NPCQS 2012 (2012. 4. 25)

NMR Studies of ^{31}P-doped Si crystals at Low temperatures down to 40 mK and at a high field of 7 T

Fukui University and Kyoto University

Takao Mizusaki

Joint Project between Japan and Korea

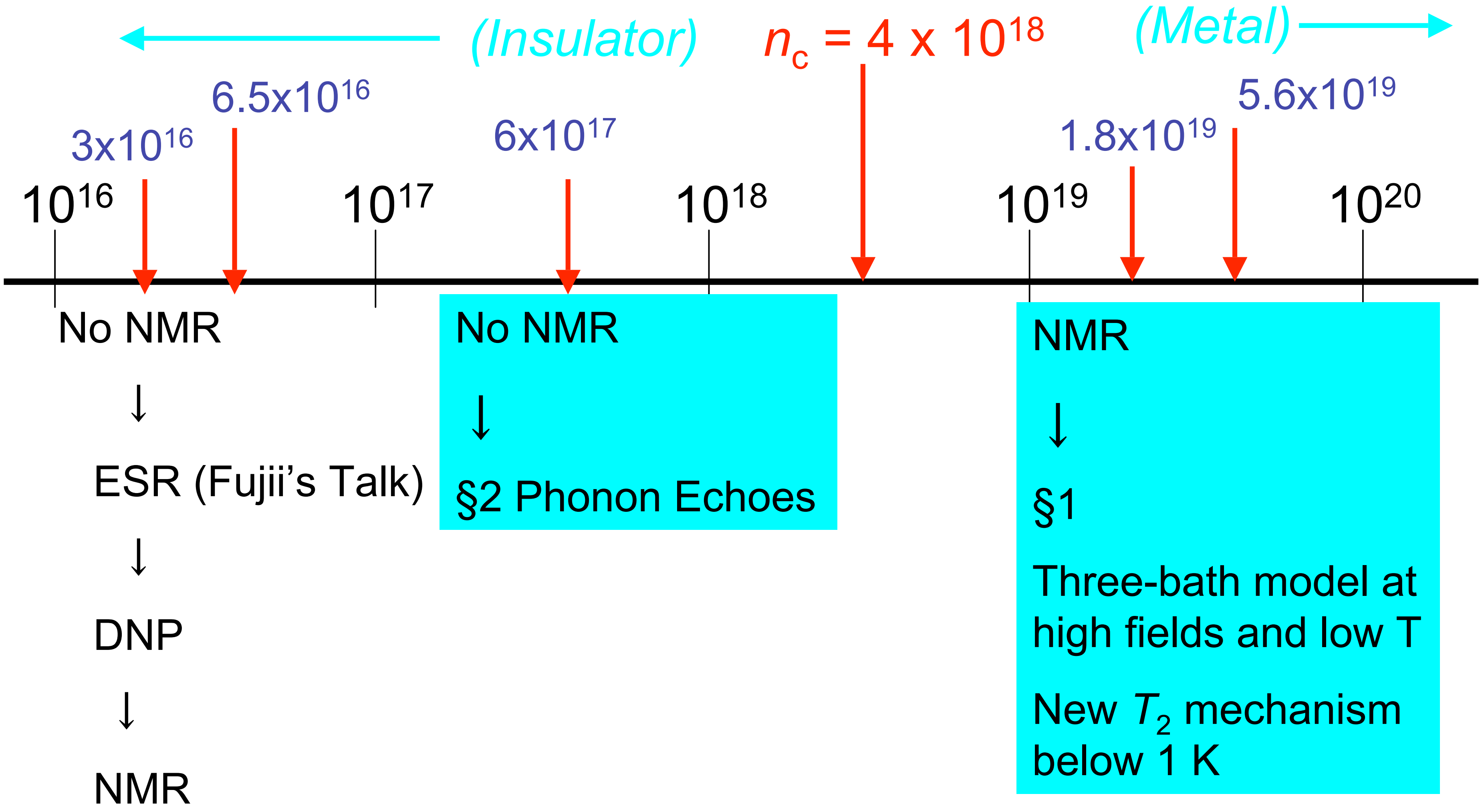
M. Jeong, M. Song, S. Lee (KAIST, Korea) +KBSI

T. Ueno, M. Matsubara (Kyoto University, Japan)+Fukui Univ.

+Vasiliev(Turku)

^{31}P NMR at low temperatures (down to 40 mK) and at a high field (7 T)

(Samples are P-doped normal Si with 4 % ^{29}Si)



§ 1. ^{31}P–NMR studies at 7 T (120 MHz) down to 40 mK

J. Phys. Soc. Jpn. 78, 075003 (2009)

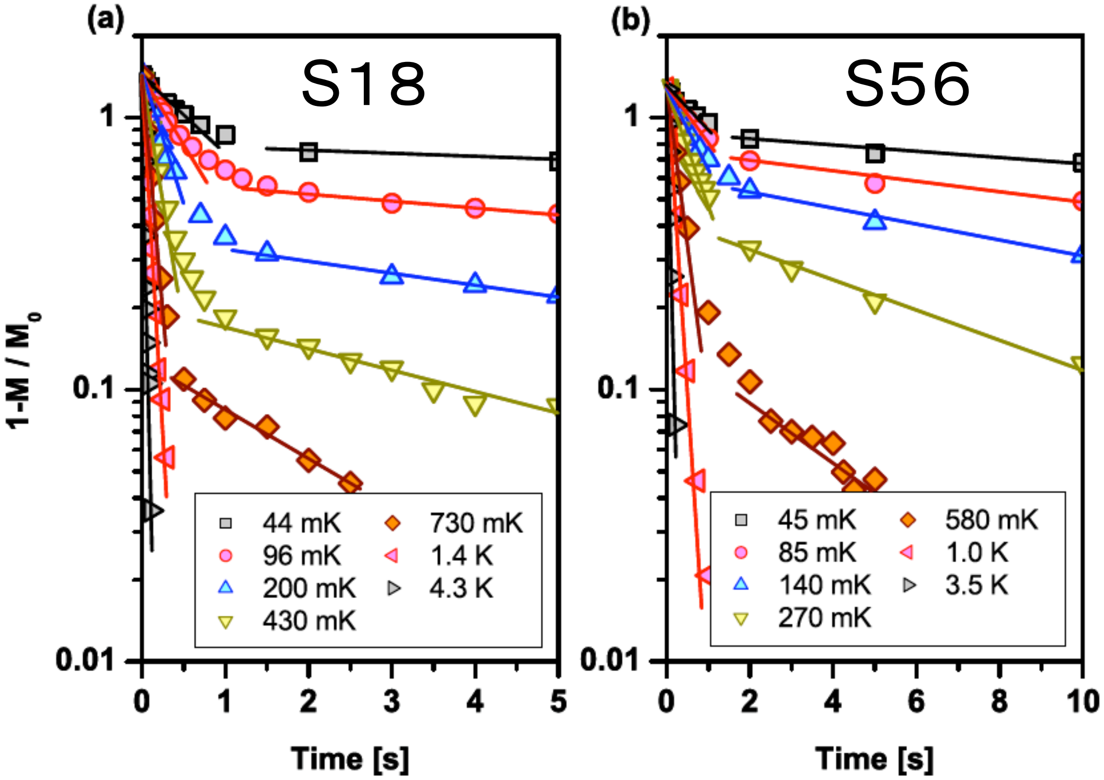
J. Low Temp. Phys. **158**, 659-665 (2010)

S18 (1.8×10^{19}/cc) and S56 (5.6×10^{19}/cc):

Metallic samples: Strongly-correlated electron system

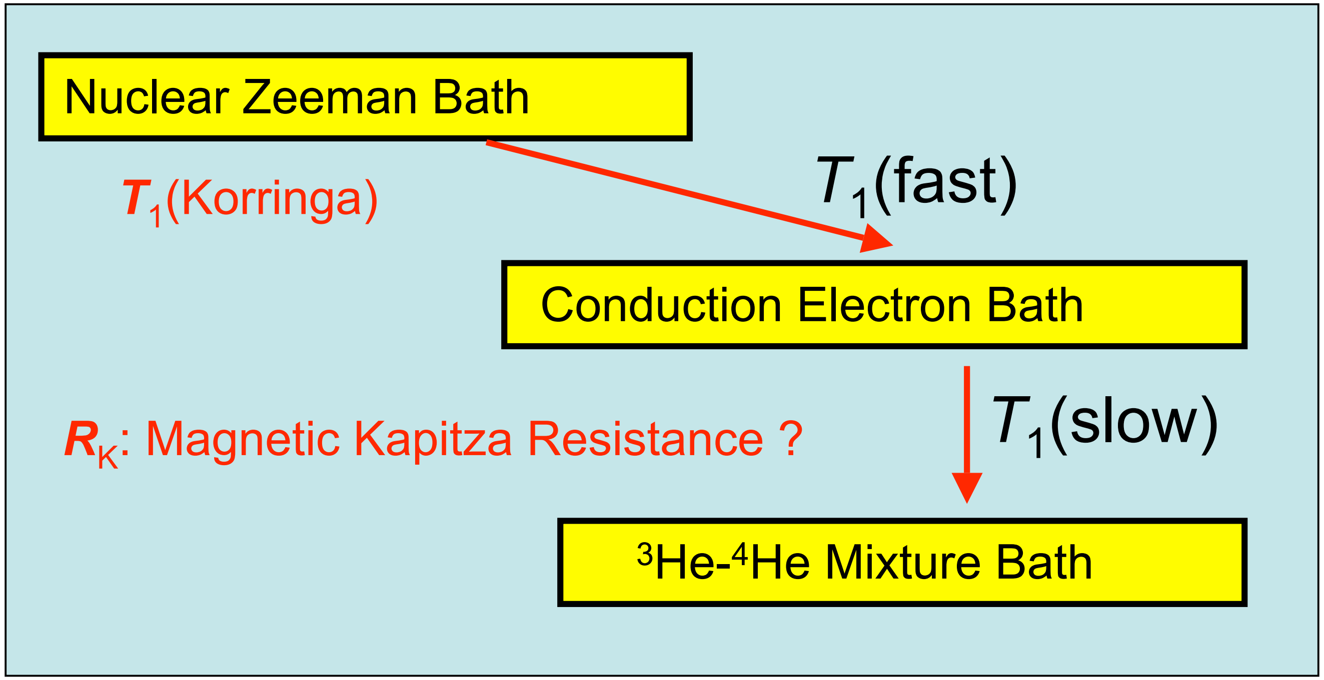
1) T_1 Measurements

Magnetization Recoveries after 180° pulse for S_{18} and S_{56}



Analysis of two-step-decay processes by three-bath model

We found two-step decay processes at low temperature below about 1 K under high fields (7 T)



$$C_Z / C_E \sim \left(\mu_N H / k_B T\right)^2 / (T / T_F) \propto (H^2 / T^3)$$

$C_Z \sim C_E$ at T = 50 mK for B = 7 T

In the case that T_1(fast) >> T_1(slow),

for T_1(fast) and for T_1(slow)

$$\frac{\partial M}{\partial t} = -\frac{M - M(T_e)}{T_1} = \frac{M - M(T_e)}{\mathrm{K}/T_e} \qquad (1)$$

