INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
34100 TRIESTE (ITALY) - P.O.B. 586 - MIRAMARE - STRADA COSTIERA 11 - TELEPHONES: 224281/2/3/4/5/6
CABLE: CENTRATOM - TELEX 460392-I

SMR/94- 25

SPRING COLLEGE ON AMORPHOUS SOLIDS
AND THE LIQUID STATE

14 April - 18 June 1982

LUMINESCENCE AND SPIN RESONANCE IN AMORPHOUS SILICON

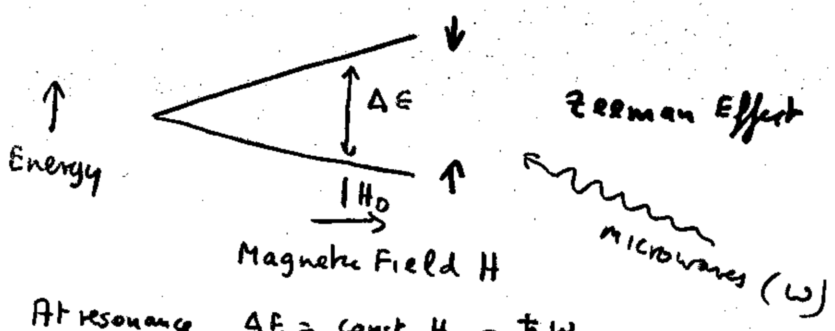
(Lecture II)

R.A. STREET

Xerox Corporation
Palo Alto Research Center
3333 Coyote Hill Road
Palo Alto, California 94304
USA

These are preliminary lecture notes, intended only for distribution to participants.
Missing or extra copies are available from Room 230.

Electron Spin Resonance ESR



At resonance $\Delta E = \text{const.}\ H_0 = \hbar\omega$

(precession frequency $\gamma H_0 = \omega$)

For defects in semiconductors

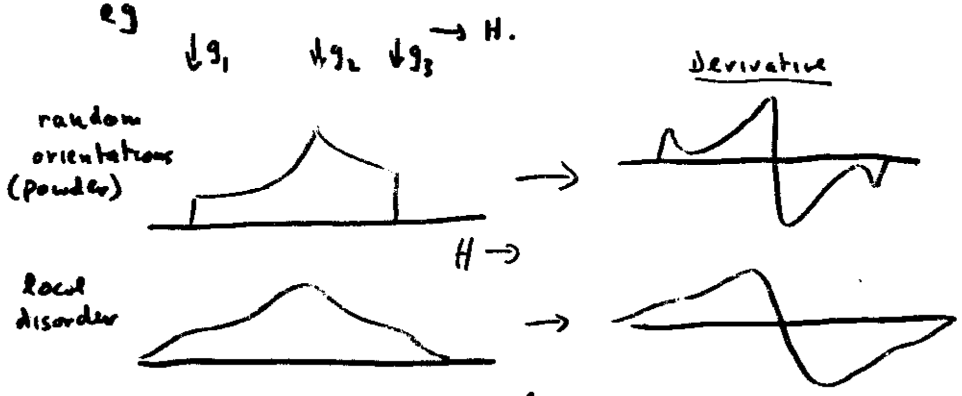
$$\mathcal{H} = \mu_B H_0 \cdot \underbrace{g}_{\text{g-tensor}} \cdot \overset{\text{spin}}{S} + \underbrace{\overset{\text{nuclear moments}}{\sum_i I_i \cdot A_i \cdot S}}_{\text{Hyperfine.}}$$

Free electron $g = g_0 = 2.0023$

in solid $g = g_0 + \Delta g_{ij}$

$$\Delta g \sim \sum \frac{\langle d | V_{so}^{i} | p \rangle \langle p | L_j | d \rangle}{(E_d - E_p)}$$

