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SPRING COLLEGE ON AMORPHOUS SOLIDS
AND THE LIQUID STATE

14 April - 18 June 1982

DEFECTS AND DEFECT MODELS
(Part II)

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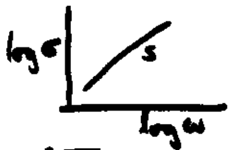
2b A.C. Conductivity (again)

QMT (quantum mechanical tunnelling) model

$$\sigma(\omega) \propto T\,\omega\,\ln^4\left(\frac{\nu_0}{\omega}\right)$$

$$s = \frac{d\ln\sigma(\omega)}{d\ln\omega} = 1 - \frac{4}{\ln\left(\frac{\nu_0}{\omega}\right)}$$



$s < 0.8$ $s \downarrow\ \omega \uparrow$ s indep of T

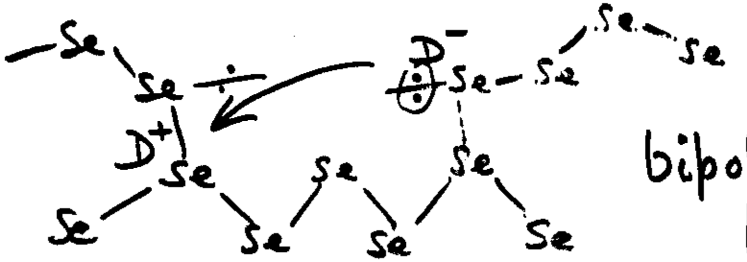
Expl results on chalcogenides (see transparencies)

s 0.8–1 s indep of ω $s \uparrow\ T \downarrow$

Also s and $\sigma(\omega)$ depend on band gap!

CBH (correlated barrier hopping) model

ELLIOTT. S.R.
- Phil Mag 36 1291 (1977)
- Solid State Comm 28 939 (1978)
- J. Non-Cryst. Sol 35-36 855 (1980)
- Phil Mag B 37 553 (1978)
- Phil Mag B 40 507 (1979)
- Phil Mag B 38 325 (1978)



