDR and input back into device design.

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