Energy Conservation between Zeeman and Electric bath:

$$(M - M(0)) \cdot H = \frac{1}{2}\gamma\,(T_e^2 - T_e^2(0)) \qquad (2)$$

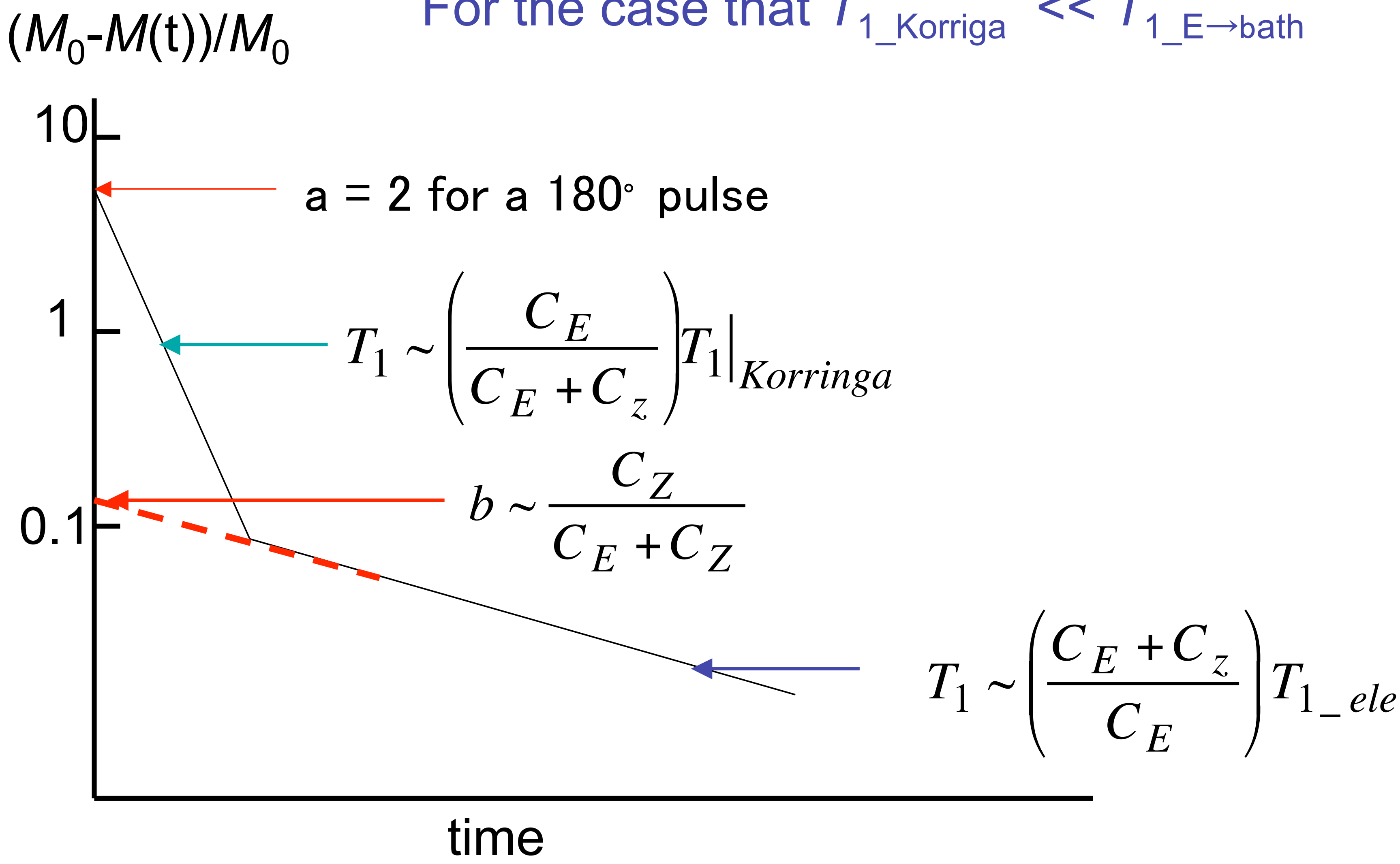
Zeeman and electric baths decay together :

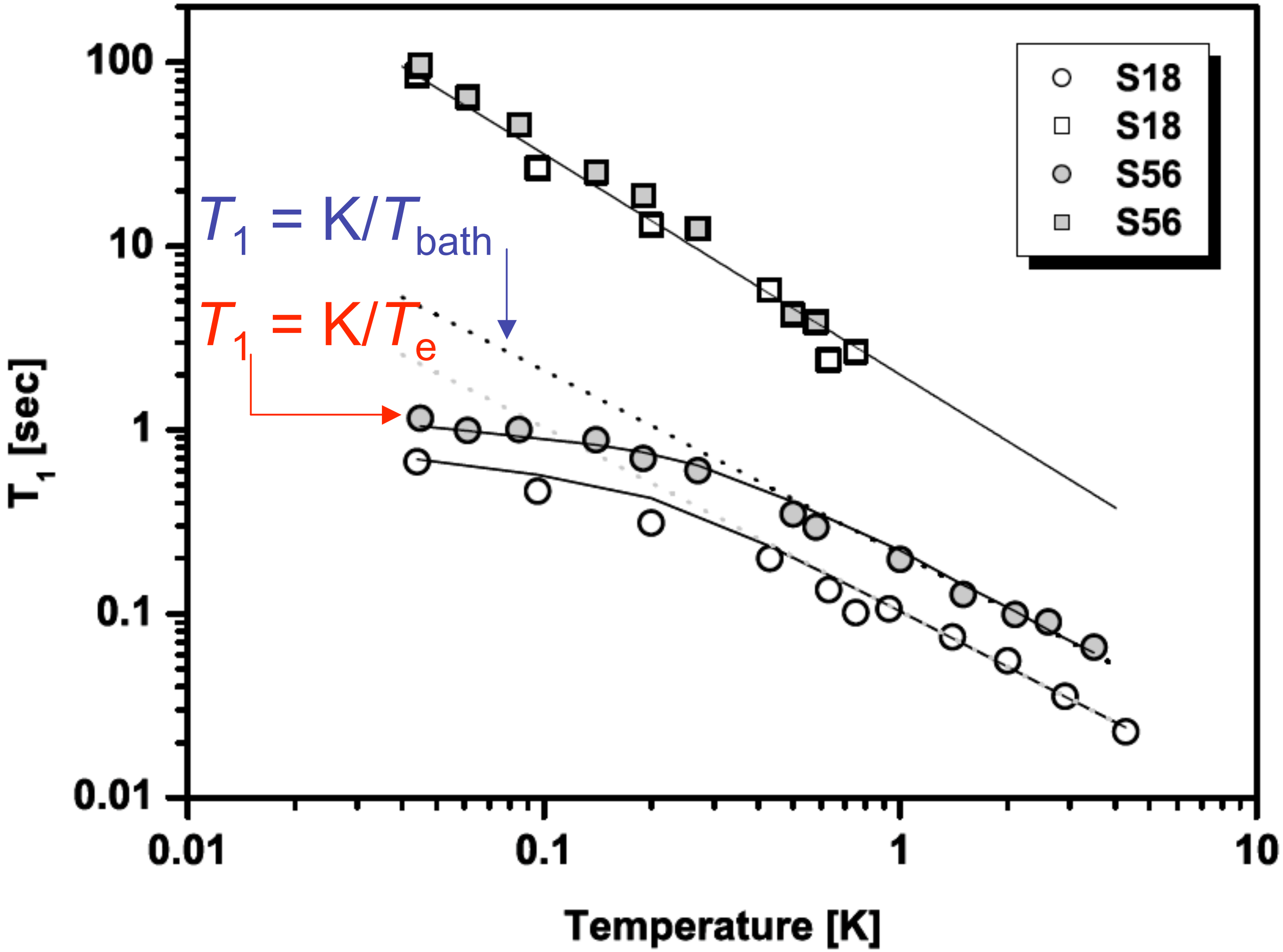
$$T = T_N = T_e \qquad (3)$$

$$(C_N + C_{ele})\frac{\partial T}{\partial t} = \frac{1}{R_K}(T - T_{He-bath}) \qquad (4)$$