bipolaron hopping

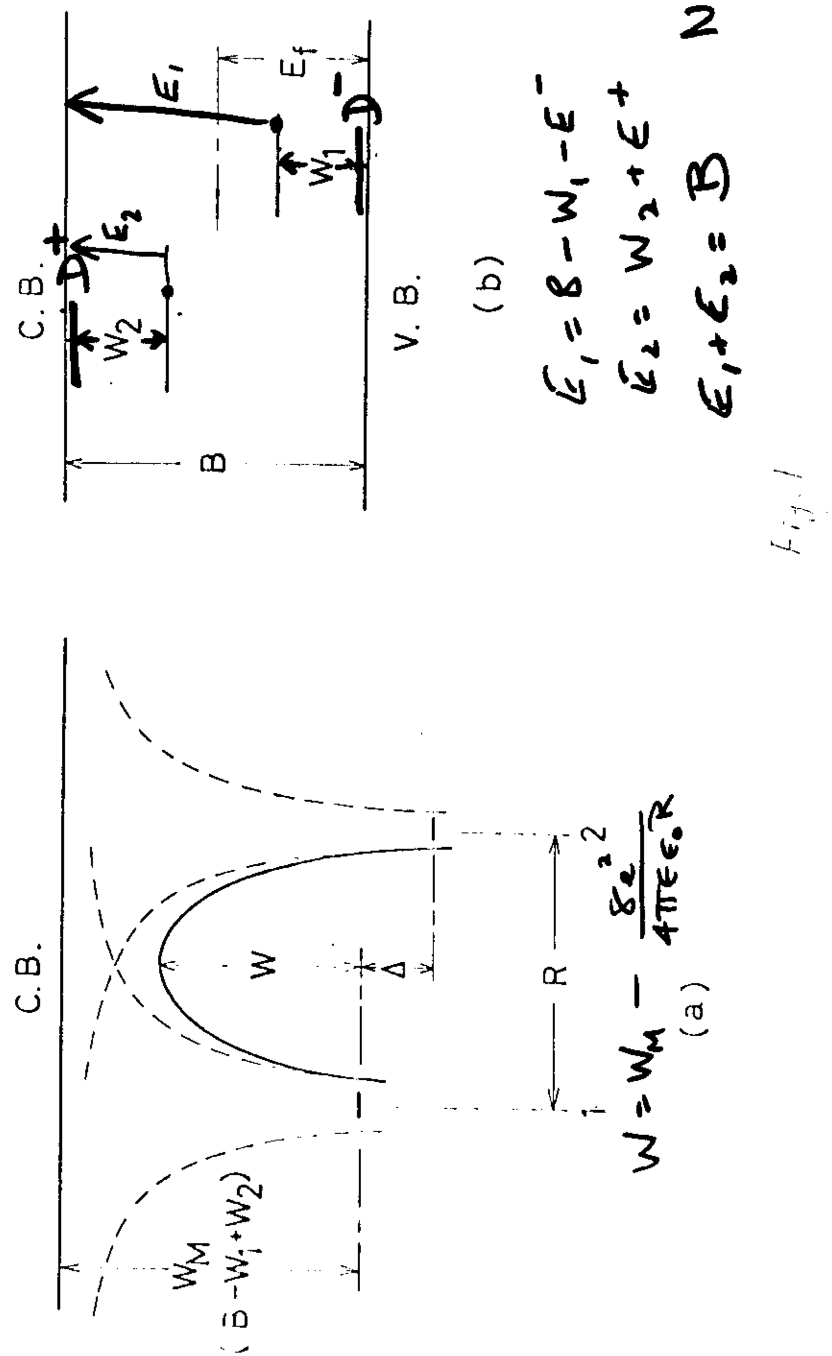
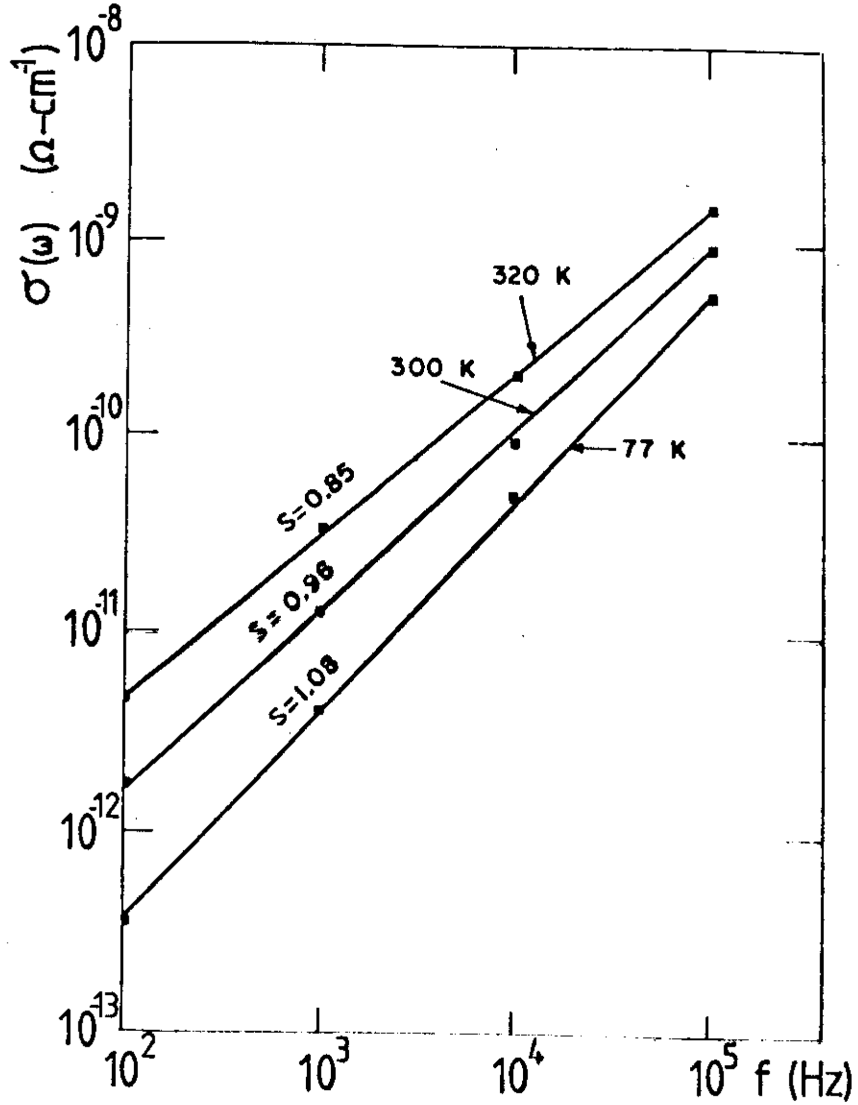