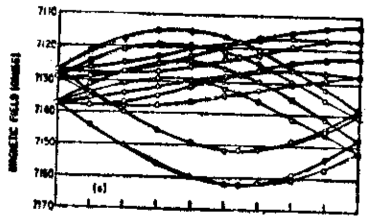
eg



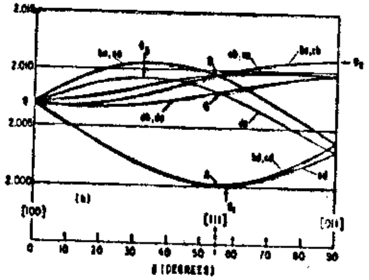
ESR xtal Si

Vacancy-Phosphorus center

ESR absorption

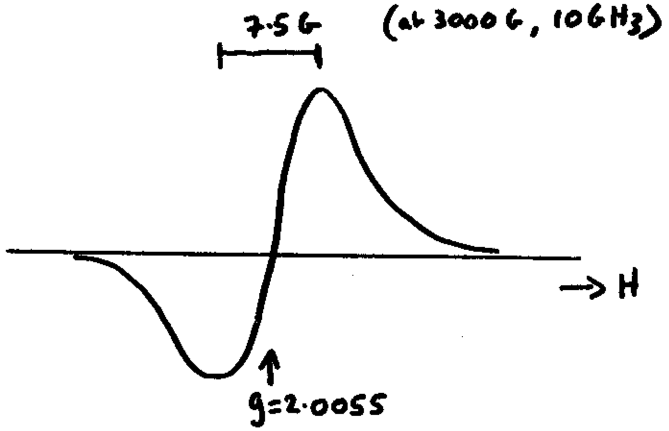


rotating sample (0$\bar{1}$1) plane



model

ESR in a-Silicon

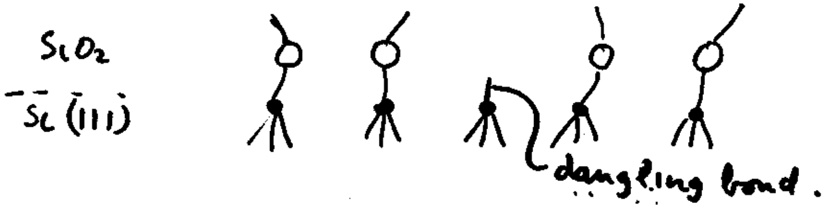


observed

- in Evaporated or Sputtered a-Si
  $N_s \sim 10^{19}/cm^3$
- in Glow Discharge or Sputtered a-Si:H
  $N_s \sim 10^{15} - 10^{18}$ cm^{-3}
- in bombarded crystalline Si
- in poly crystalline Si.

Inhomogeneous line ie. distribution of g-values

xtal Si / SiO$_2$ interface



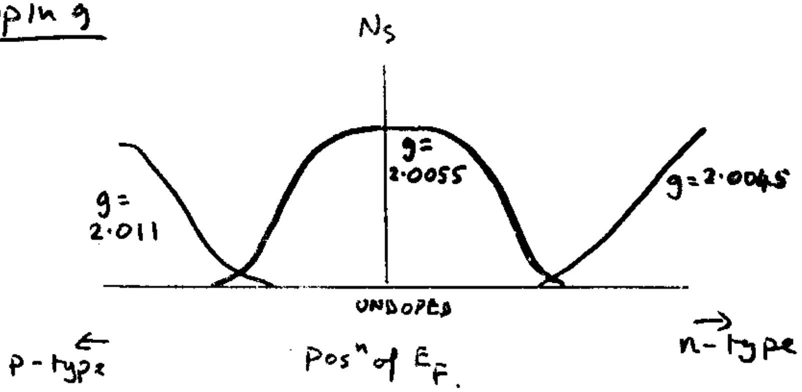
Observation ESR $g_{\uparrow} = 2.0012$
$g_{\rightarrow} = 2.0082$
$N_s \sim 10^{12}/cm^2$ surface spins