Characteristic Behavior of Three-Bath Model

For the case that $T_{1\_Korriga} \ll T_{1\_E \rightarrow bath}$

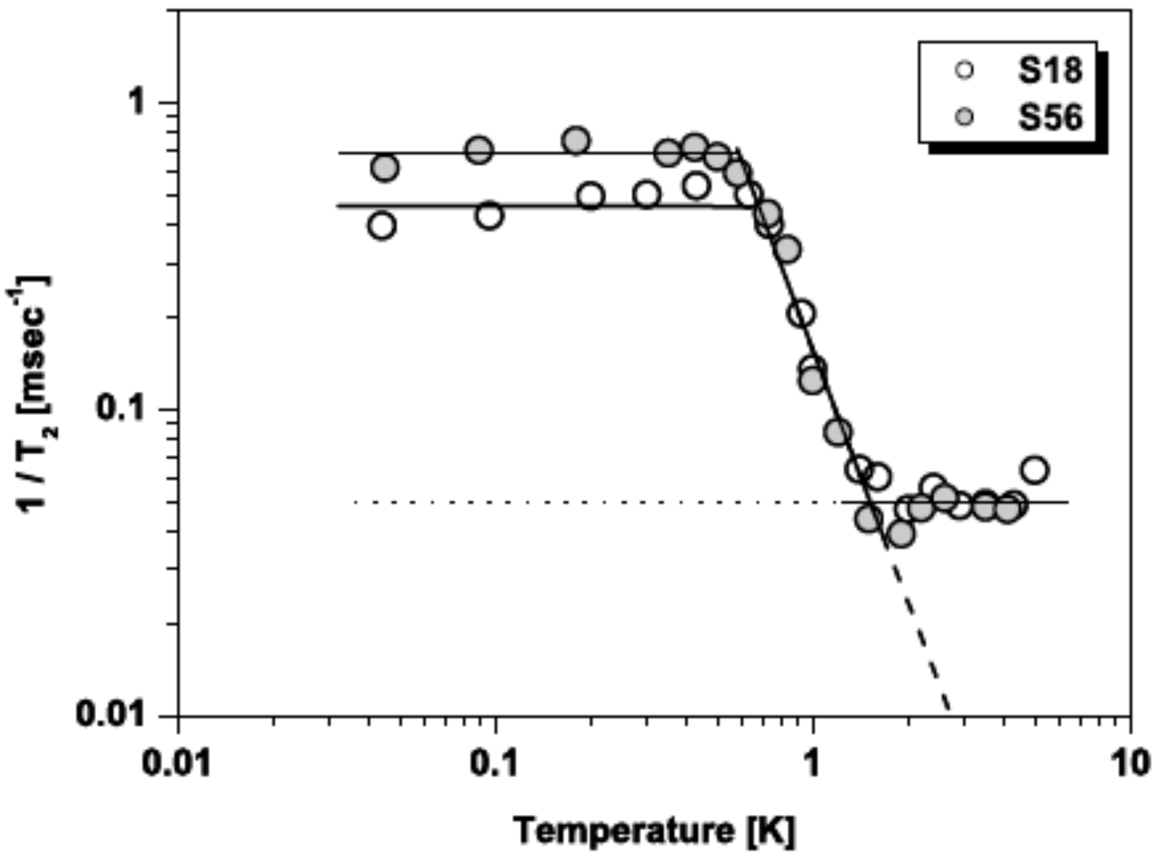




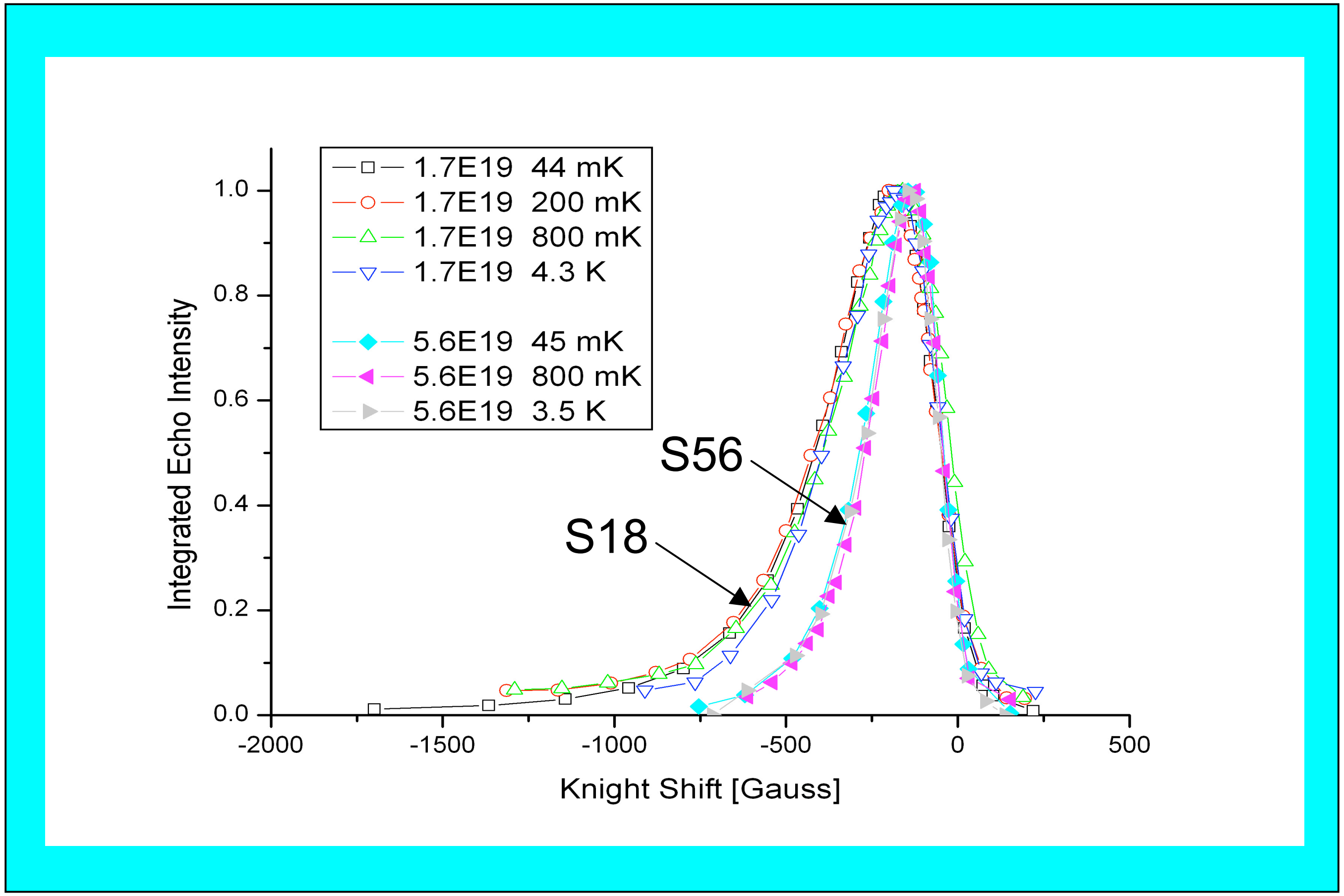
T_1(slow) may be determined by Kapitza resistance between conduction electron and ^3He-^4He bath

2) T_2 measurement

First observation of T_2 below 1 K.



NMR spectrum for S18 and S56



Knight shift of ^{31}P-NMR from Lamor frequency

Inhomogeneous broadening of $1/T_2^* \sim 10^6\ sec^{-1}$

$$1/T_2 = (1/T_2)_{dip} + (1/T_2)_{excess}$$

1) $(1/T_2)_{dip}$ is determined by the rigid lattice for 4 % ^{29}Si-^{31}P dipole.
   $(1/T_2)_{dip}$ is independent of T and n.

2) We found $(1/T_2)_{excess}$.

$$(1/T_2)_{excess} = \begin{cases} \sqrt{M_2}, & T < 0.6\ K \\ M_2 \tau_c, & T > 0.6\ K \end{cases}$$

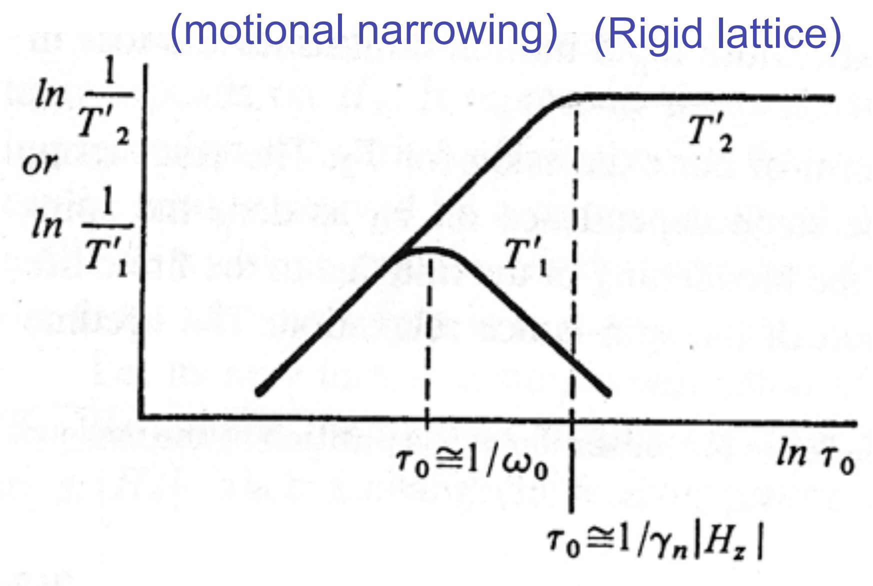
$$\tau_c = \tau_0 (T/T_F)^{-m}, \quad m = 4 \sim 5$$

1) $\sqrt{M_2}$ depends on the concentration *n.*

Thus fluctuating fields responsible for T_2 is either the dipole interaction between P-P or the RKKY.

2) $\tau_c(T)$ strongly depends on T and dipole between ^{31}P-^{3}1P is too small. Thus electrons have to be involved →RKKY.

Motional Narrowing (from Slichter's book)



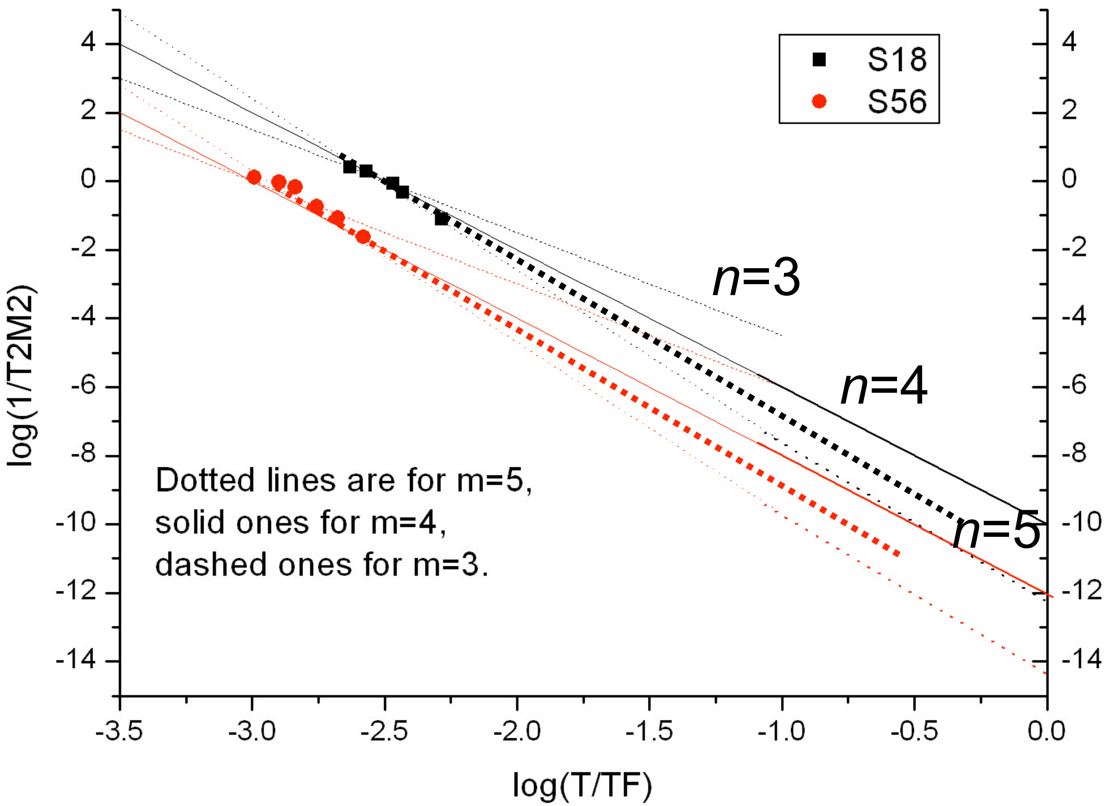
$1/T_1 \sim M_2\tau_c / (1+(\omega\tau_c)^2)$

$1/T_2 \sim M_2\tau_c,$

where M_2 is the 2nd moment of the fluctuation field.

But if $\tau_c > 1/\sqrt{M_2}$, then $1/T_2 \rightarrow \sqrt{M_2}$ (Rigid Lattice)

Temperature-dependence of $\tau(T)$



$$\tau(T) \sim (a / v_F)(T / T_F)^{4\sim 5}$$

$(1/T_2)_{excess}$ Mechanism–Motional Narrowing of RKKY

$$H_{RKKY} = \sum_{k \neq l} A(R_{kl}) I^k \cdot I^l, \qquad \left[I_x^1 + I_x^2,\ \ I^1 \bullet I^2\right] = 0$$

1) Non-identical spins due to inhomogeneous broadening→
“ Truncation of the RKKY “

$$H_{RKKY} = \sum_{k \neq l} A(R_{kl}) I_z^k\, I_z^l, \qquad \left[I_x^1 + I_x^2,\ \ I_z^1 I_z^2\right] \neq 0 \qquad \rightarrow 1/T_2$$

, where $(I_1^+ I_2^+ + I_1^- I_2^-)$-terms are cancelled in phase factor by inhomogeneous broadening and only $(I_z^1 I_z^2)$ - term is left.

