(Spin Dependent Variable Range Hopping and) Spin Dependent Charge Pumping in Metal-Insulator-Semiconductor Systems

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This work involved the collaboration of many other, including

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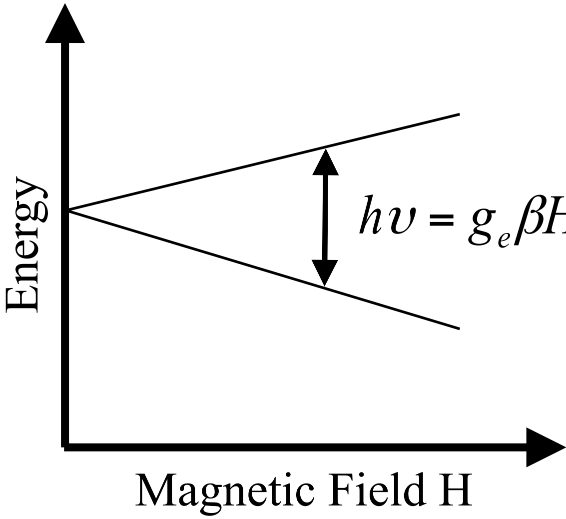
Penn State work supported by: US Army Research Laboratory and NIST

EPR

- The most powerful analytical tool for the study of point defects in semiconductors (and insulators) is Electron Paramagnetic Resonance (EPR)
- Electrically Detected Magnetic Resonance (EDMR) has the analytical power of EPR plus enormously enhanced sensitivity and the capability for exclusive sensitivity to defects directly involved in the electronic behavior in semiconductor devices

EPR: Isolated (free) Electron



An unpaired electron at a paramagnetic site in a device:

In relatively simple cases this expression is modified:

g tensor: g_e becomes a tensor: g_e altered by spin orbit coupling

A tensor: electron interacts with nearby magnetic nuclei

Examples

Si ≈ 4.7% spin ½

C ≈ 1.1% spin ½

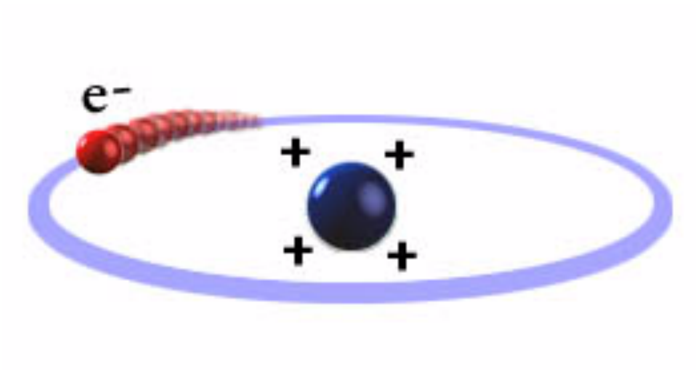
N ≈ 100% spin 1

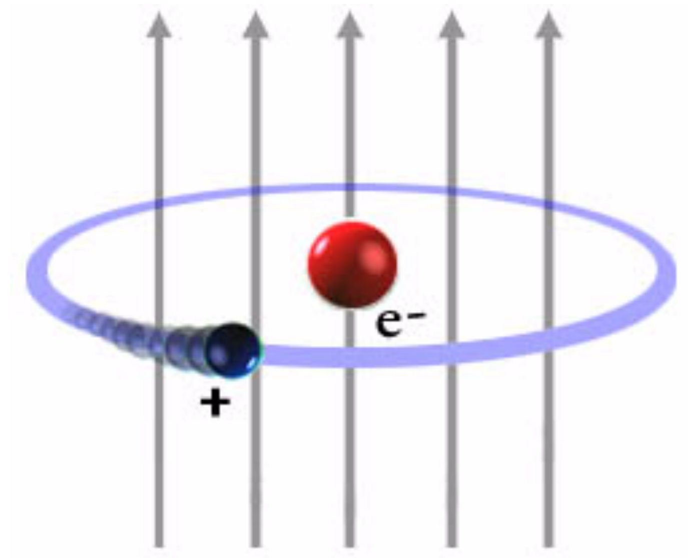
O ≈ 0%

H ≈ 100% spin 1/2

$$g_e = 2.0023219 \quad h\upsilon = g\beta H + M_I A$$

Spin Orbit Coupling: g tensor



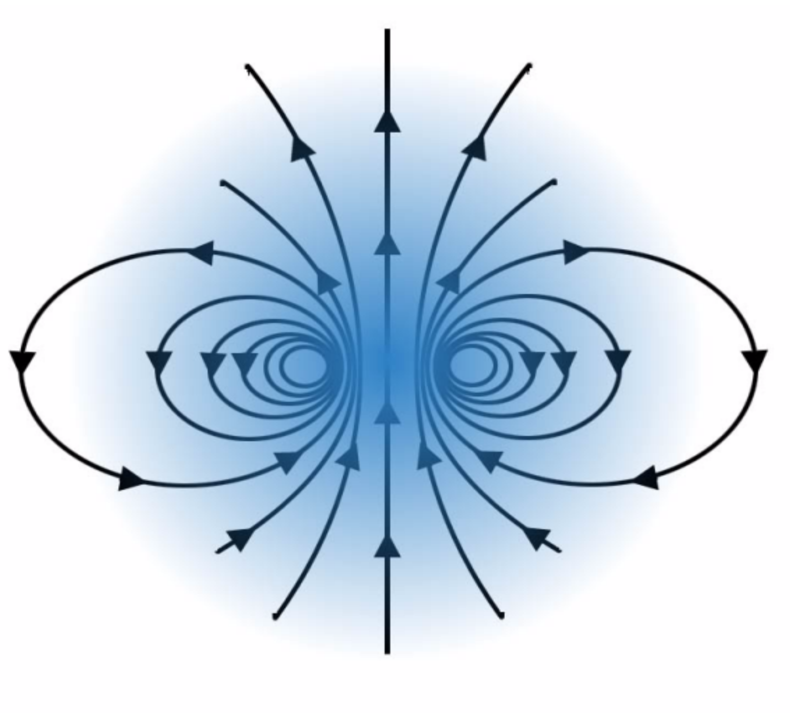


The greater the nuclear charge and orbital angular momentum quantum number, the greater the spin orbit coupling.

The g tensor deviates from the free electron value because of spin orbit coupling.

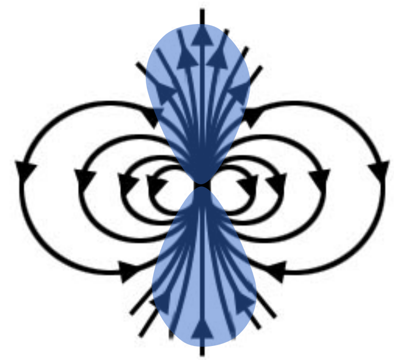
Electron-Nuclear Hyperfine Interactions

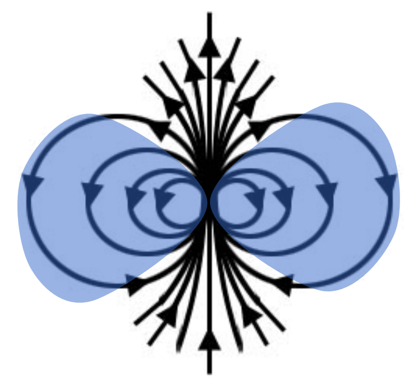
Interactions with (isotropic) s-orbital electrons and interactions with p-orbital electrons



$$A_{iso} = \frac{8}{3}\pi\left|\alpha(0)\right|^2 g_N\beta_N$$

4/5 $g_N b_N$ár^{3}ñ$^{-1}$ = 2b





-2/5 $g_N b_N$ár^{3}ñ$^{-1}$ = -b

Electrically Detected Magnetic Resonance (EDMR)

Conventional EPR has a sensitivity of about 10^{10} total paramagnetic defects
It is also sensitive to ALL paramagnetic defects in a sample

1. We want to identify defects in *transistors*
2. We want to know what different defects do to device performance

A main problem for electronic materials science is performing resonance inside fully processed transistors in integrated circuits

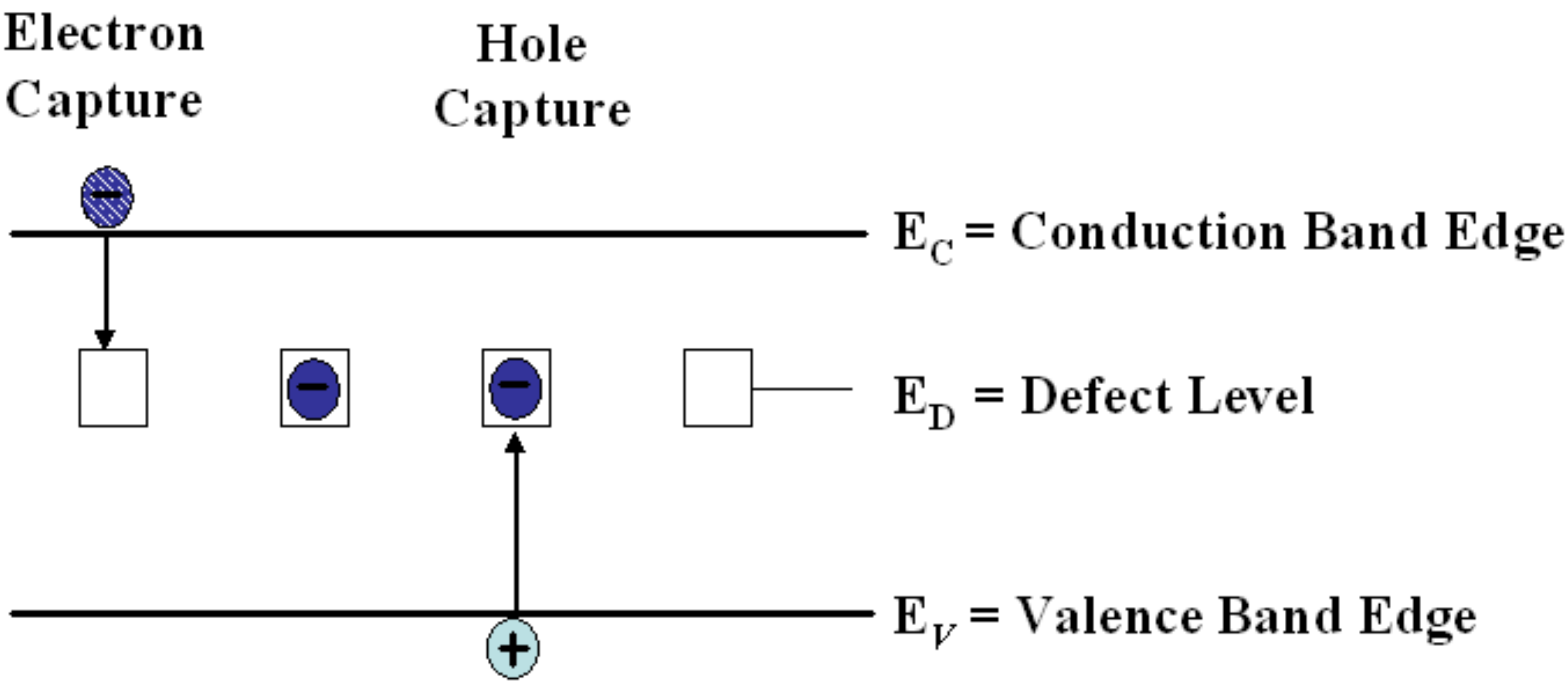
EDMR provides sensitivity about **7 orders of magnitude higher** than conventional EPR