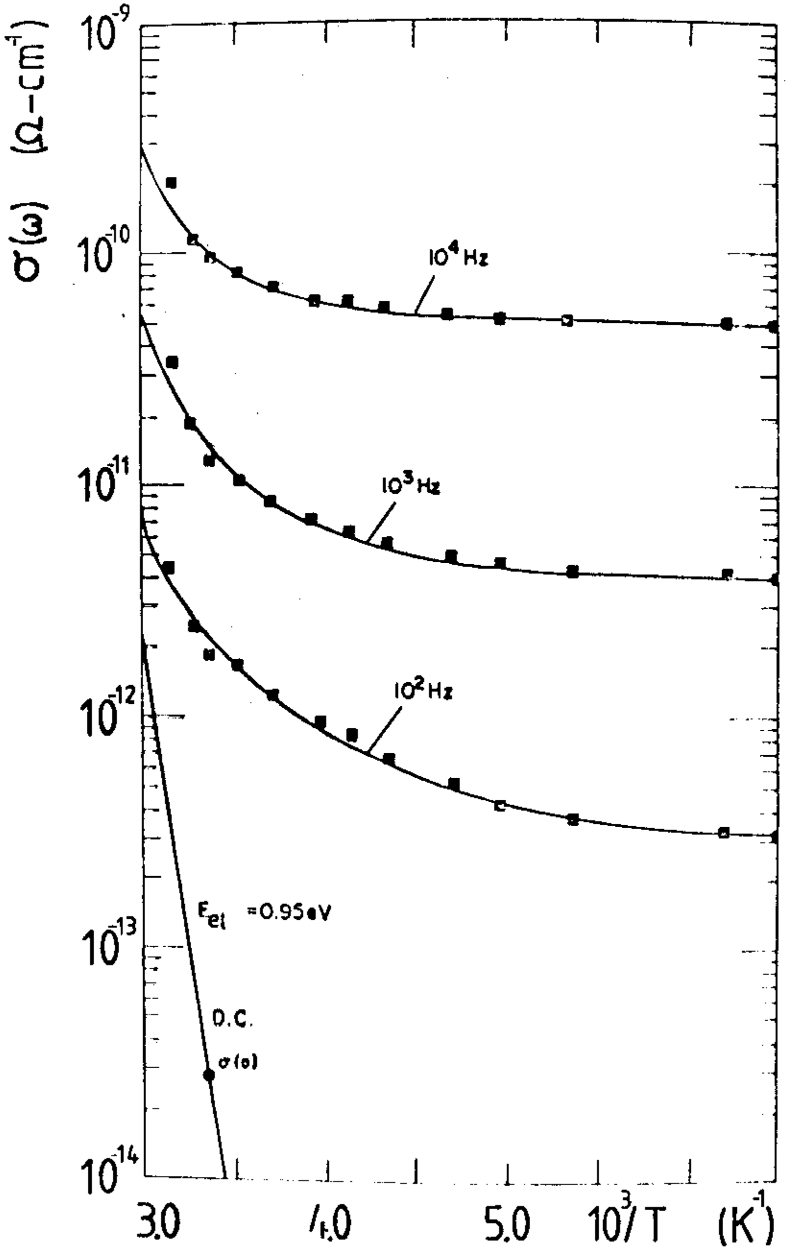
Fig. 1

3

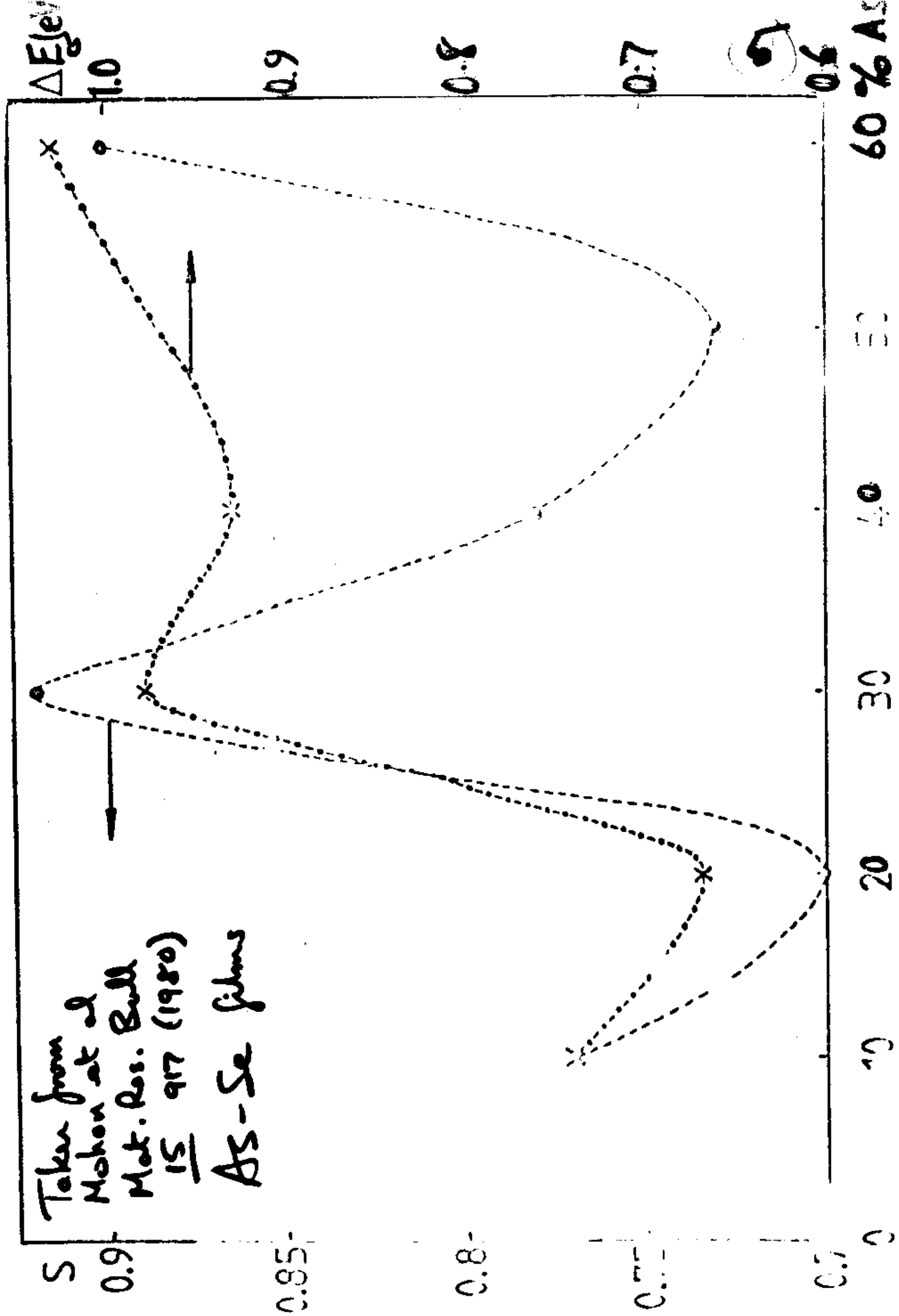


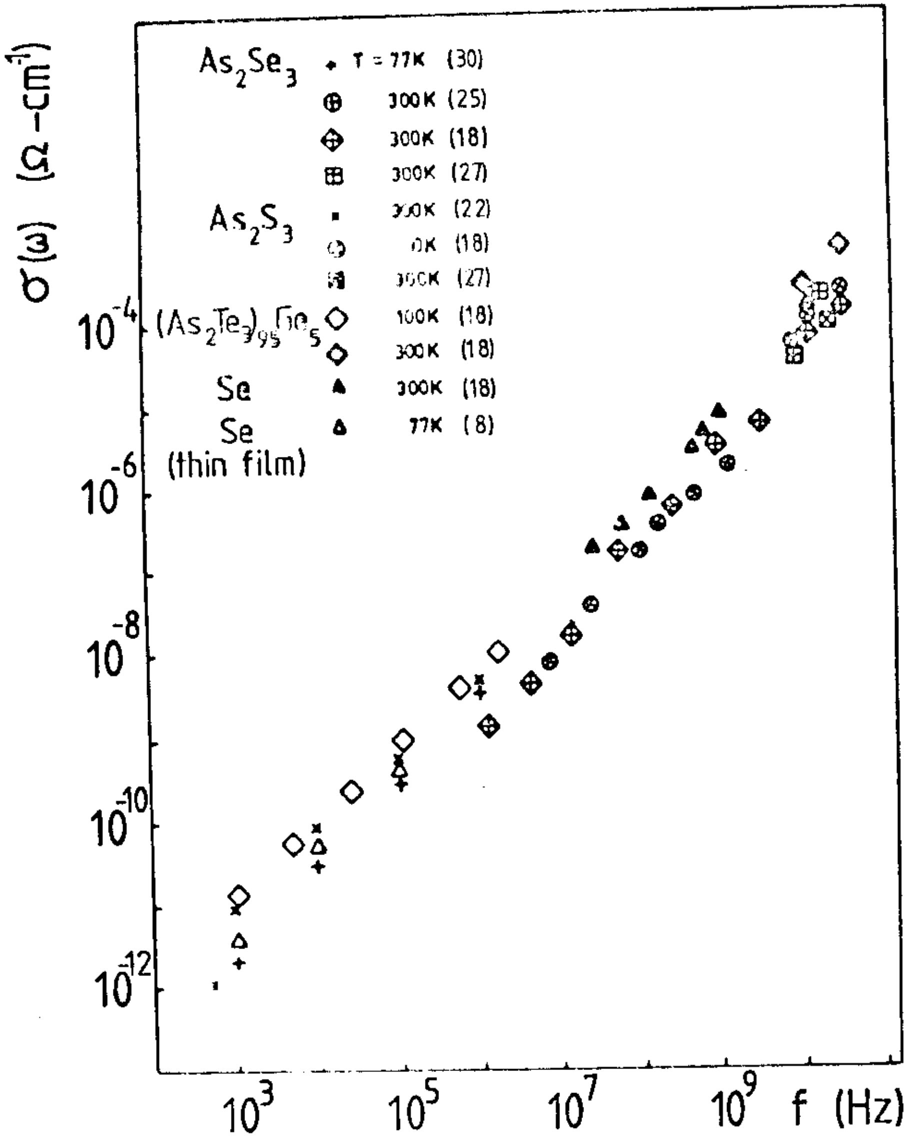
Thin films a-Se
Lakatos + Abkowitz Phys Rev 3 1791 (1971)

4



Lakatos + Abkowitz Phys Rev 3 1791 (1971)





Chalcogenide glasses

$$\left\{ \begin{array}{l} s \sim 1 \\ \sigma(\omega) \text{ indep of } T \\ \sigma(\omega) \text{ indep. of material!} \end{array} \right.$$

Electric field $E(t) = E\sin\omega t \rightarrow$ polarization $P(t)$

$$P(\omega) = \epsilon_0\, \chi(\omega)\, E(\omega)$$