2) Low density of conduction electrons → (E_F~100 K) →

large RKKY

$$1/T_2 = \sqrt{M_2} = \sqrt{A(R_{kl})^2} \sim (hyperfine)^2 / E_F$$

$$\sim (120 MHz)^2 / (10^4 GHz) \sim 1 ms^{-1}$$ for Rigid Lattice case

Motional Narrowing formula for T_2

$$\frac{1}{T_2} = \frac{\mathrm{Re}\int_0^{\infty} \langle [I_x, H_{RKKY}(o)][I_x, H_{RKKY}(t)] \rangle dt}{\hbar^2 Tr\{I_x^2\}}$$

where

$$H_{RKKY} = \sum_{k \neq l} A(R_{kl}) I_z^k I_z^l, \qquad \left[I_x^1 + I_x^2,\ I_z^1 I_z^2 \right] \neq 0$$

Assuming

$$\left\langle \sum_{k \neq l} \sum_{k'l'} A(R_{kl}(0)) A(R_{k'l'}(t)\} \right\rangle$$

$$= \left\langle \sum_{k \neq l} \sum_{k'l'} A(R_{kl}) e^{-iH_m t/\hbar} A(R_{k'l'}) e^{iH_m t} \right\rangle = \sum_{kl} A(R_{kl})^2 \delta_{kk',ll'} e^{-t/\tau_c(T)}$$

$$1/T_2 = M_2 \tau_c(T), \qquad where \quad M_2 = \frac{1}{9} \sum_k A(R_{k,l})^2$$

§ 3. First observation of Phonon Echoes in P–Doped Si

J. Phys.:Conf. Ser. **150**, 042078 (2008)

The set-up for "phonon echoes" is the same as NMR (120 MHz), where the sample is immersed in liquid ^{3}He-^{4}He mixtures.

We measured three samples;

(L-P) : Low-doped Si ($n = 6 \times 10^{17}$) in powder form, → Echoes

(L-B) : Low-doped Si ($n = 6 \times 10^{17}$) in plate(bar) with thickness of 0.1 mm, → No Echo

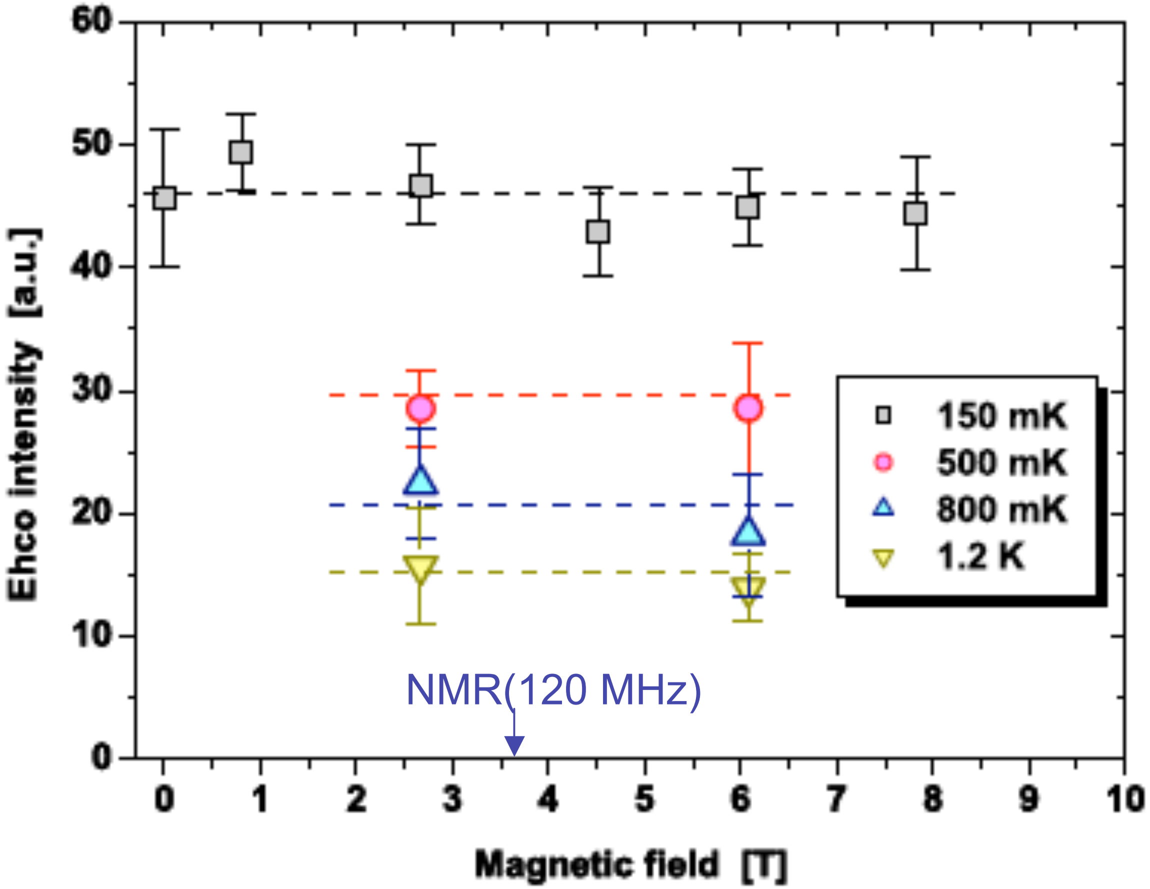
(H-P) : High-doped Si ($n = 6 \times 10^{19}$) in powder form → NMR

metallic sample

1) Why were Phonon echoes observed for powder sample?

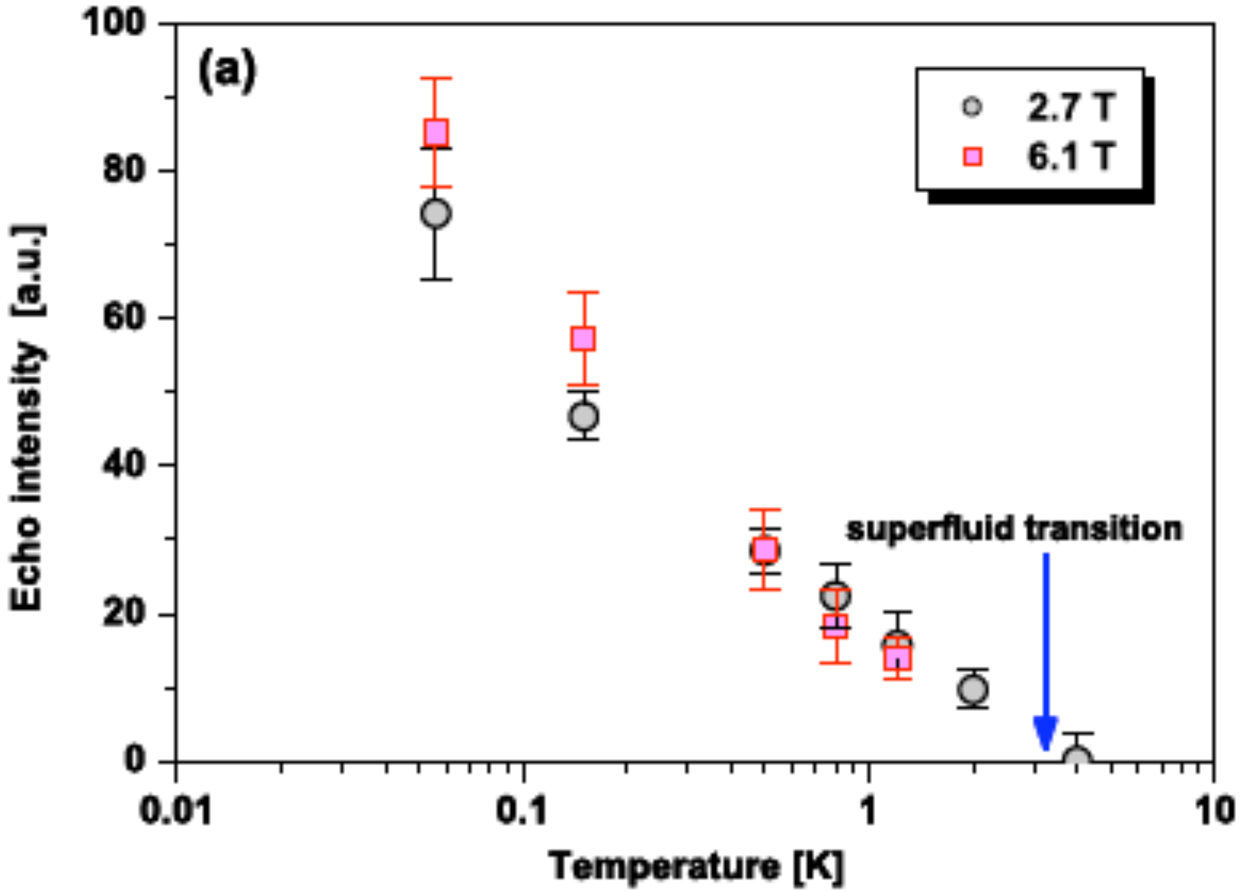
D / Sound velocity ~10 μm/ 10 km/s~1/100 MHZ → Phonon

2) Echo intensity at 2τ = 150 μs msec does not depend on fields but strongly depends on temperatures



3) Temperature-dependence of echo intensity
No echo is observed above T_λ

Echo Intensity vs. T at 2τ = 150 μsec

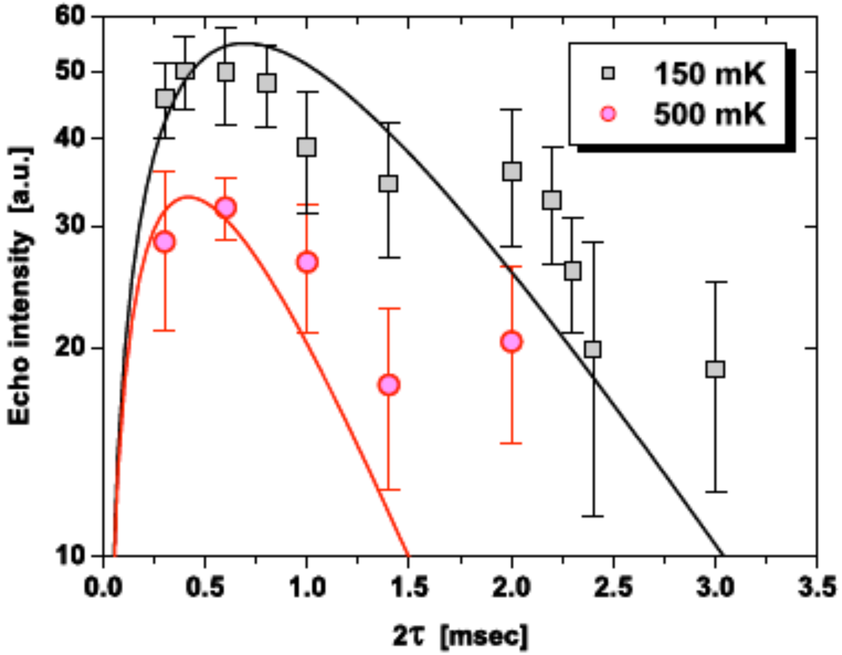


Low-doped Si ($n = 6x10^{17}$) in powder form, immersed in ^3He-^4He mixtures ($n \sim n_c = 4 x10^{18}$/cc)