<u>Solution</u>: EDMR, spin dependent recombination (SDR), and a new approach spin dependent charge pumping (SDCP)

Electrically Detected Magnetic Resonance (EDMR)

Spin Dependent Recombination (SDR)

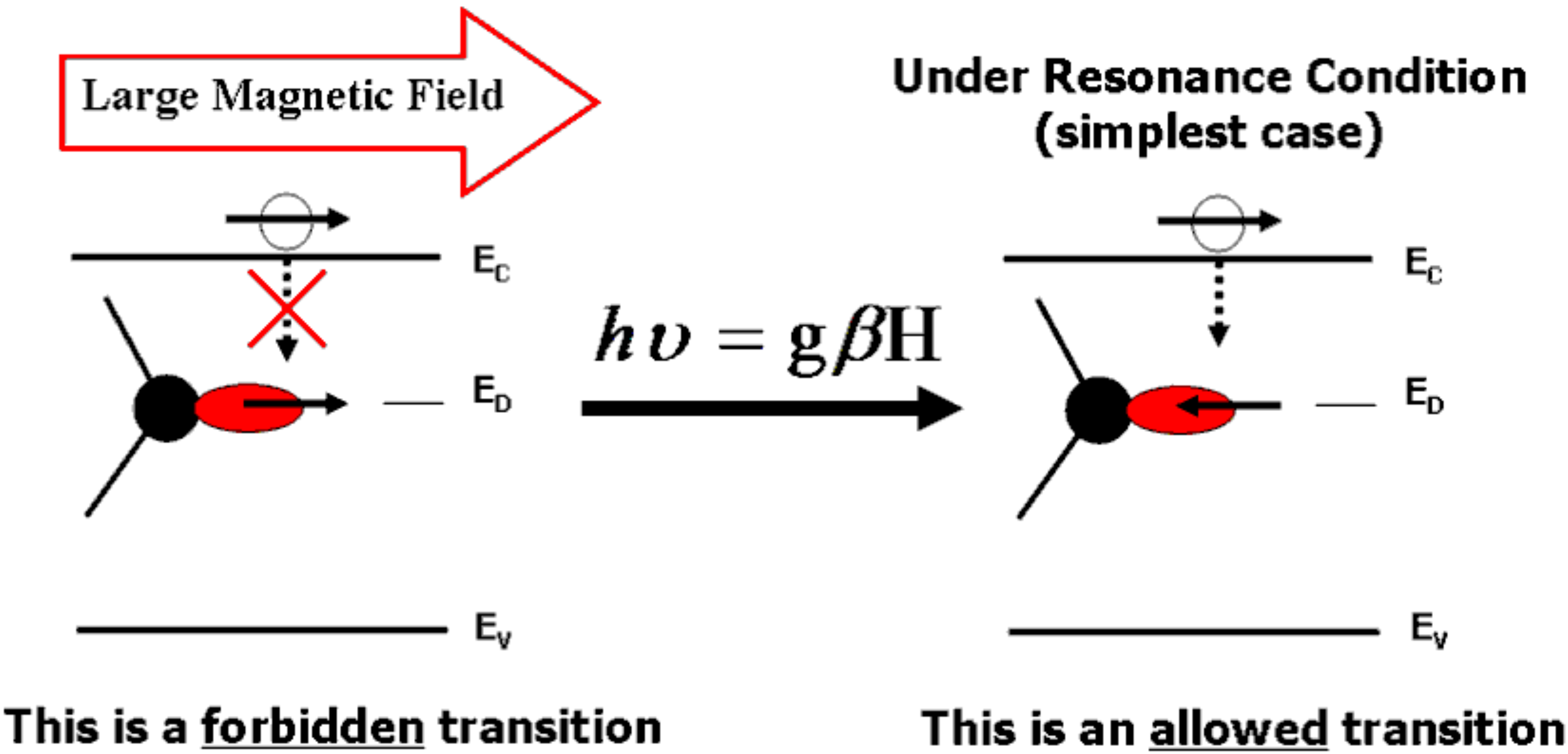
<u>Shockley-Read-Hall Model</u>



Electrically Detected Magnetic Resonance (EDMR)

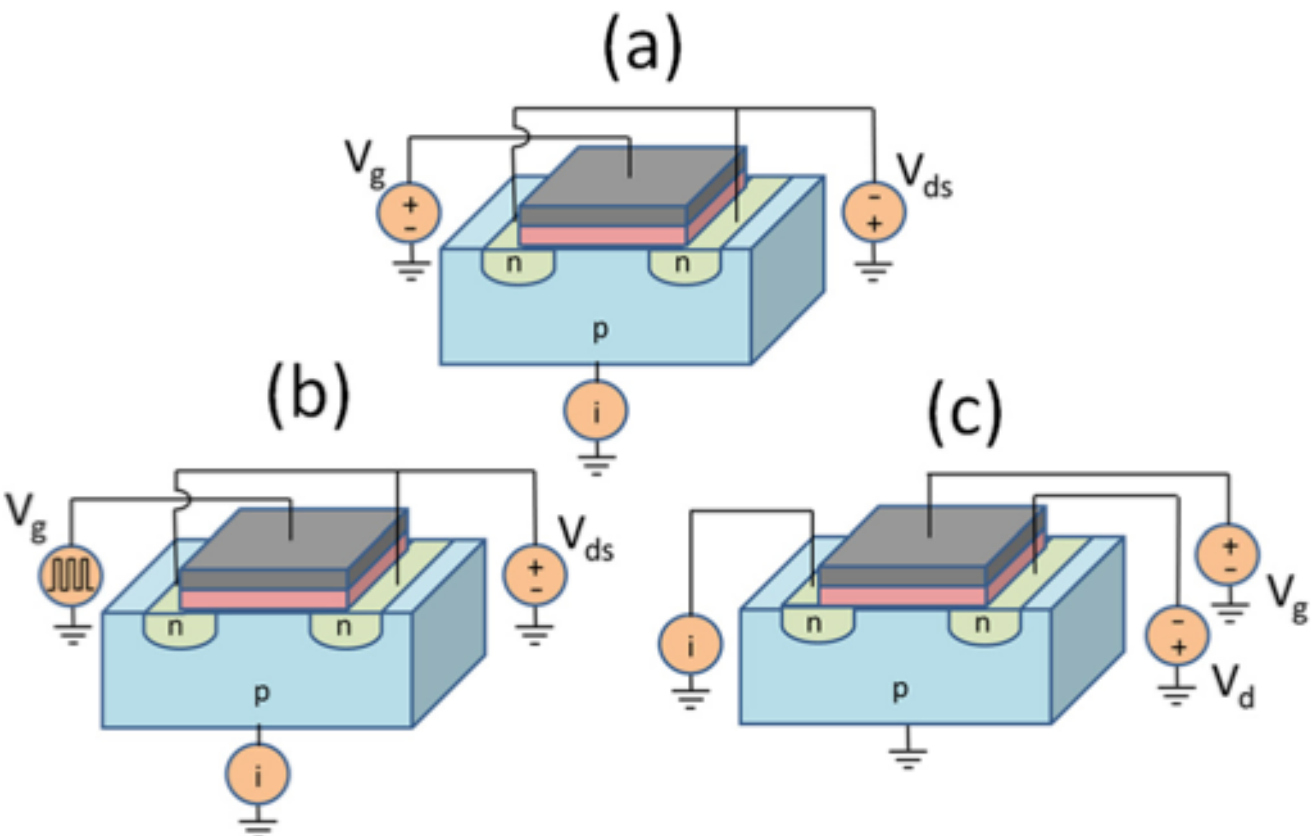
Spin Dependent Recombination (SDR)

Pauli Exclusion Principle

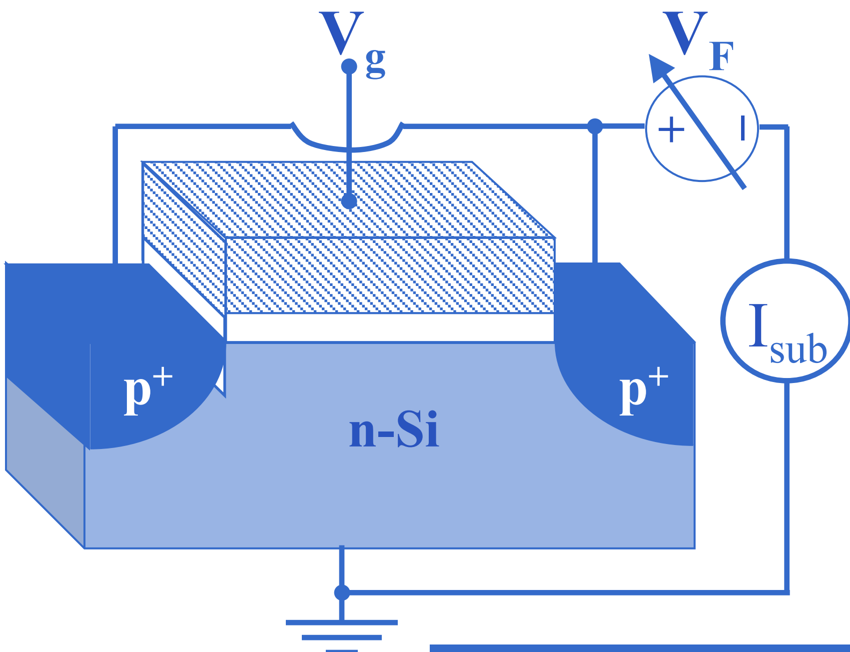


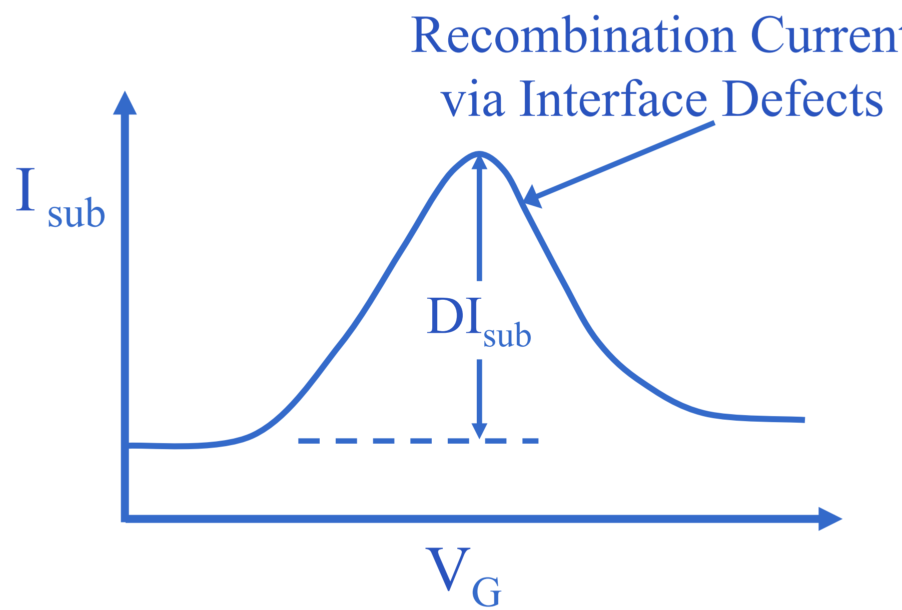
EDMR Schemes for MOSFETs

a) DCIV
b) Spin-Dependent Charge Pumping
c) Bipolar Amplification Effect



DC-IV/Gate-Controlled Diode Measurement





$$\Delta I_{SUB} = \frac{1}{2} A_G q n_i \sigma v_{th} D_{it} q V_F \exp\left(\frac{qV_F}{2kT}\right)$$