identified as dangling bonds

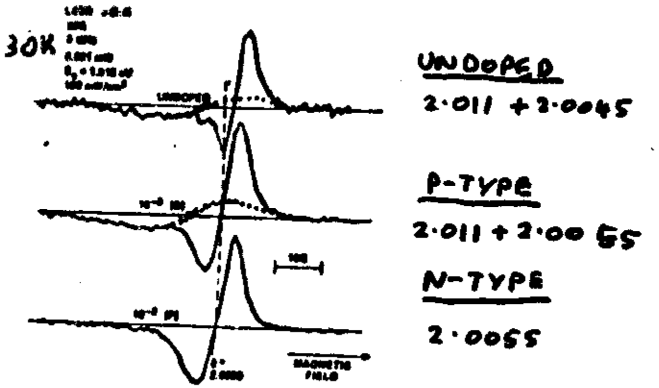
Take powder pattern + disorder broadening
$\Rightarrow g \approx 2.0055$

Implies that ESR in a-Si is also dangling bond.

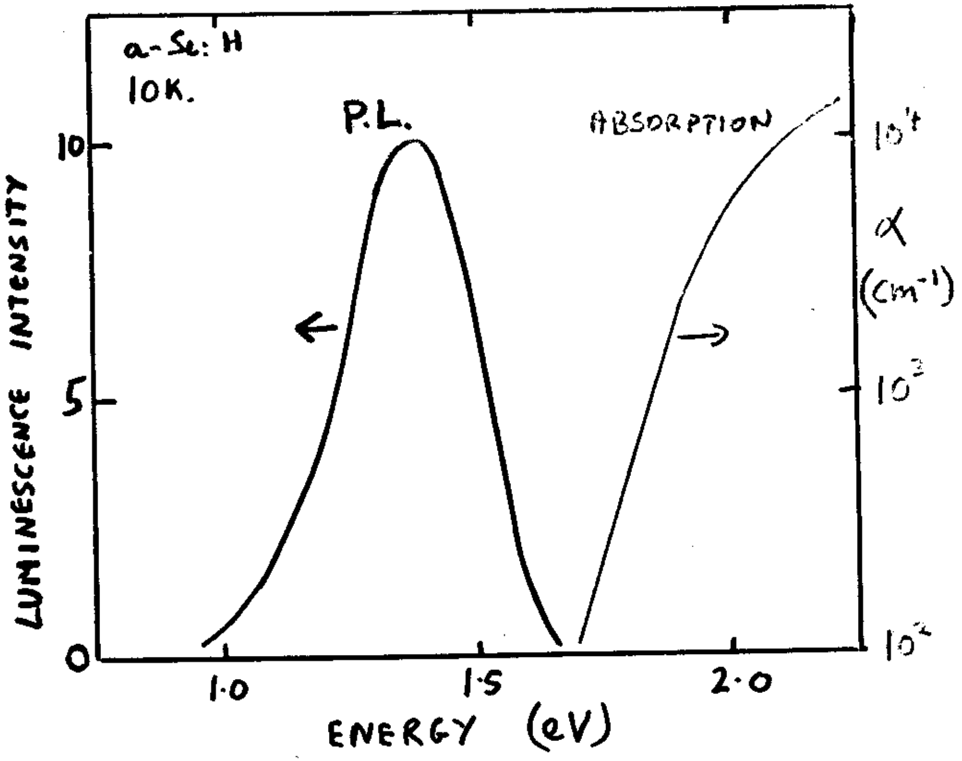
Doping



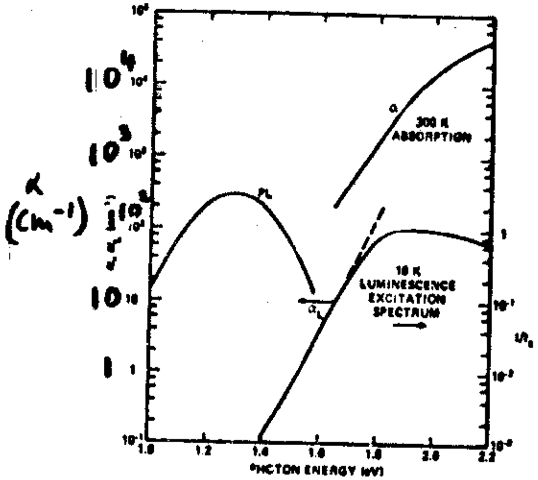
LIGHT INDUCED ESR



LUMINESCENCE IN a-Si:H



Phonon Coupling?