Dynamical Polarization Phonon Echoes in Piezoelectric materials

1) Echoes is formed by non-linear terms of elastic constant

$$F = 1/2\, C_2S^2 + (1/6\, c_3S^3) + 1/24 C_4S^4$$



$$\ddot{S} - 2\Gamma \dot{S} + \omega_0^2 (1 - \beta S^2) S = f(t)$$

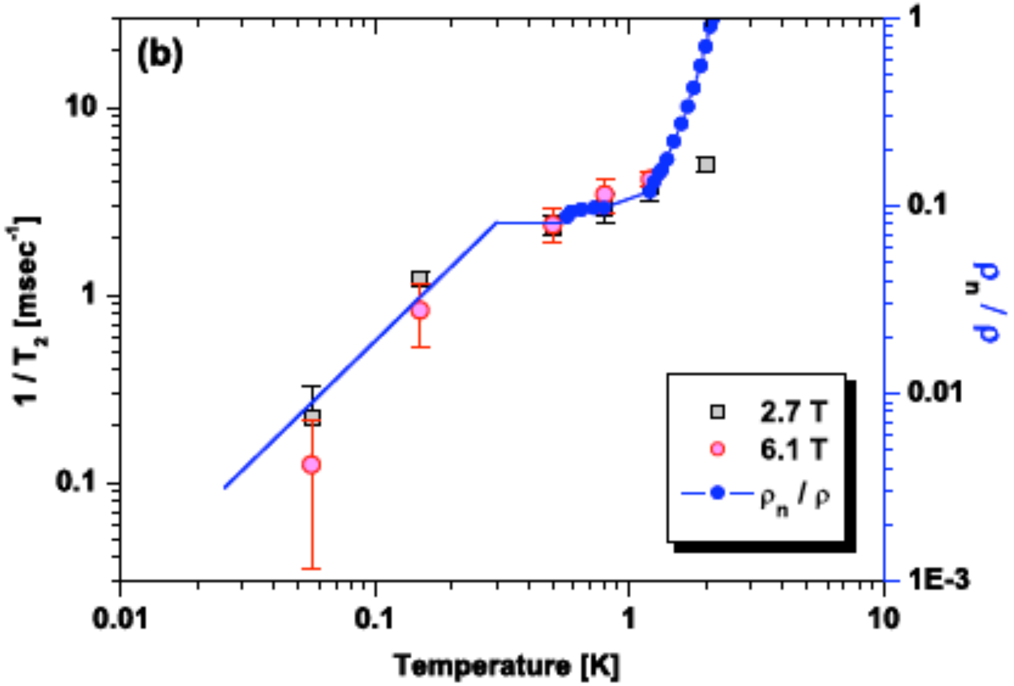
$$E(2\tau) \approx (T_2/2)\beta E_1 E_2^2 (1 - e^{-2\tau/T_2}) e^{-2\tau/T_2}$$

where $\Gamma = \dfrac{2}{T_2}$ *and* $\beta = c_4 / 2c_2$

Coupling with rf-field (E-field) determine E_1 and E_2.→ Piezoelectric

$\beta E_1 E_2^2$ is a fitting parameter for an experiment

T_2 (T) and the dissipation mechanism of phonon echoes



Drag force of sphere with radius *a*, moving with velocity $\dot{S}$, due to elastic collision of quasi particles in ^3He-^4He mixture in Knudsen regime →

$$F_{drag} = -2\Gamma\dot{S}, \qquad \Gamma = 2/T_2,$$

$$\frac{2}{T_2} = \frac{A\rho_n v_n}{a\rho}$$

$\rho_n = \rho_n(4) + \rho_n(3)$

v_n = *group velocity of quasi particle*

Why P-doped Si near n_c has piezoelectricity .

P-clusters exist for $n < n_c$ (see ESR (c and d)).

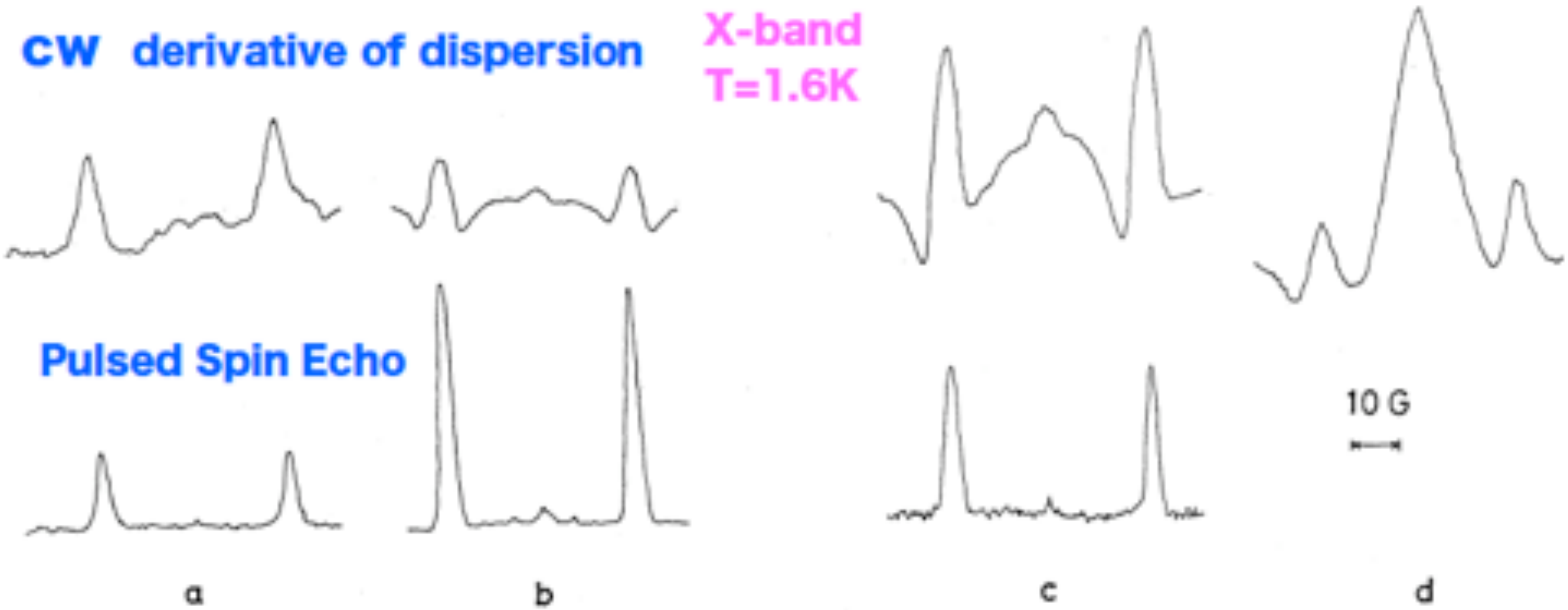


Fig. 1. ESR spectra of phosphorus doped silicon at 1.6 K. Upper traces are obtained by the conventional steady state method and lower traces are obtained by the spin echo method using a boxcar integrator. Sample; a: $c=3.0\times10^{16}$, b: $c=6.6\times10^{16}$, c: $c=2.0\times10^{17}$ and d: $c=3.1\times10^{17}$.

M. Chiba and A. Hirai, J. Phys. Soc. Jpn., 33, 730 (1972)

$n_c = 4 \times 10^{18}$/cc

Note that cluster (2P, 3P and 4P) signals can be observed even for $n \ll n_c$.

Thank you for your attention

Outline

§ 1. NMR in metallic samples

(n = 1. 8x10^{19} and 5.6 x 10^{19} /cc)

down to dilution temperatures at 7 T.

Three-bath model: T_1(fast) and T_1(slow) for $T < 1$K

T_2 : new mechanism for $T < 1$ K

§ 2. Photon echoes (n = 6x10^{17}/cc) in insulator

Dynamical Polarization Phonon Echoes by

piezoelectric character of P-doped Si near n_c

(*Critical concentration* n_c = 4x10^{18}/cc)

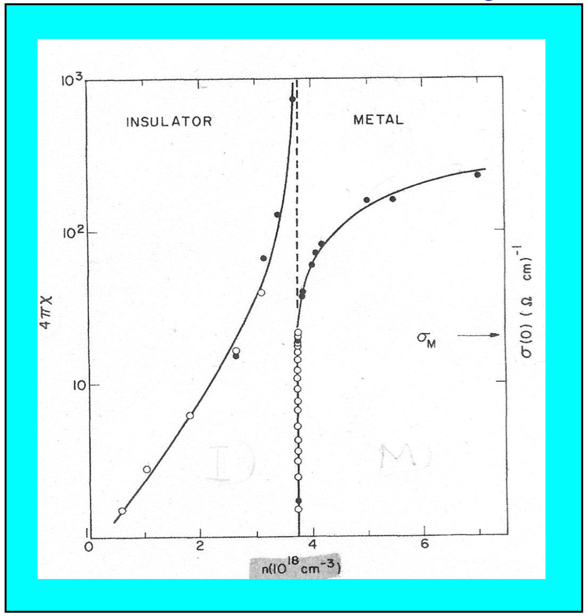
Metal-Insulator Transition

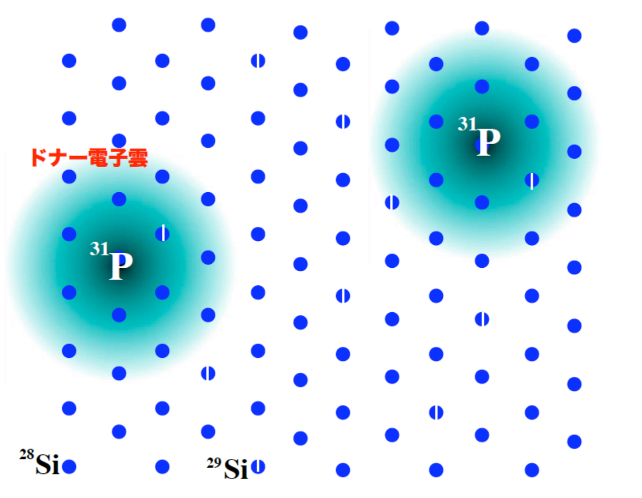
Critical concentration n_c = 3.7 x 10^{18}/cc)

P-doped Si: $n > n_c$: Metal: n-type semiconductor

strongly- correlated electron system

$n < n_c$: Insulator: isolated donor P





Metal-Insulator Transition in a doped semiconductor, T. F. Rosenbum et al.