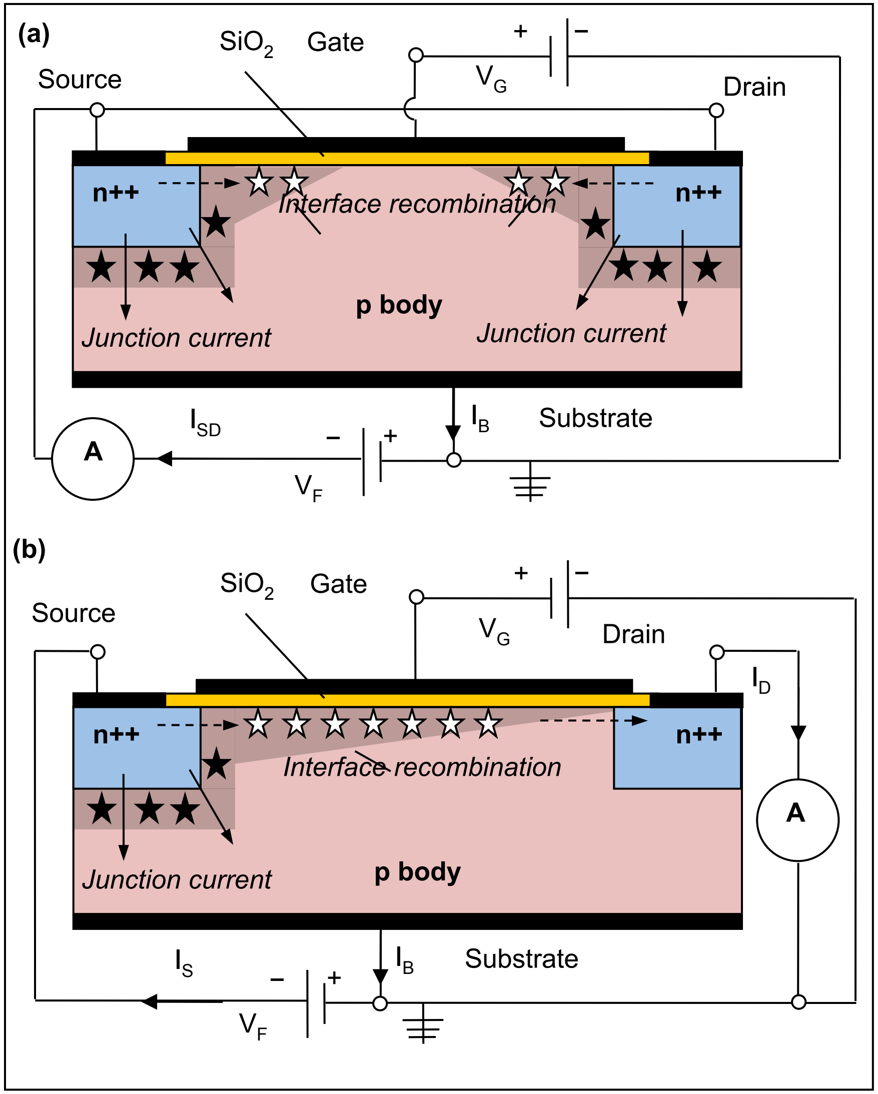
Sensitive to interface defects within ~(q|V_F|)

V_F controls the recombination energy window

Fitzgerald *et al.,* Surf. Sci. (1968), Neugroschel, *et al.*, IEEE TED, (1995)

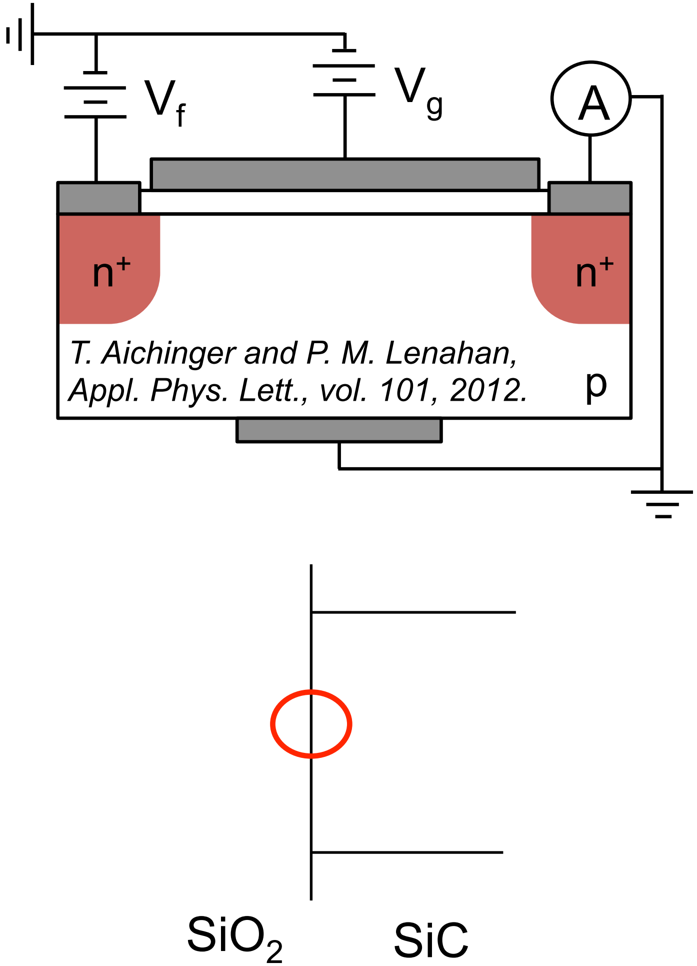
Bipolar Amplification Effect (BAE)

The method (i) greatly amplifies the spin dependent fraction of the investigated transistor current and (ii) concentrates the sensitivity to exclusively the semiconductor-insulator interface.

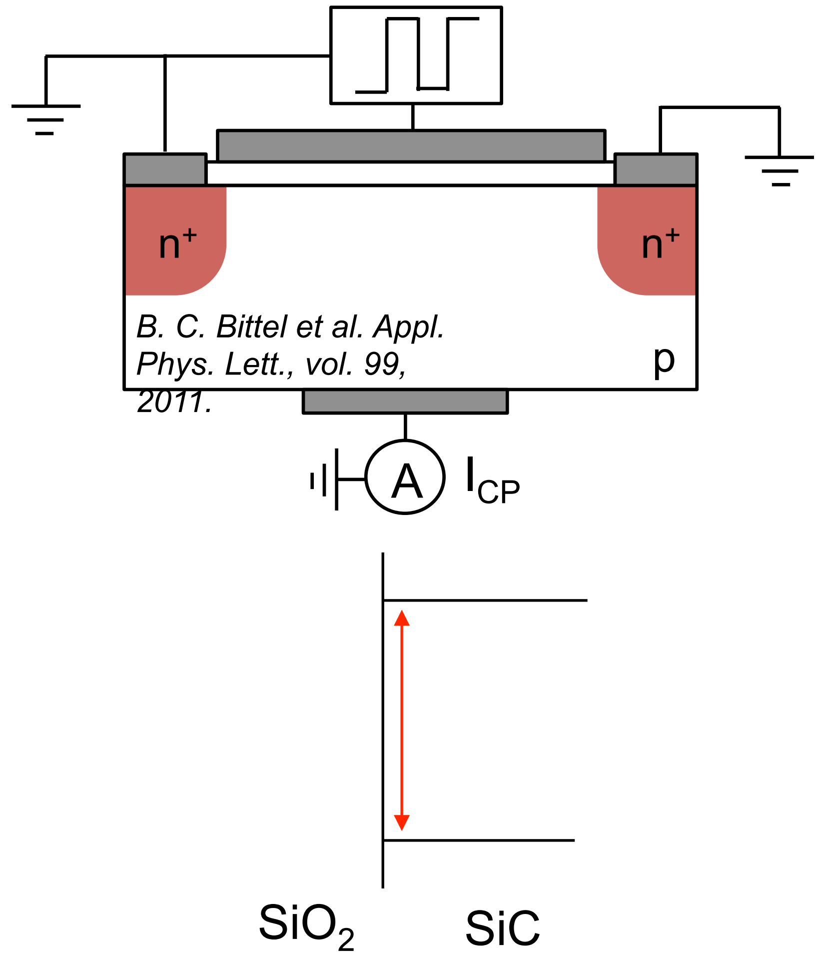


SDCP vs SDR (DCIV/BAE)