Detailed balance

$$\tau^{-1} = \frac{8\pi n^2}{\lambda^2}\left(\frac{g_1}{g_2}\right) N^{-1}\int \alpha \, d\nu$$

Recombination rate $= \underline{y_L G} = N_{occ}\tau^{-1}$

$$\leq N\tau^{-1} = \frac{8\pi n^2}{\lambda^2}\left(\frac{g_1}{g_2}\right)\int \alpha \, d\nu$$

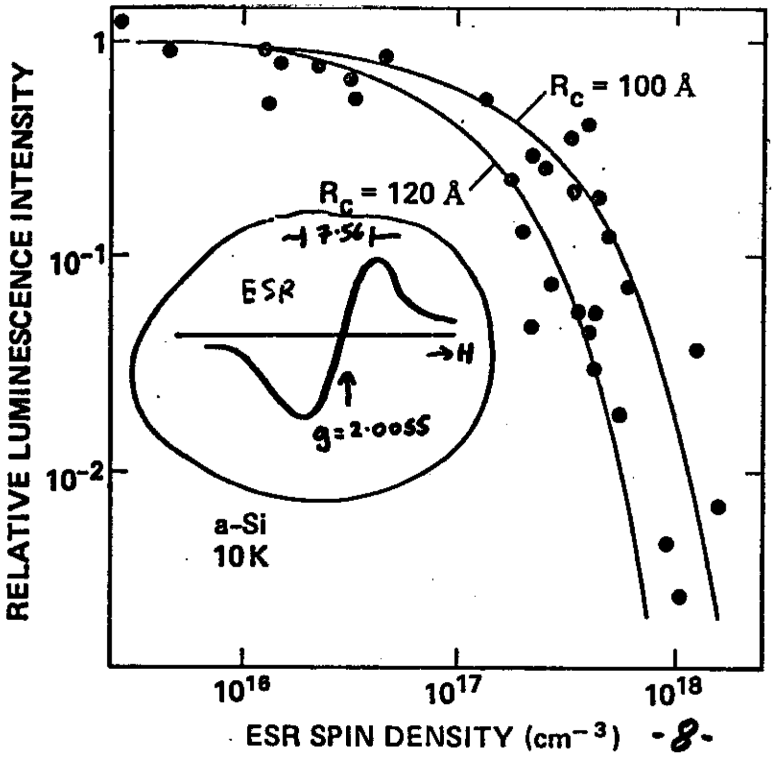
therefore gives lower bound on $\int \alpha \, d\nu$