P.R. **B27**, 7509 (1983)

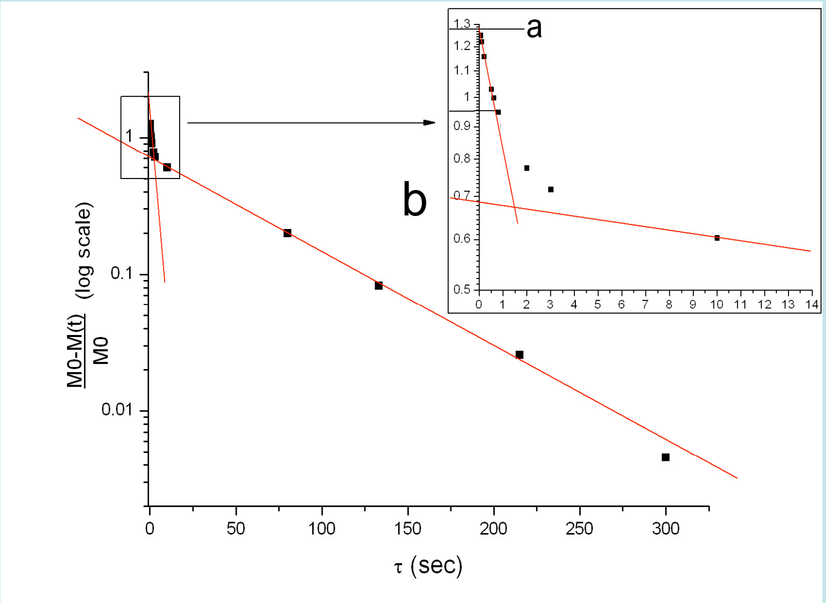
n_c = 3.7 x 10^{18}cm^{-3}

$n_c^{-1/3}$ = 60 Å = 2 a_B

a_B = 30 Å for m_{eff} = 0.3 m_e

T_1 measurement for sample for S_{56}

Recovery of magnetization after 180 pulse below 1K



S_{56} at T=140 mK

New features in T_1

at 7 T and low temperatures

Above $T = 1$ K, the recovery is a single-exponential decay.

Below 1 K, the magnetization is decayed in two steps.

$$\frac{M_0 - M(t)}{M_0} = (a-b)\cdot e^{-\frac{t}{T_1(fast)}} + b\cdot e^{-\frac{t}{T_1(slowt)}}$$

Hamiltonian to describe the entangled state of nuclear spin Q-bits

$$H_{en} = \mu_B B \sigma_z - g_n \mu_n B I_z + A\sigma \cdot I + (dipole)$$

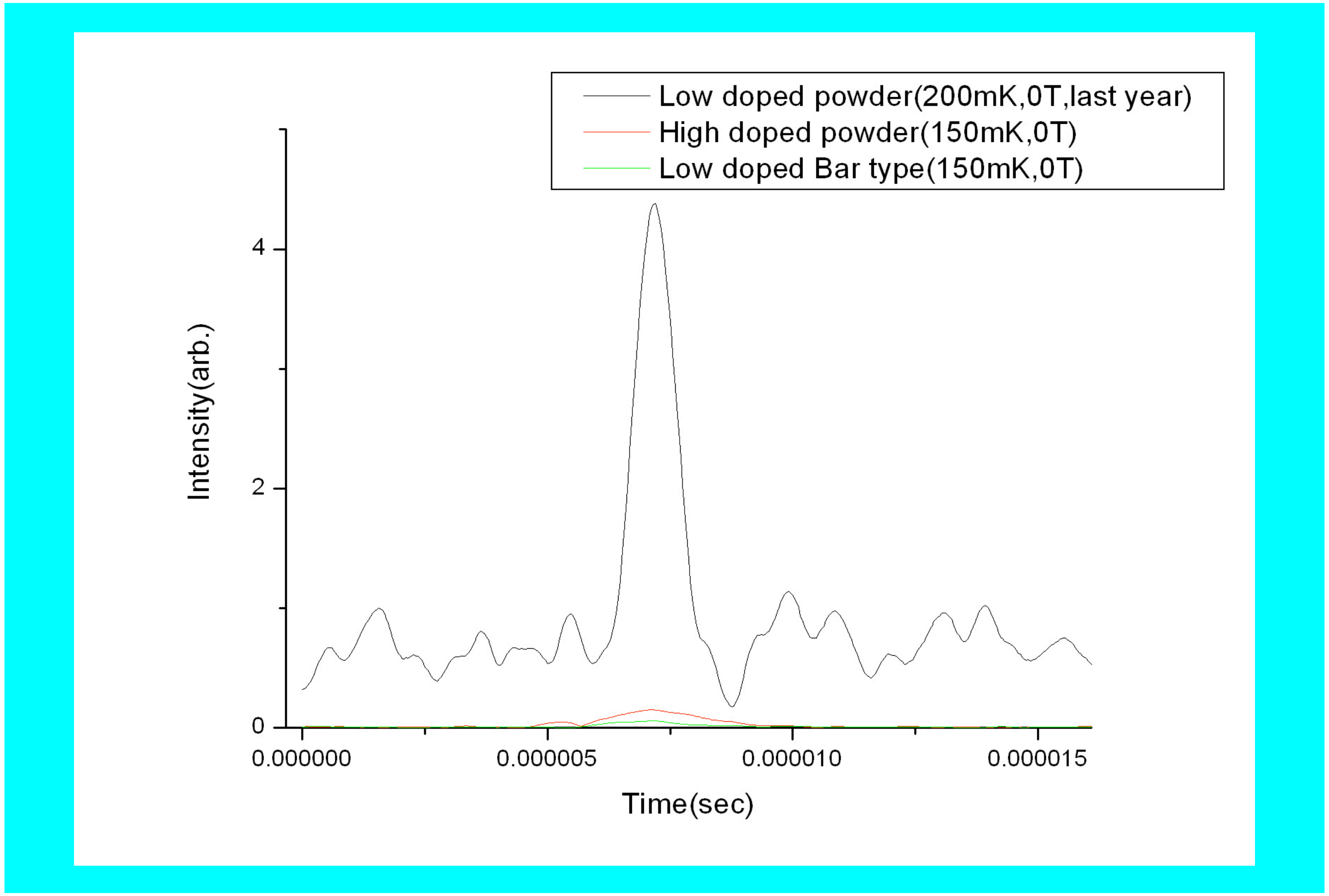
$$(Zeeman) \qquad\qquad (Hyperfine)$$

$$H_{e-e} = \sum_{i\sigma} (\varepsilon_i - \mu) n_{i\sigma} + \sum t_{ijo} c^{+}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$(Hubbard\ Model)$$

T_2 in metallic sample reflects nuclear spin dynamics in the entangled states (ensemble average)

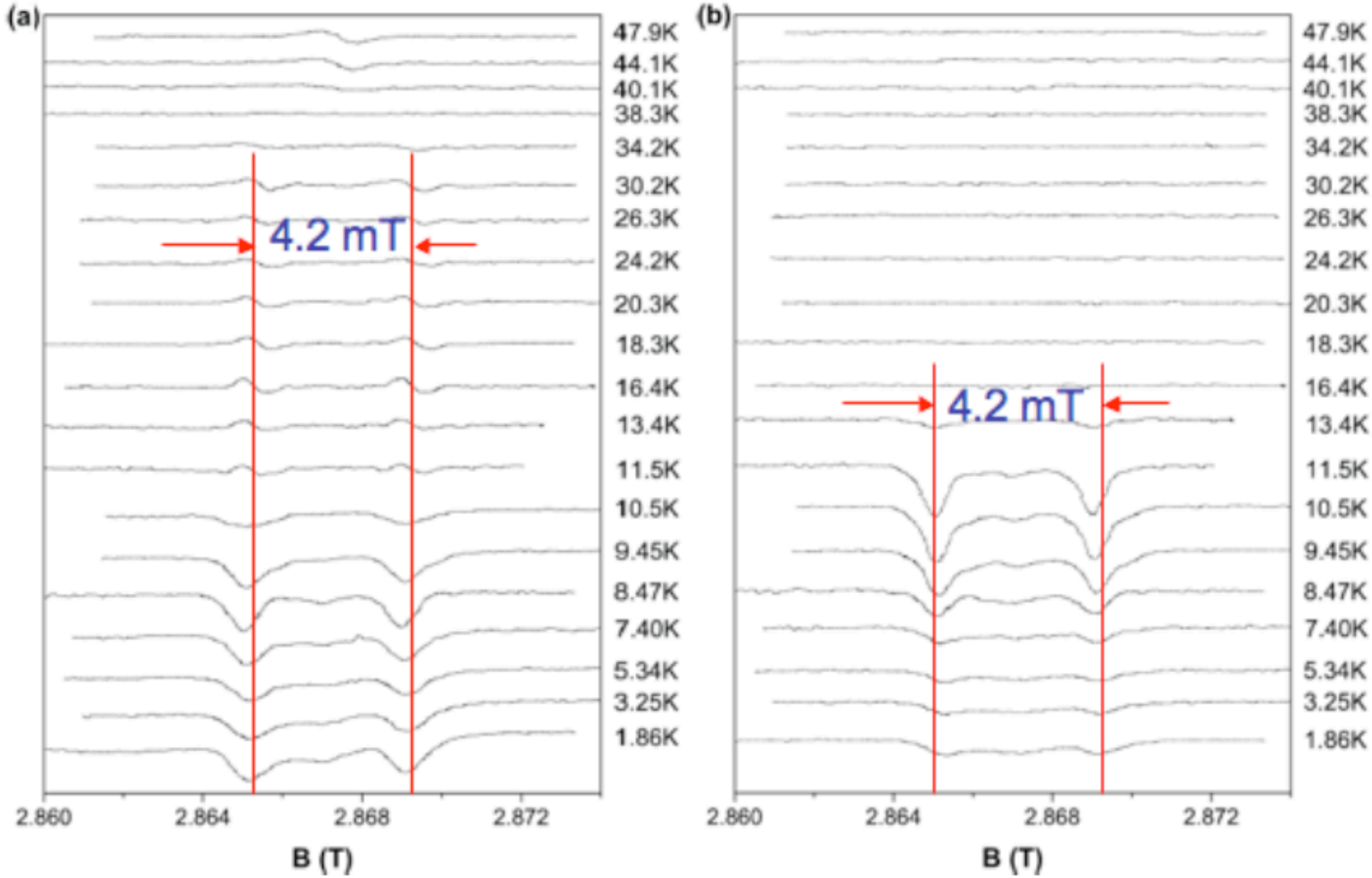
Phonon Echo signal by dynamical polarization echoes



§3. ESR in insulator sample (n = 6.5 x 10^{16}/cm^3)