BAE

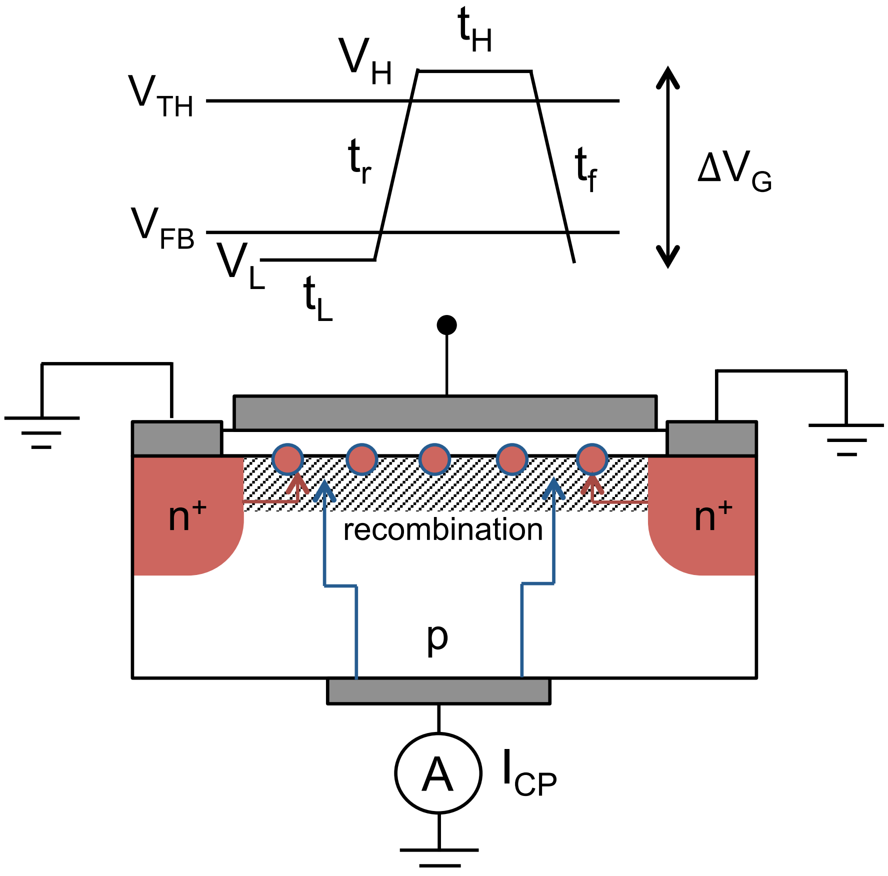


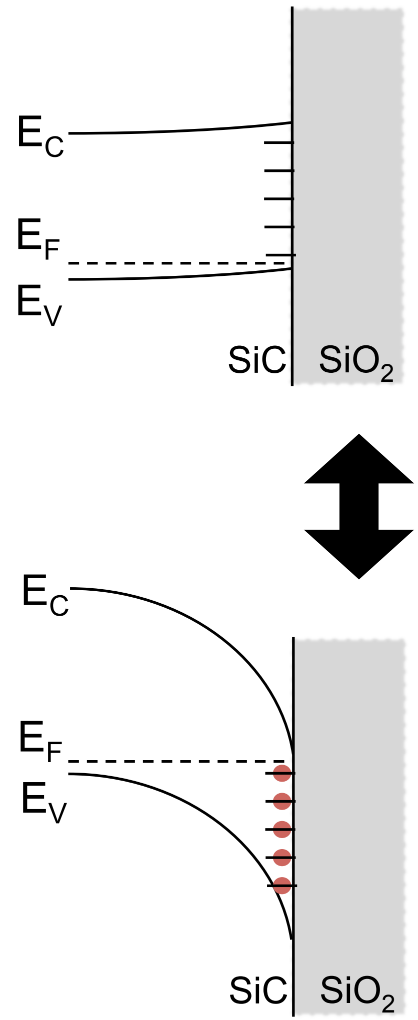
SDCP



- Large improvement in sensitivity over BAE

Charge Pumping Basics



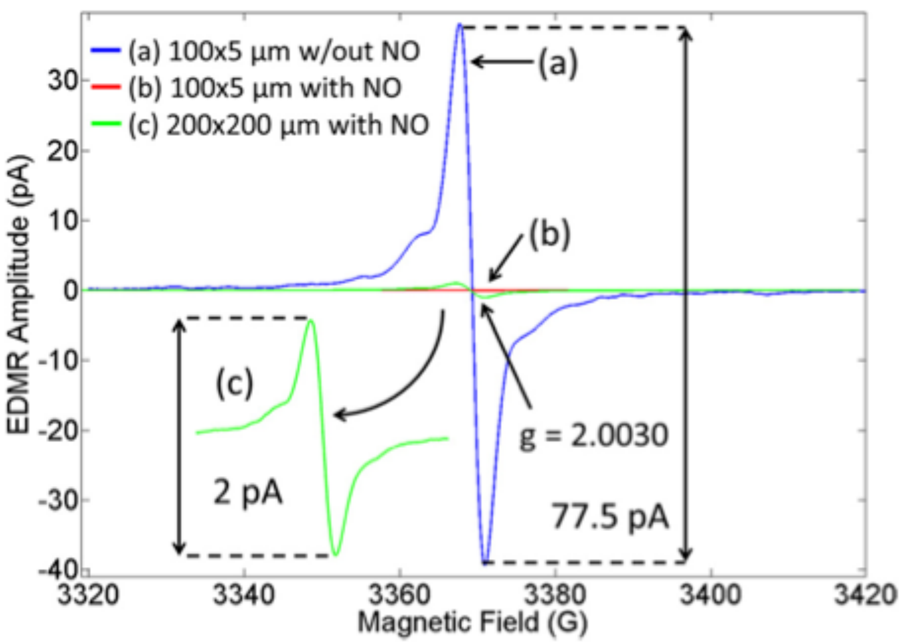


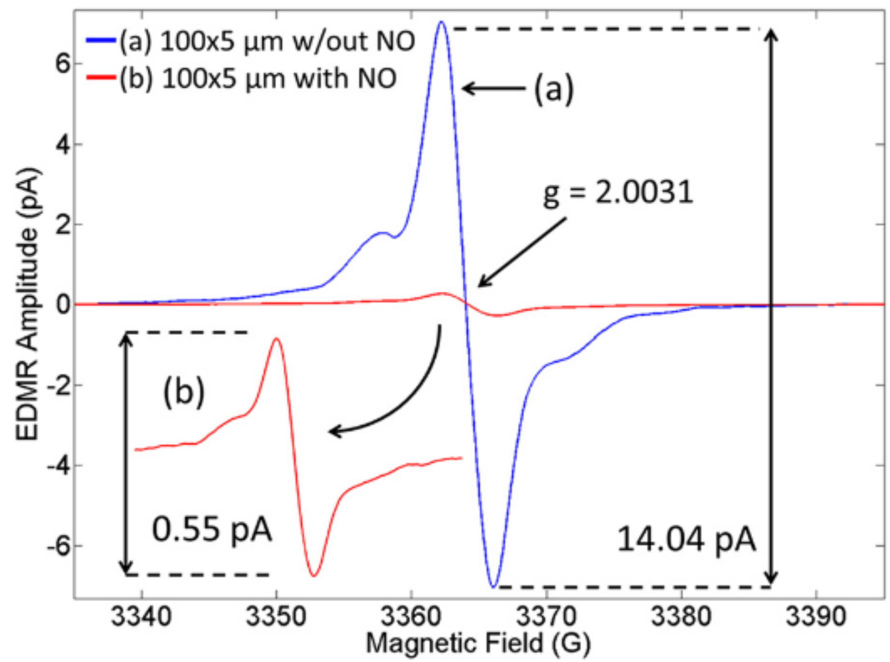
J. S. Jespers and P. G. A. Brugler, IEEE Trans. Electron Dev., vol. 16, 1969.
G. Groeseneken et al., IEEE Trans. Electron Dev., vol. 31, 1984.

High sensitivity and access to nearly the whole band gap

- SDCP's higher sensitivity and near full band gap access allows us to:
  - rule out the presence of some defects
  - explore very nearly the entire band gap

BAE and SDCP: NO/no NO from "Better" 4H-SiC nMOSFETs



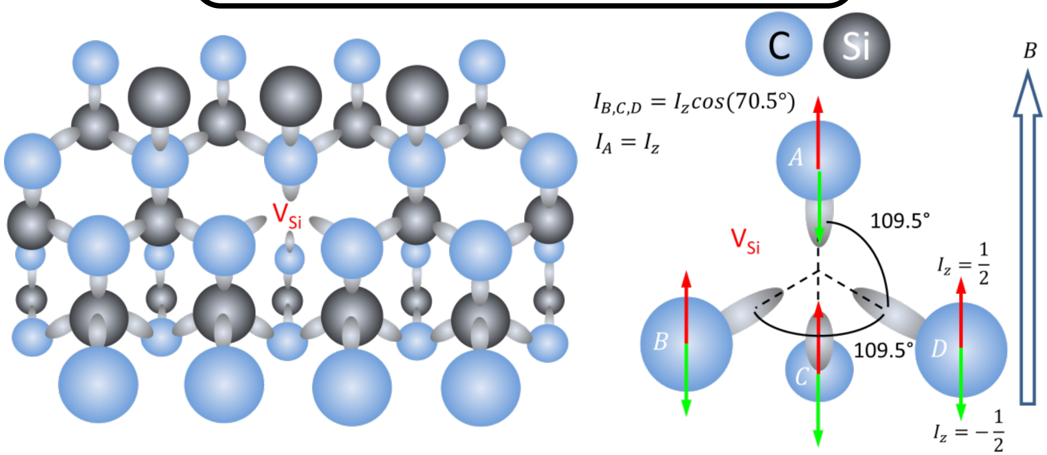


C. J. Cochrane *et al.,* Appl. Phys. Lett.**102**,193507 (2013).

Near Interface Trap: V_{Si}

Using the natural abundances of ^{29}Si (4.7%) and ^{13}C (1.1%) standard first order perturbation theory, yield this spectrum with **B||c** .

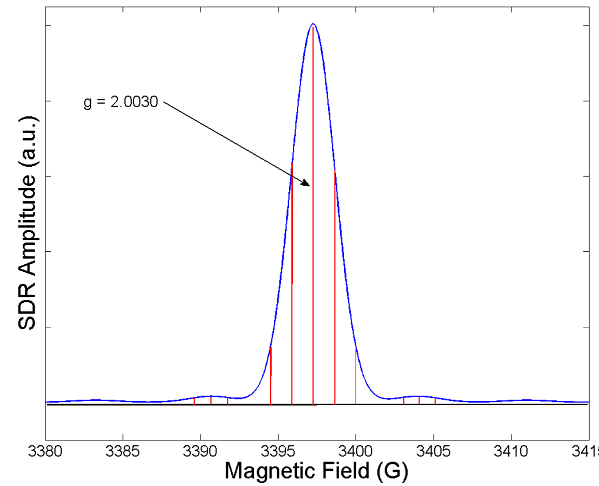
Si: A_{iso} = 2.96 G for V_{si}^{-} (I) and V_{si}^{-} (II)
C: V_{si}^{-} (I): A_x = 27.35 G, A_y = A_z= 10.1 G
C: V_{si}^{-} (II): A_x = 28.36 G, A_y =A_z = 11.1 G

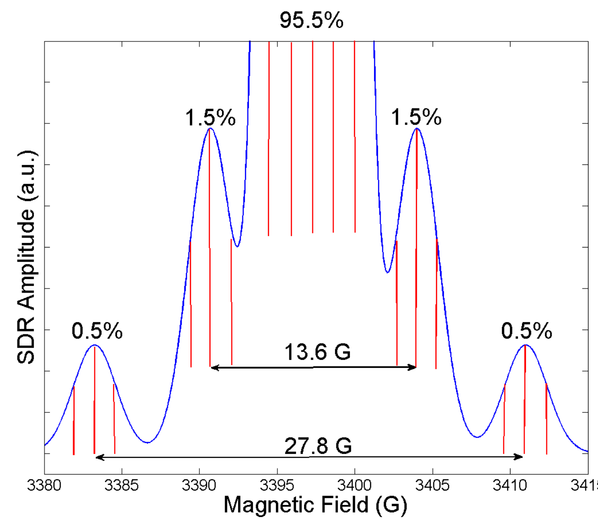


$R = \#\ of\ NN\ Si^{28}\ atoms,\ r = \#\ of\ NN\ Si^{29}\ atoms,\ p_{Si^{29}} = probability\ of\ Si^{29}$

$S = \#\ of\ NN\ C^{12}\ atoms,\ s = \#\ of\ NN\ C^{13}\ atoms,\ p_{C^{13}} = probability\ of\ C^{13}$