<u>but</u> too large by $\sim 10^4$

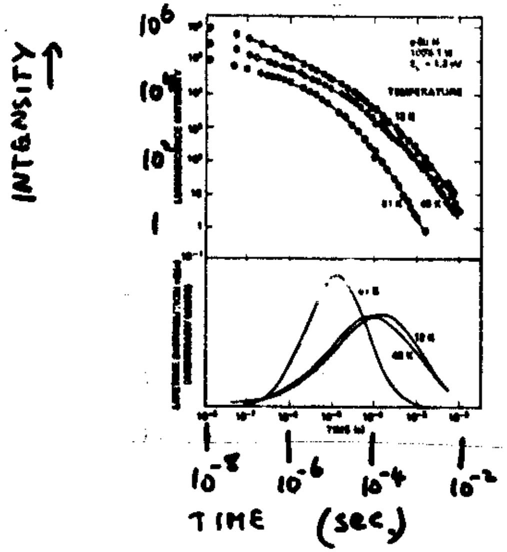
$\therefore$ Phonon coupling

Estimate Zero Phonon Energy $\sim$ 1.6 – 1.7 eV

Stokes Shift $\sim$ 0.4 eV



Luminescence Decay



Decay times extend from 10^{-7} sec to 10^{-2} sec

mostly $10^{-4}-10^{-3}$ sec

$\Rightarrow$ very weak overlap

$\Rightarrow$ tunnelling between localized states

$$\tau = \underset{\overset{\uparrow}{10^{-8}}}{\tau_0} \exp(2R/R_0) \qquad R/R_0 \sim 5$$

Calculation of Non-Radiative Transition Rate to Defects

1) Define critical Transfer Radius R_c
as distance for which
Non-Rad Rate = Rad. Rate.

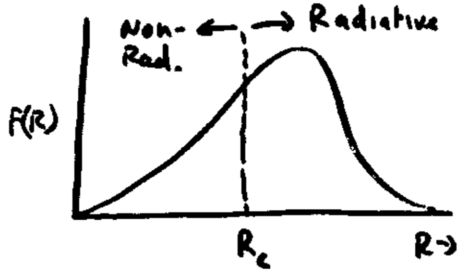
$$\omega_0 \exp(-2R_c/R_0) = \tau_R^{-1}$$

or
$$R_c = \frac{R_0}{2} \ln(\underbrace{\omega_0}_{10^{12}\ \text{sec}^{-1}} \overbrace{\tau_R}^{10^{-4}\ \text{sec}})$$

$$R_c \cong 10\, R_0$$

2) For a random distribution of defects
nearest-neighbour distance given by

$$F(R) = 4\pi R^2 N \exp(-4/3\, \pi R^3 N)$$

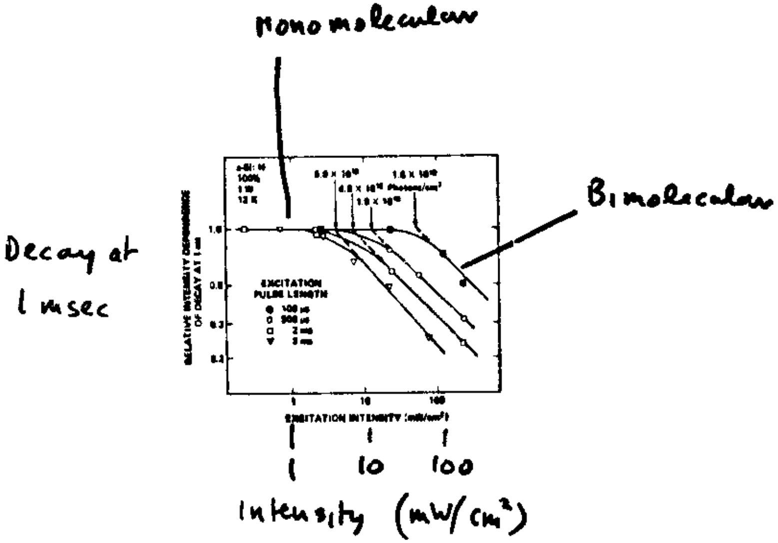


So Luminescence efficiency
given by

$$\eta_L = \int_{R_c}^{\infty} F(R)\, dR = \exp(-\tfrac{4}{3}\pi R_c^3 N)$$

Data $\Rightarrow$ $R_0 \sim 10$ Å

Recombination Kinetics



Interpreted as transition from Geminate to non-geminate recombination

Transition occurs at a pair density $\sim 10^{18}$ cm^{-3}

$\Rightarrow$ Pair radius ~ 50 Å