J. Phys.:Conf. Ser. **150**, 022078 (2008),

J. Physics: Condensed Matters, **22**, 206001 (2010).



f_o = 80 GHz (~3 T), ω_m= 330 Hz,

Temperature-dependence of ESR signals

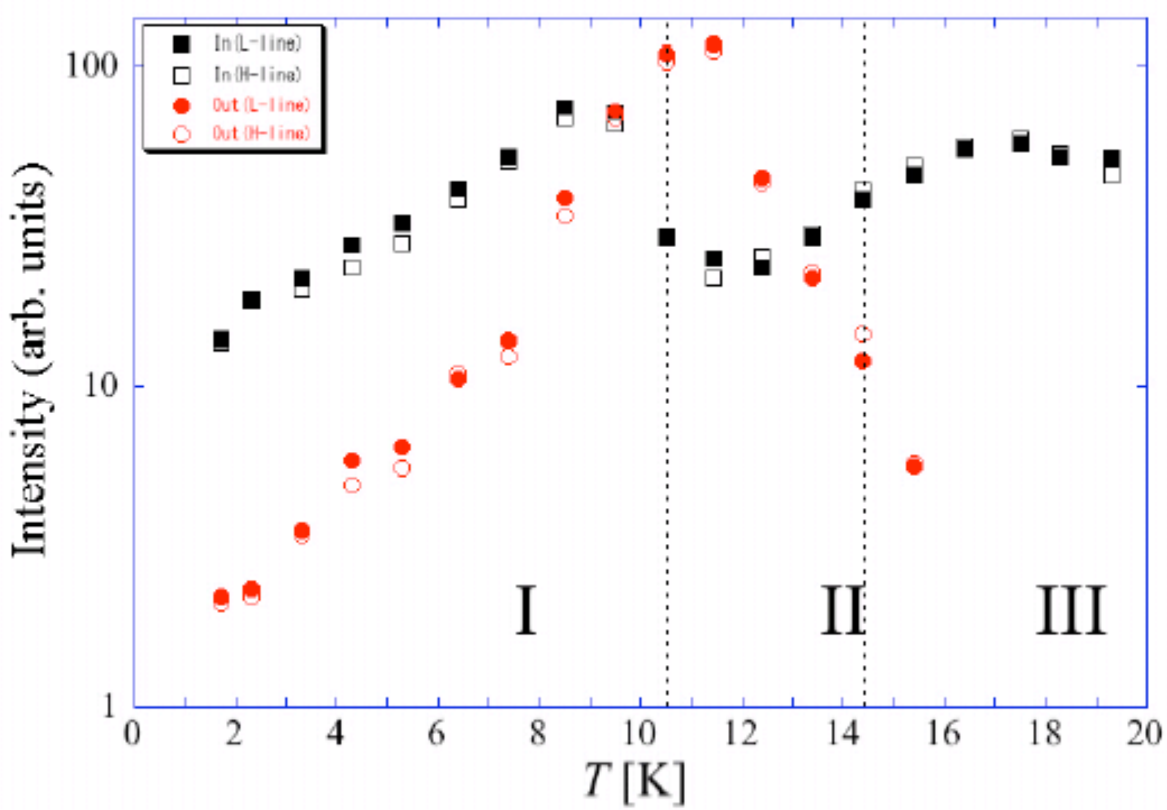


Fig. 3 Temperature dependence of normalized intensities. Squares are for in-phase and circles are for out-of-phase and solid symbols are for L-lines and open ones for H-lines

Numerical Solution for Bloch Equation

１）
$$h(\omega', \omega_{res}) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(\omega' - \omega_{res})^2}{2\sigma^2}\right)$$

から波束ω’ を取り出し、Bloch方程式に従うとする.

２）δω= ω−ω’ でスピンの運動 (Bloch Eq.)を解く（$t > 5T_1$）

3）
$$M_{\alpha-IN}(\delta\omega) = \frac{\omega_m}{2\pi} \int_0^{2\pi/\omega_m} M_\alpha(t, \delta\omega) \cos\omega_m t \, dt$$

4）
$$M_\alpha^{IN}(\omega - \omega_{res}) = \int_{-\infty}^{\infty} M_{\alpha-IN}(\omega' - \omega) h(\omega', \omega_{res}) d\omega'$$

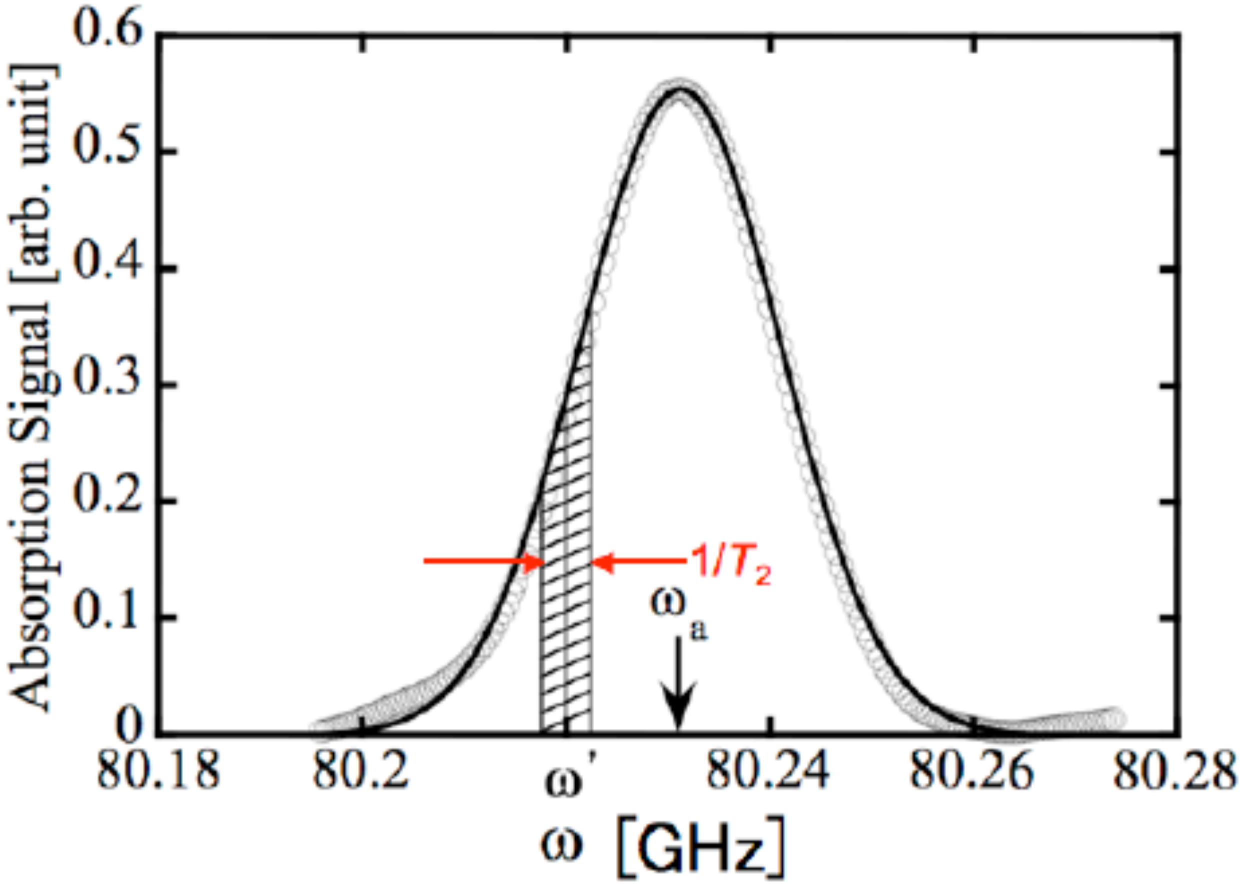


Fig. 4 ESR absorption line shape observed at a high temperature of 17 K in the region III.

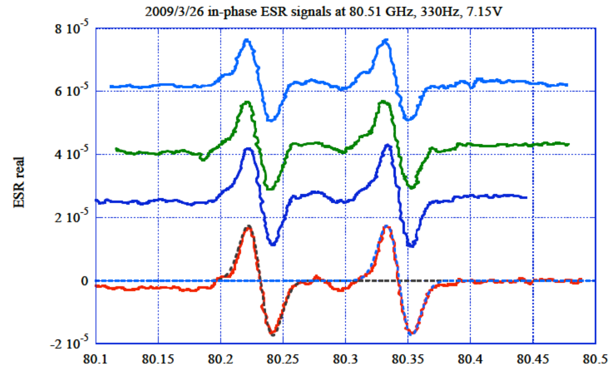
Numerical Simulation of Bloch Equation (T_1 unknown)

$$\frac{dM_z}{dt} = \gamma B_1 M_y - \frac{M_z - M_0}{T_1}$$

$$\frac{dM_x}{dt} = -\gamma b_z M_y - \frac{M_x}{T_2}$$

$$\frac{dM_y}{dt} = \gamma b_z M_x - \gamma B_1 M_z - \frac{M_y}{T_2}$$

$$b_z = \frac{\delta\omega}{\gamma} + B_m \cos\omega_m t$$



$$h(\omega,\omega_{res}) = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{(\omega-\omega_{res})^2}{2\sigma^2}\right)$$