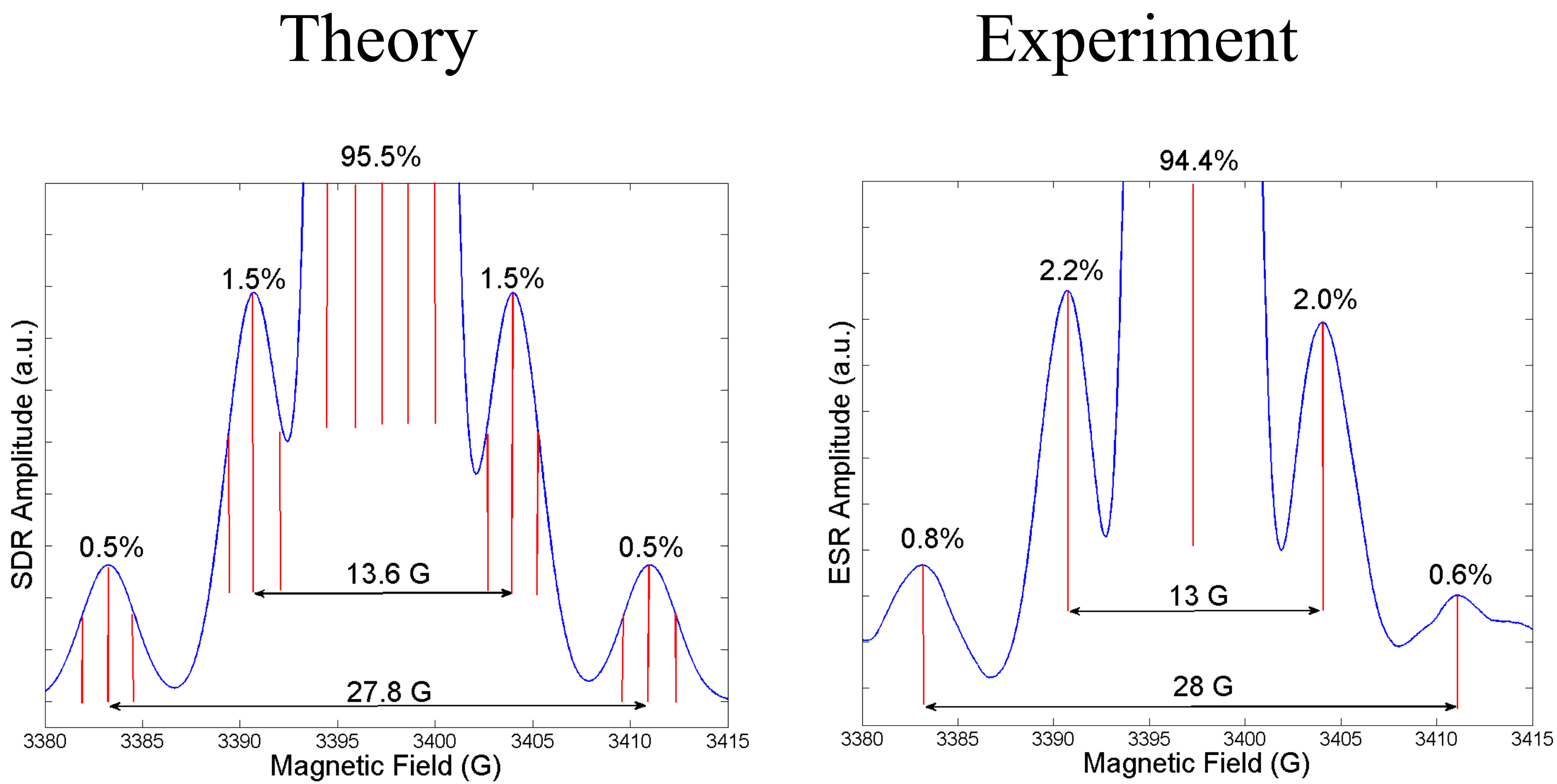
$$P(r\ Si^{29}\ AND\ s\ C^{13}) = \binom{R}{r} p_{Si^{29}}{}^{r} (1 - p_{Si^{29}})^{R-r} \cdot \binom{S}{s} p_{C^{13}}{}^{s} (1 - p_{C^{13}})^{S-s}$$





T. Wimbauer, et. al, Phys. Rev. B. 56, 7384 (1997)
N. Mizuochi, et. al, Phys. Rev. B. 66, 235202 (2002)
J. Isoya, et. al, Phys. Stat. Sol. (b) 245, No. 7, 1298-1314 (2008)

Near Interface Trap: V_{Si}^{-} Theory vs. Experiment



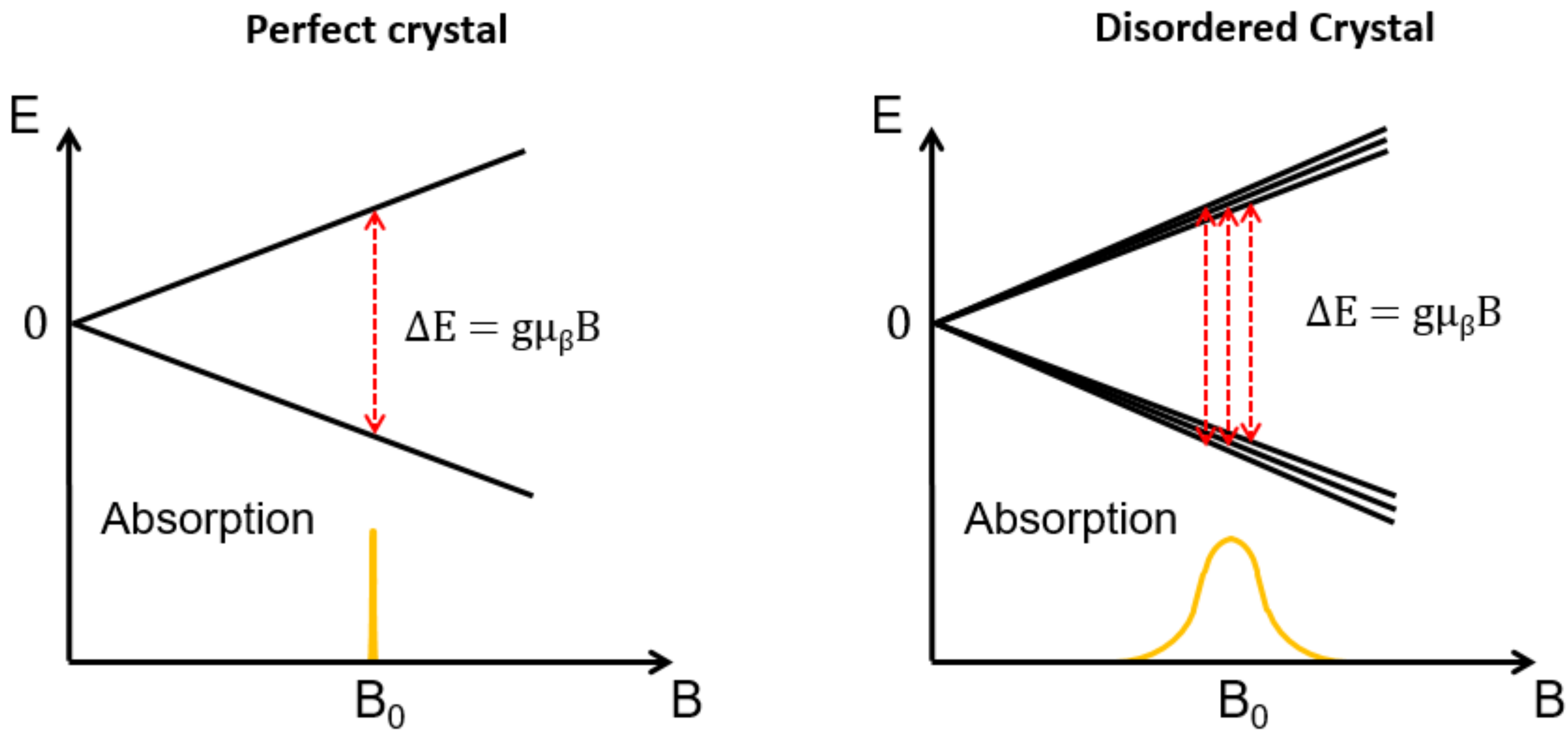
C.J. Cochrane, P.M. Lenahan, A.J. Lelis, Appl. Phys. Lett. 100, 023509 (2012)

What else is going on at the 4H-SiC/SiO_2 interface?

Even after the elimination of most of the V_{Si}, the effective channel mobilities remain mediocre

Could EDMR measurements provide additional insight?

Plausibility Argument for Disorder



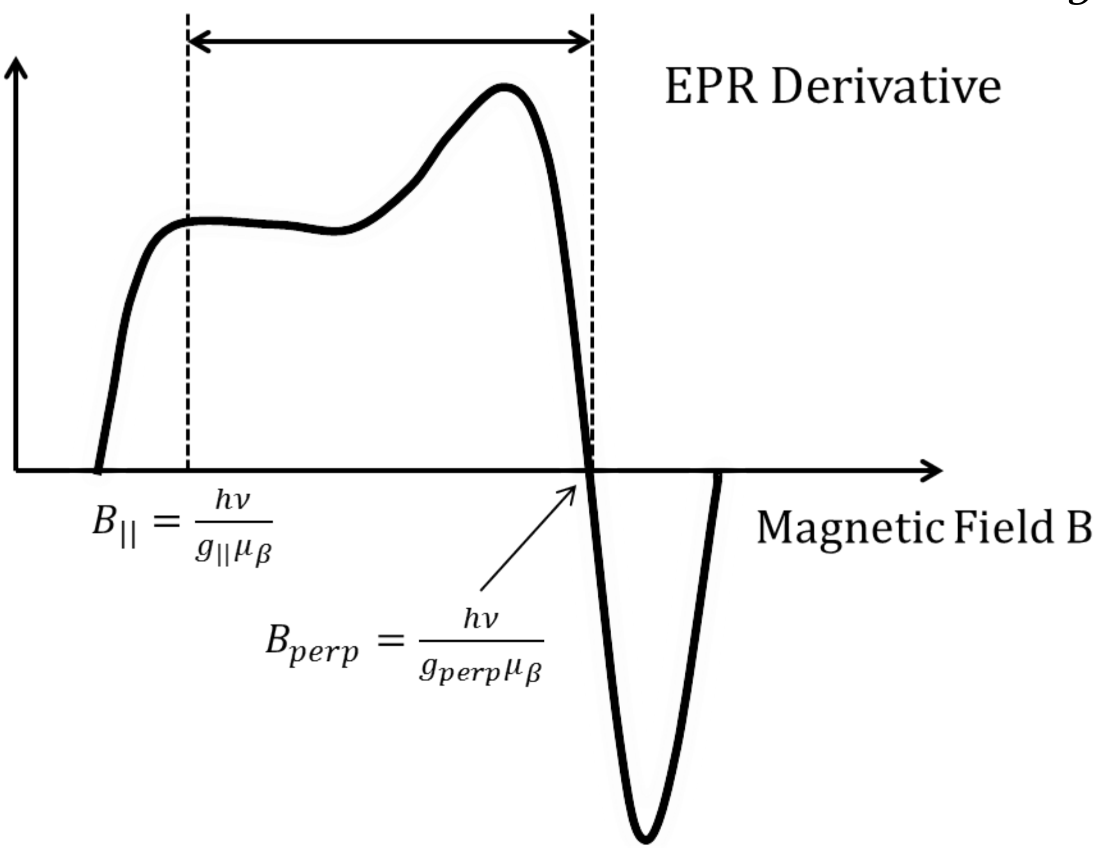
A comparison of EDMR measurements at high and very low frequencies could be a probe of disorder in a highly defective crystalline environment

Plausibility Argument for Disorder

$$\Delta B = \frac{h}{\mu_\beta}\left(\frac{1}{g_{perp}} - \frac{1}{g_{||}}\right)\nu$$

$\Delta B_g \cong \nu[\Delta g]h/4\mu_B$

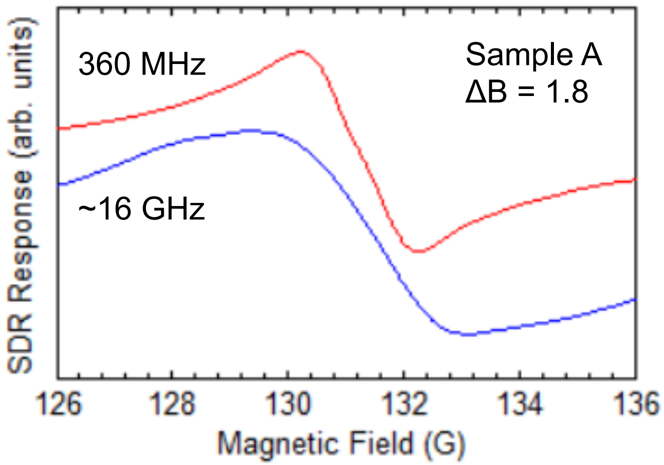
$\Delta B_g \cong \boldsymbol{\nu} * \boldsymbol{\Delta g} * constant$



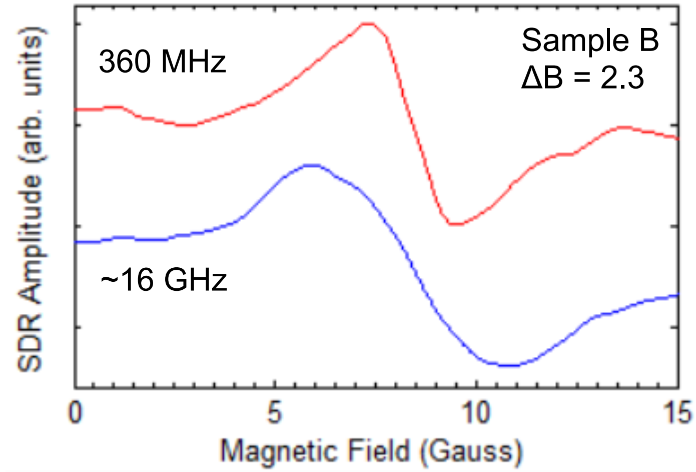
- **If line width is dominated by g, the line width will be proportional to frequency.**

Multi frequency BAE

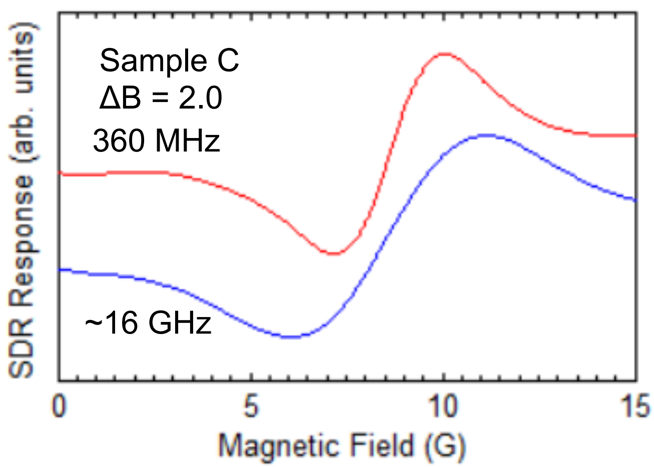
nMOSFET – no NO



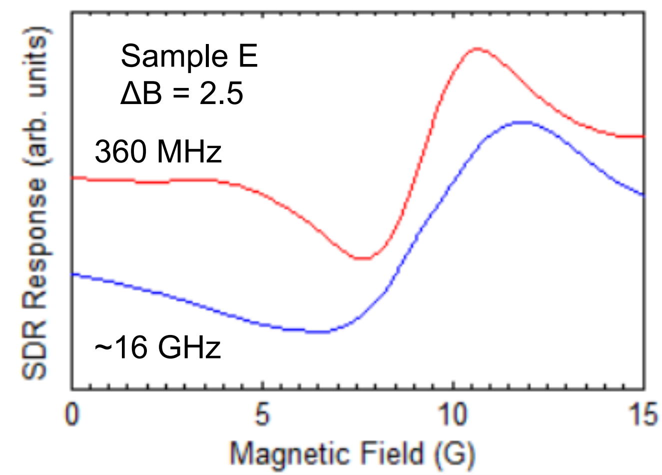
nMOSFET – NO



nMOSFET – NO

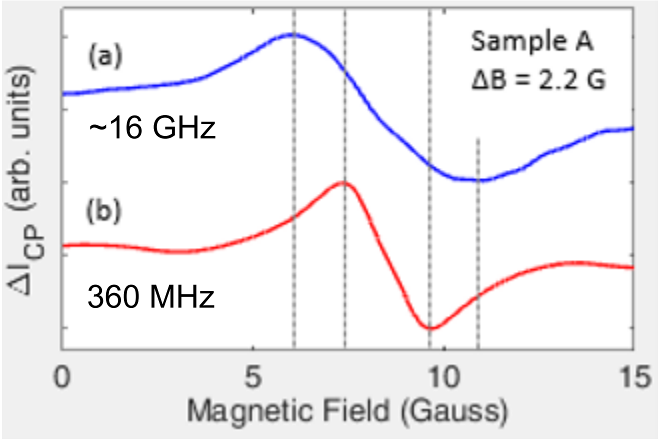


pMOSFET – NO

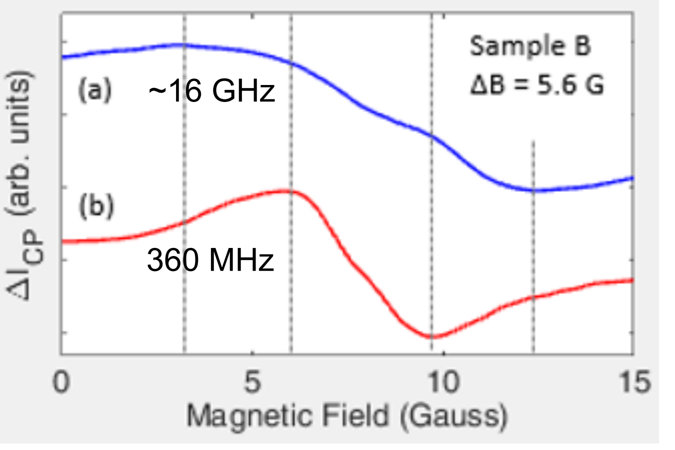


Multi frequency SDCP

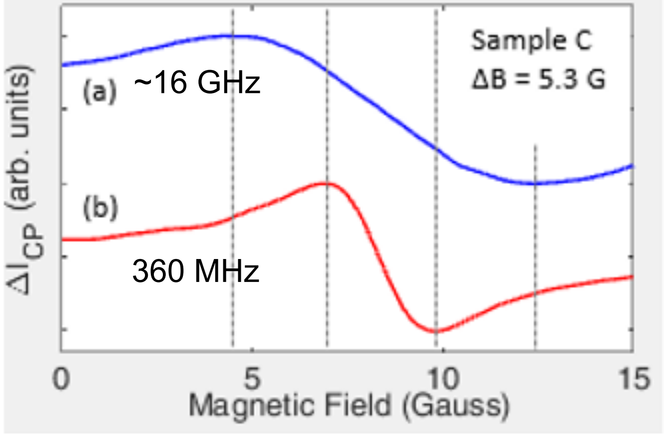
nMOSFET – no NO



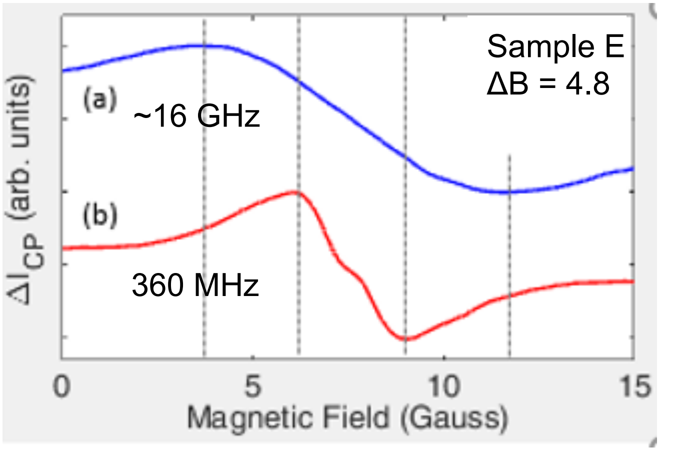
nMOSFET – NO



nMOSFET – NO



pMOSFET – NO



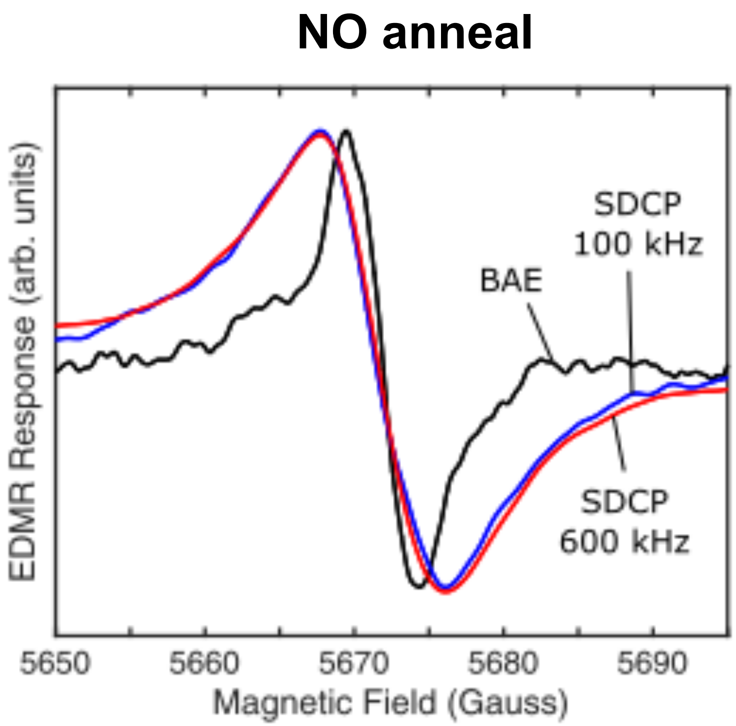
Summary Multi frequency EDMR

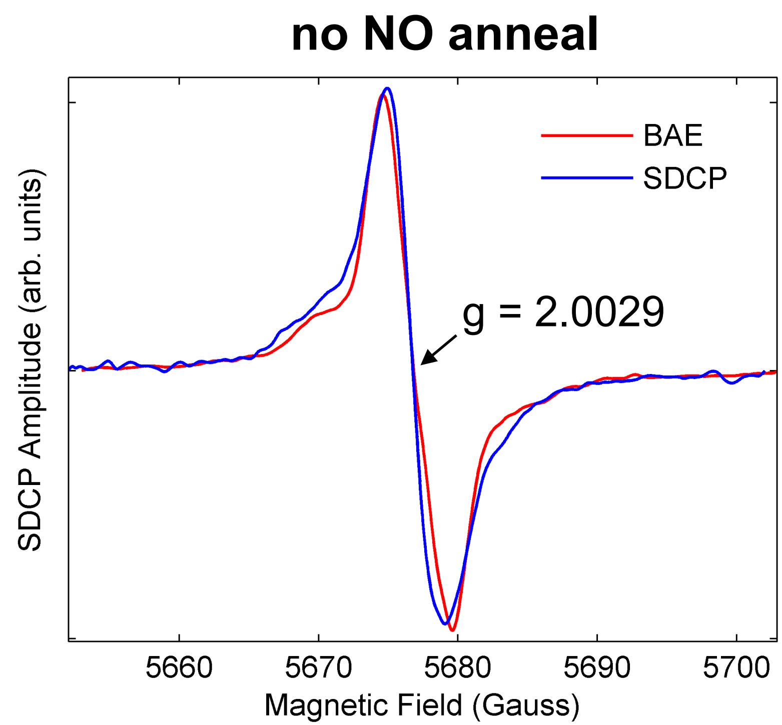
Sample Name	N processing?	ΔB (BAE)	ΔB (SDCP)
A	NO	1.8	2.2
B	YES	2.3	5.6
C	YES	2.0	5.3
E	YES	2.5	4.8