Passage conditions

$$\varepsilon_A = \frac{\gamma B_1^2}{B_m \omega_m},$$ Adiabatic passage

$$\varepsilon_R = \frac{B_m}{B_1}\omega_m T_1,$$ Rapid Passage

$$\varepsilon_F = \omega_m T_1,$$ Fast passage

$\sigma/\gamma = 2.5\times10^{-4}$T

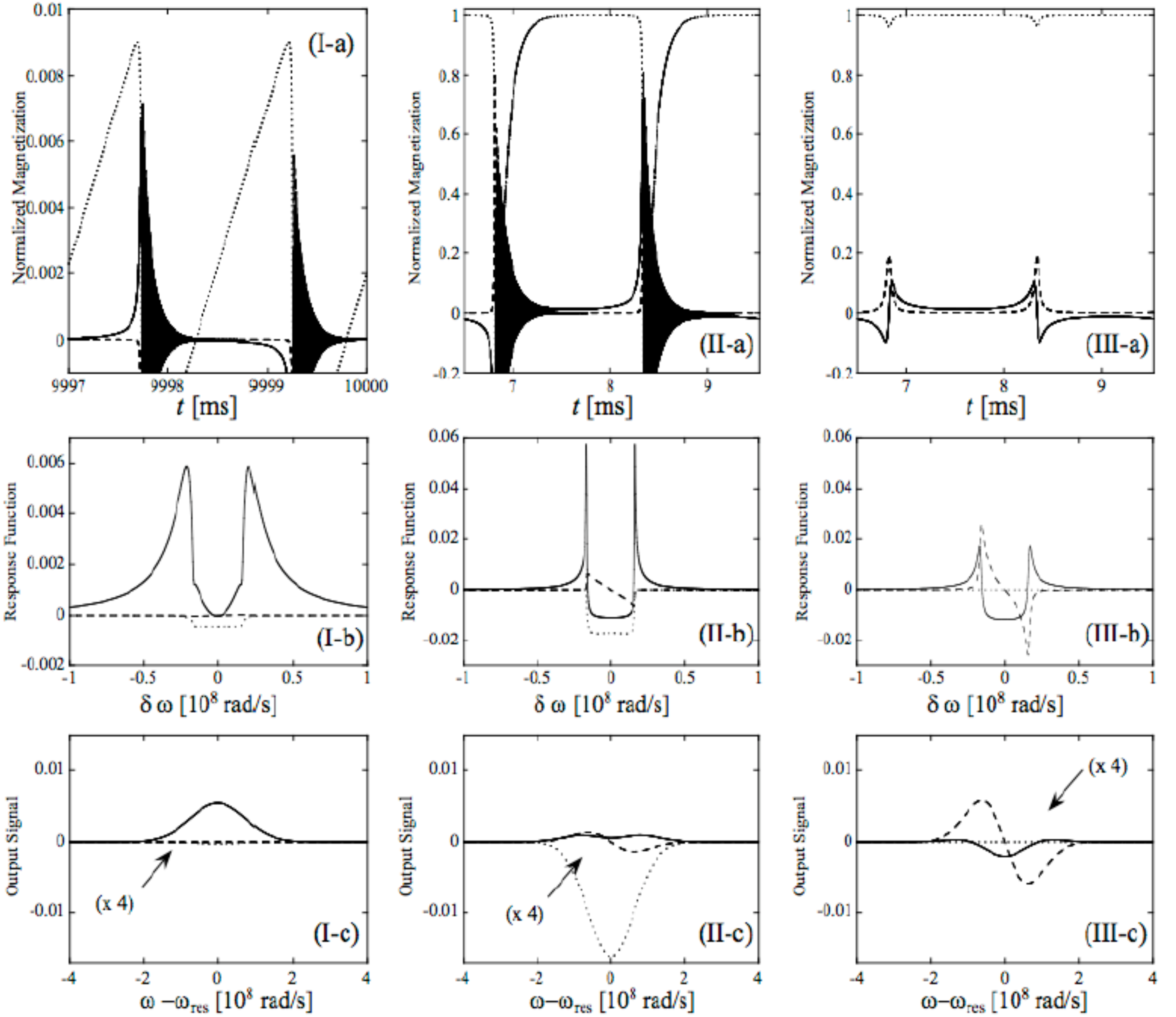
$\omega_m/2\pi = 330$ Hz

$B_m = 9.1\times10^{-5}$ T

$B_1 = 2.2\times10^{-6}$T

$T_2 = T_1$ for $T_1 < 10^{-4}$ s

$T_2 = 1\times10^{-4}$ s for $T_1 > 10^{-4}$ s



(I-a)
(II-a)
(III-a)
Normalized Magnetization
t [ms]
(I-b)
(II-b)
(III-b)
Response Function
δ ω [10^8 rad/s]
(I-c)
(II-c)
(III-c)
Output Signal
(x 4)
ω −ω_res [10^8 rad/s]

T_1- Dependence of Intensity for various passage conditions

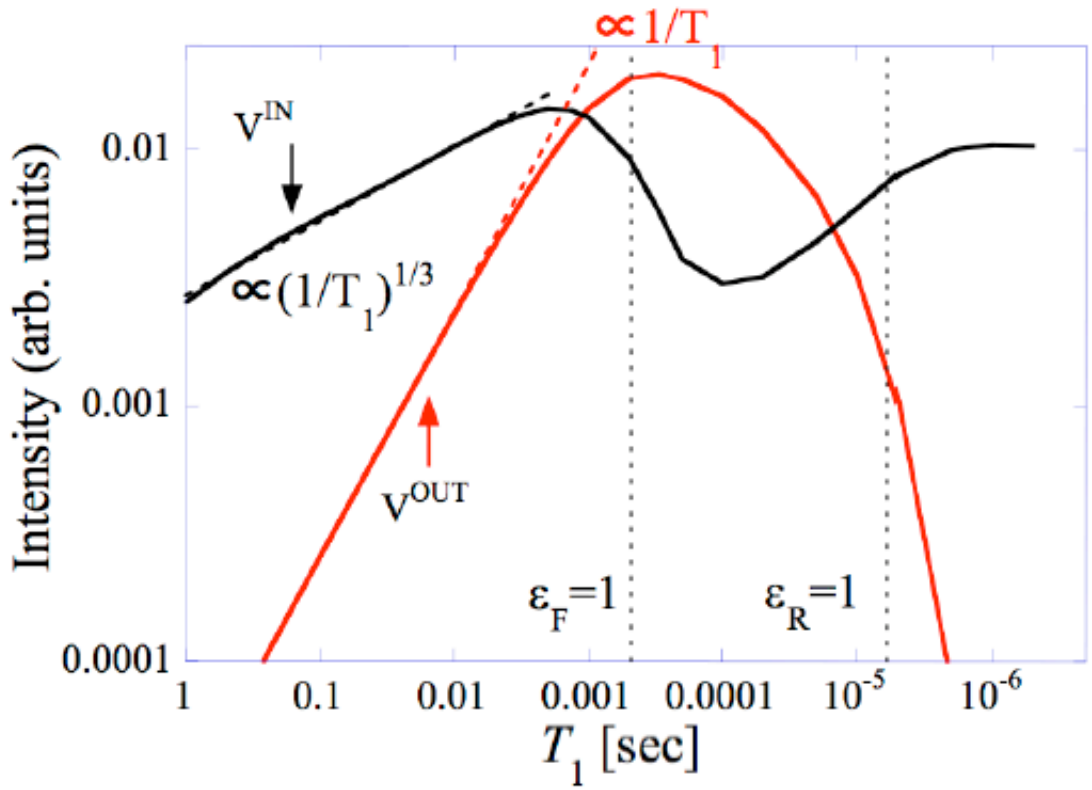
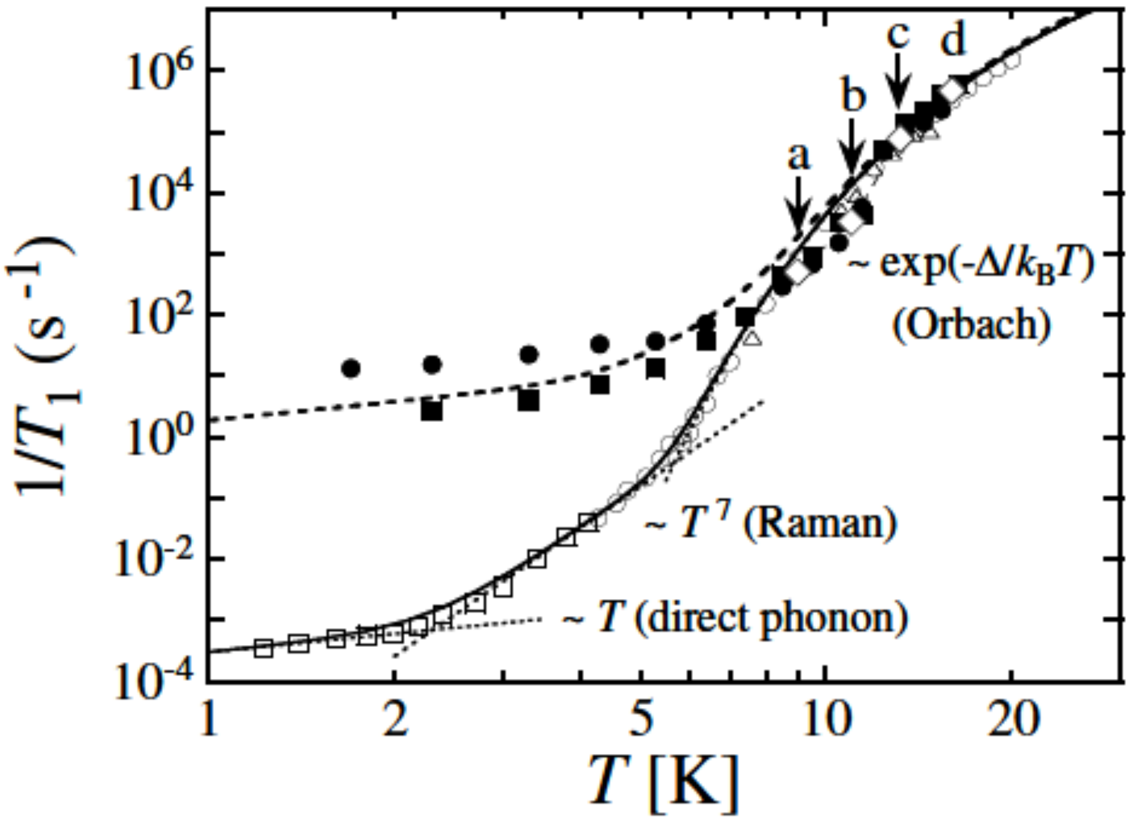


Fig. 6 Intensities of V^{IN} and V^{OUT} as a function of T_1. The mixing parameter A=4 is used to calculate $M^{\mathrm{IN}} = M_x^{\mathrm{IN}} + 4\, M_y^{\mathrm{IN}}$

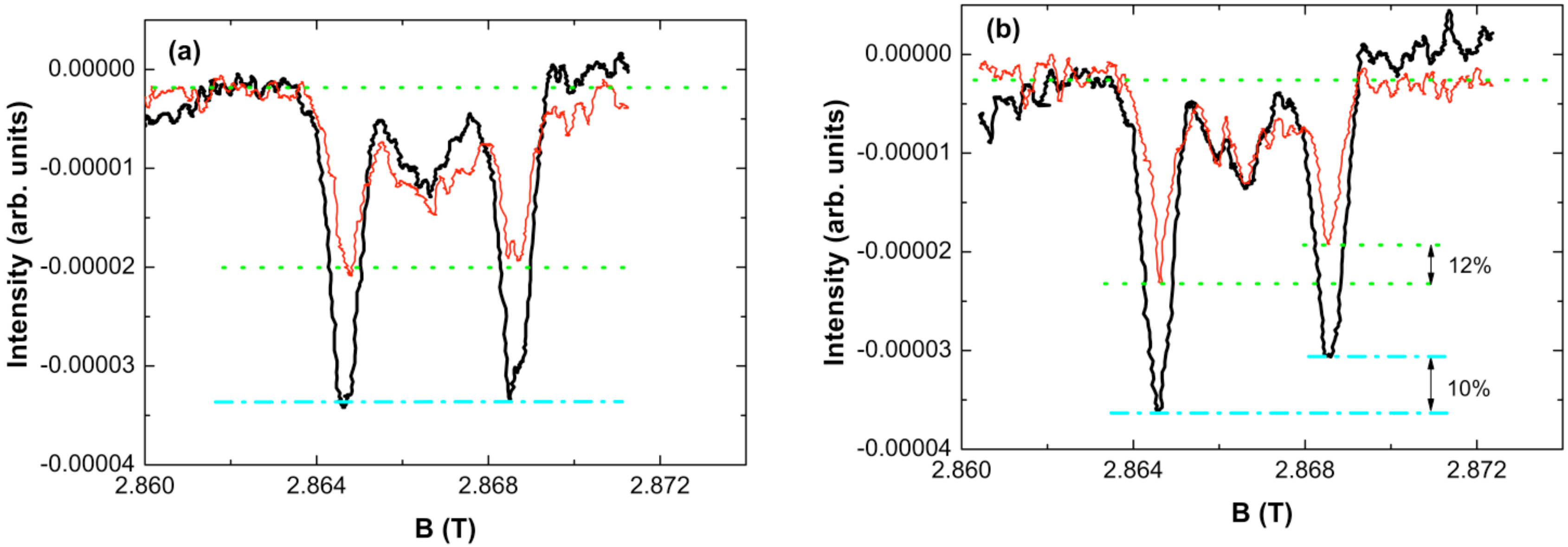
$T_1(T)$ at B = 3T

First observation of T_1 at high fields



T_1(T=0.1 K) is expected to be 10 sec at B = 3 T.

Dynamic Nuclear Polarization of ^{31}P (DNP) ?



(black lines: in-phase signals, red lines: out-of-phase.)

$$\frac{\Delta I}{I_+ + I_-} = 10\%$$

$$= 10^3 \times \left. \frac{\mu_N H}{2k_B T} \right|_{T=6.9\,K,\,H=3\,T}$$