- N creates disorder at interface
- Disorder may limit MOSFET performance
- Consistent with anisotropic strain due to N reported by Dycus *et al.*

J. H. Dycus et al., Appl. Phys. Lett., vol. 108, 201607 (2016)

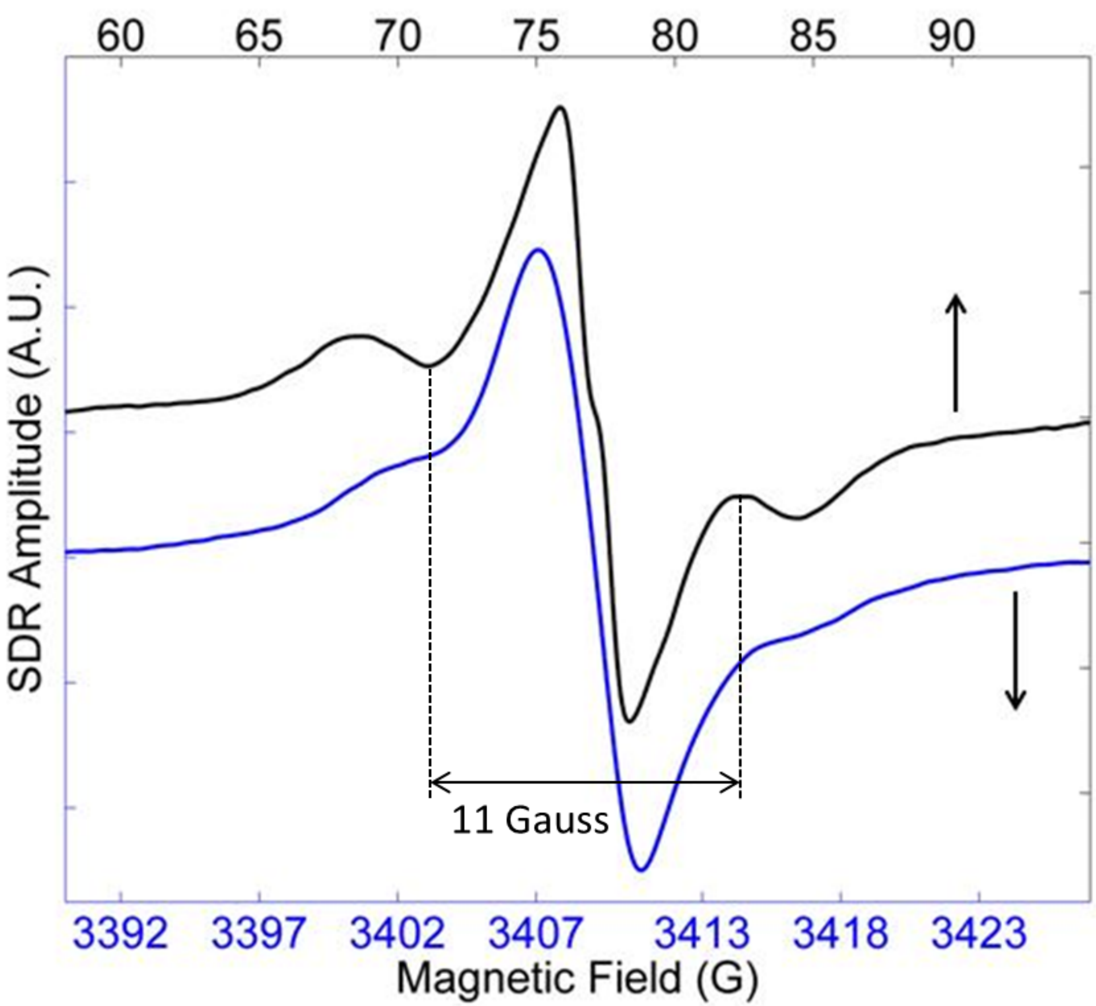
BAE vs SDCP – NO anneals



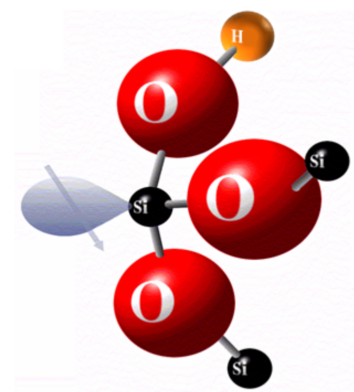


- BAE: Mid gap; SDCP: Most of gap
- no NO: BAE and SDCP same – same defect detected
- NO: BAE and SDCP different – N changes V_{Si} energy levels

High/Low Frequency EDMR Comparison (no NO anneal)

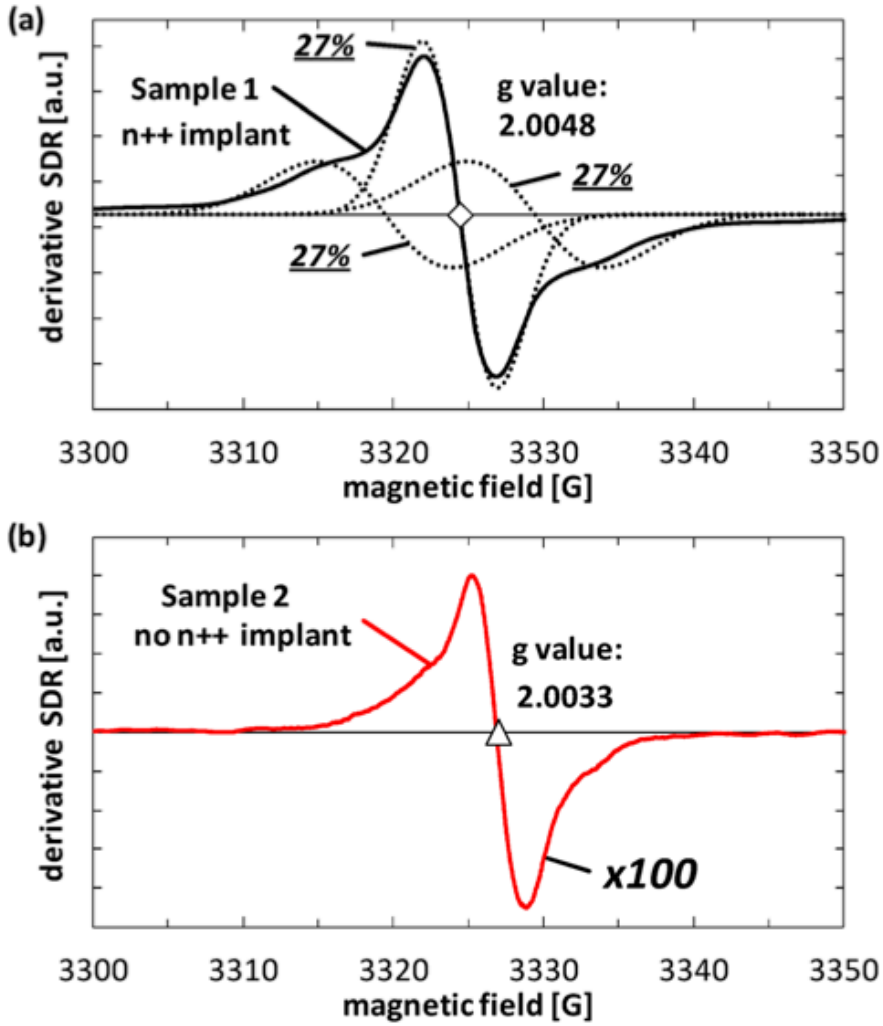


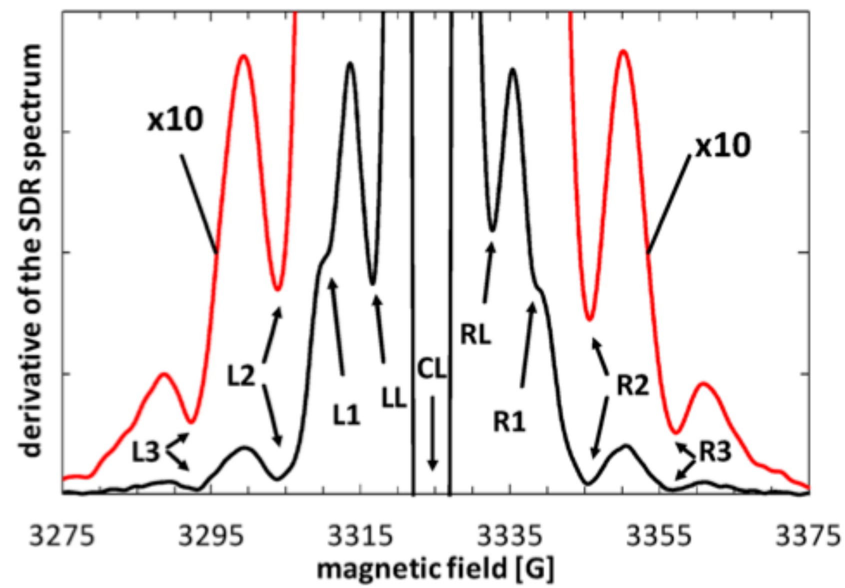
Low frequency EDMR trace sharpens the center line and allows clear observation of the two side peaks separated by about 11 Gauss.



This is the 10.4 Gauss doublet.

Nitrogen Implant Signal (in some Infineon devices)





Nitrogen substitutional Carbon antisite complex

T. Aichinger et al. - Experiment
B.R. Tuttle, S.T. Pantelides et al. – DFT Theory

4H-SiC MOSFET: Searching for dangling bonds

Cdbs:
From Cantin et al:
g-parallel = 2.0023
g-perpendicular = 2.0032

Sidbs:

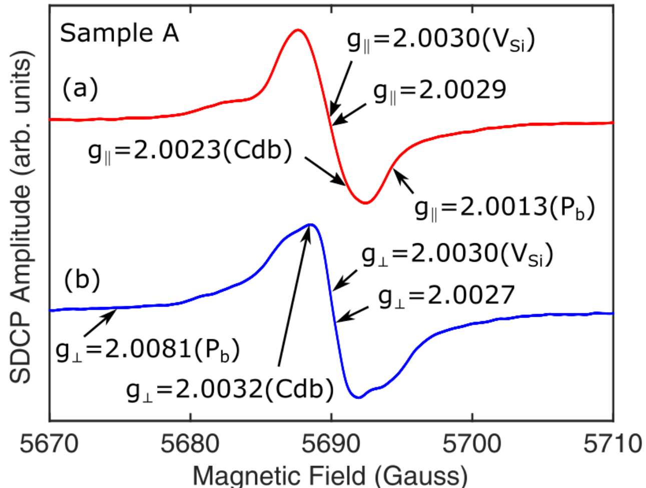
$$g_{ij} = g_e + \Delta g_{ij},$$

$$\Delta g_{ij} = -2\lambda \sum_{i,j,n\neq 0} \frac{\langle 0|L_i|n\rangle\langle n|L_j|0\rangle}{E_n - E_0}$$

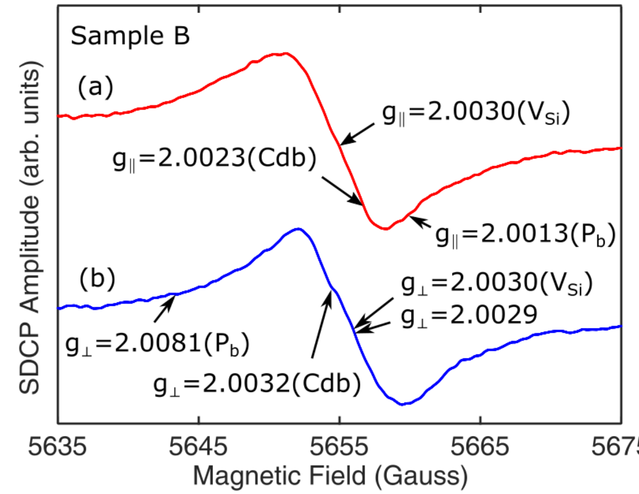
From theory:
g-parallel = 2.0023
g-perpendicular = largest deviation from g_e

J. L. Cantin, et al., Phys. Rev. Lett., vol. 92, p. 5502-1, 2004.

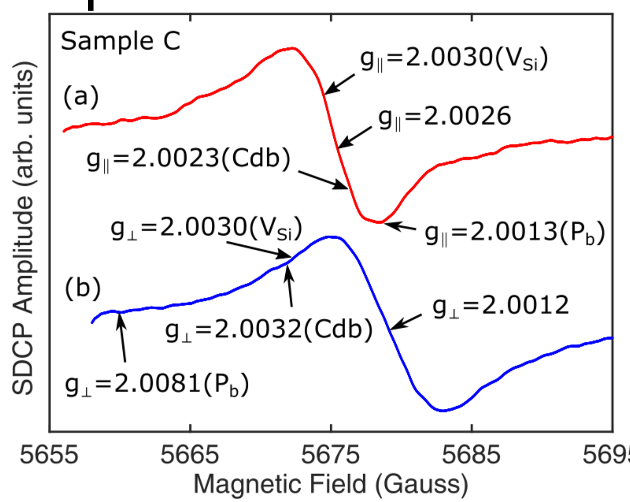
nMOSFET – no NO



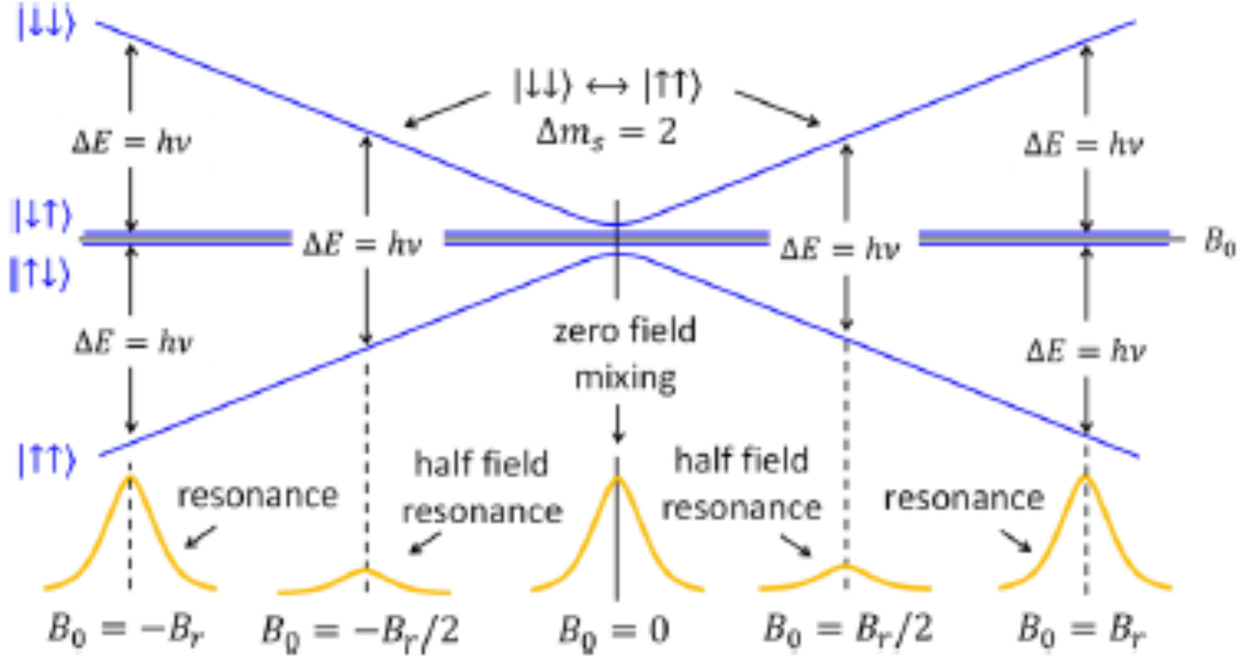
nMOSFET – NO



pMOSFET – NO



EDMR Defect Density: Half Field



Energy level diagram of two paramagnetic sites in proximity

- Half field physics pointed out by Slichter and others.
- Power of the technique demonstrated by Eaton *et al*.

Slichter, Principles of Magnetic Resonance, Eaton *et al*. J. AM. Chem. Soc. **105** 6460 (1983)

EDMR Defect Density: Half Field

The magnetic dipole-dipole interaction:

$$\widehat{\mathcal{H}}_d = \frac{\mu_0}{4\pi}\frac{(g\mu_B)^2}{|\boldsymbol{r}|^3}\left[\widehat{\boldsymbol{S}}_1 \cdot \widehat{\boldsymbol{S}}_2 - \frac{3\left(\widehat{\boldsymbol{S}}_1 \cdot \boldsymbol{r}\right)\left(\widehat{\boldsymbol{S}}_2 \cdot \boldsymbol{r}\right)}{|\boldsymbol{r}|^2}\right]$$

mixes these energy levels and weakly allows for a forbidden half field transition.

From second order perturbation theory:

$$\Psi_n = \Psi_n^{(0)} + \sum_{n'} \frac{\langle n' | \mathcal{H}_p | 0 \rangle}{E_n - E_{n'}} \Psi_{n'}^{(0)},$$

Where:

$$\langle n' | \mathcal{H}_p | 0 \rangle \approx (g\mu_B)^2 / r^3$$

EDMR Defect Density: Half Field

The mixing is about:

$$|\langle n' | \mathcal{H}_p | 0\rangle / (E_n - E_{n'})| \approx [(g\mu_B)^2 / r^3]\, 1/g\mu_B H_0 = [g\mu_B / r^3]\, 1/H_0$$

or:

$$g\mu_B / r^3 \; 1/H_0 = H_{local} / H_0 \, ,$$

So, the lower the resonance field the greater the mixing. The strength of the no longer strictly forbidden transition is, from Fermi's golden rule:

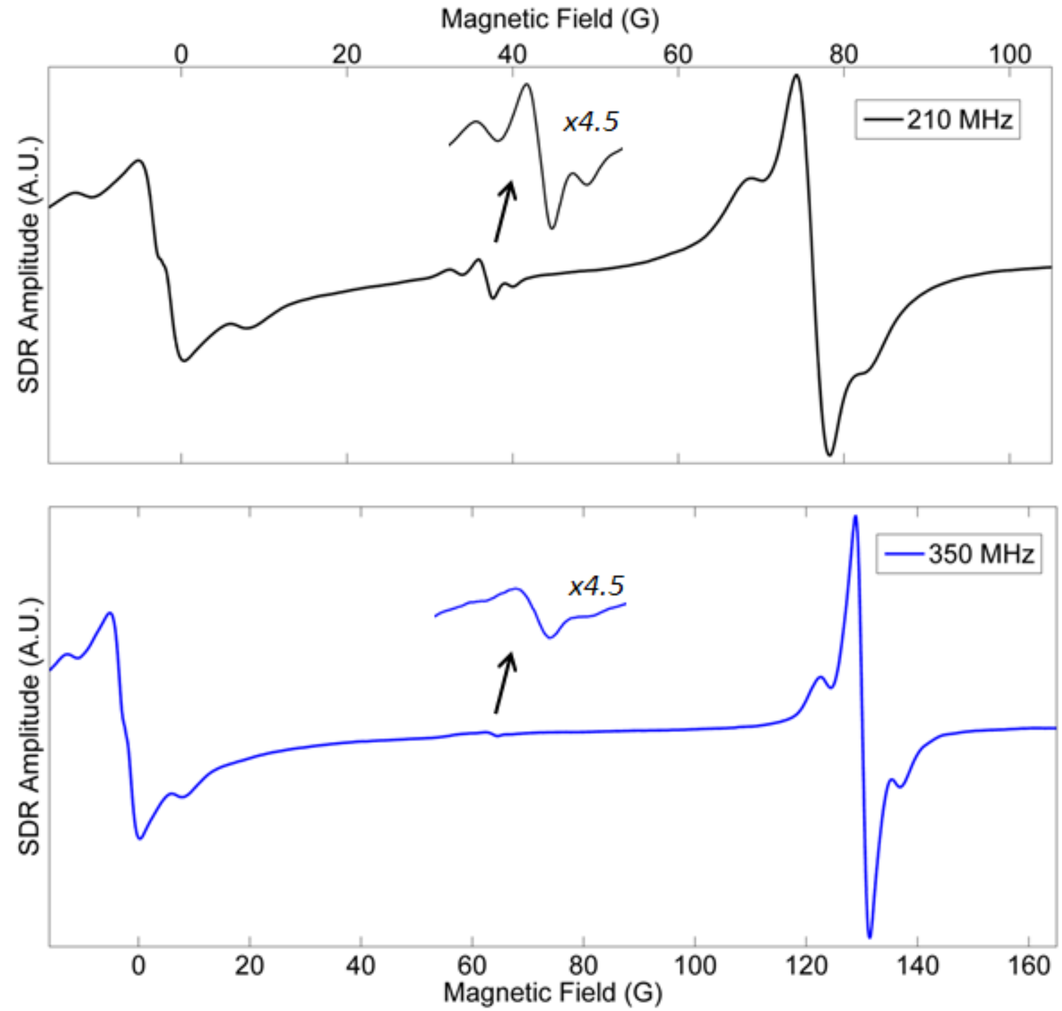
$$W_{a \to b} = 2\pi/\hbar \; |\langle a | F | b \rangle|^2 \; \delta(E_a - E_b - \hbar\omega)$$

Half-Field EDMR Response in GE Lateral pMOSFET

With some gross assumptions, this leads to:

$$r_d \approx \left(\frac{6,937}{\nu^2 {a_0}^3}\frac{1}{R}\right)^{\frac{1}{3}} \text{Å}^2\text{GHz}^{2/3}$$

In the most defective samples, this half-field response is clearly observable



Conclusions

- EDMR, especially in the form of SDCP, is a powerful tool for the exploration of heterointerfaces such as that of SiC/SiO_2
- The introduction of N in device processing can greatly reduce the density of silicon vacancy centers, but apparently introduces disorder and changes in defect energy levels
- The SiC/SiO_2 interface is fundamentally different and much more complex than the Si/ SiO_2 interface