susceptibility $= \chi'(\omega) - i\,\chi''(\omega)$

dielectric loss

$$\sigma(\omega) = \epsilon_0\, \omega\, \chi''(\omega)$$

For a Debye response (osc. charge or dipole time constant τ)

$$\chi''(\omega) = \chi(0)\,\frac{\omega\tau}{1+\omega^2\tau^2}$$

For a single τ, loss peak when $\omega\tau = 1$ and $\sigma(\omega) \propto \omega^2$ for $\omega\tau < 1$

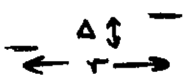
In non-cryst. systems there will be a distr^{n} of τ

$$\sigma(\omega) = \int_0^\infty \alpha\, n(\tau)\,\frac{\omega^2\tau}{1+\omega^2\tau^2}\,d\tau$$

In QMT $\quad \tau = \tau_0 \exp 2\alpha r \quad$ with a spread in r (random distr^{n})

In CBH $\quad \tau = \tau_0 \exp\left(\frac{W}{kT}\right) \quad$ with W correlated with r

Pair approximation: α = polarizability of a pair of sites



$$= \frac{e^2 r^2}{12kT\cosh^2(\Delta/2kT)} \times 4 \text{ for bipolarons}$$

Integrate Δ over the range $0-\Delta_0$ assuming a flat distribution $\rightarrow$ factor $\frac{2kT}{\Delta_0}\tanh\left(\frac{\Delta_0}{2kT}\right)$

Integrate over a random distr^{n} of r

$$dp(r) = 4\pi N r^2 dr$$

$$\sigma(\omega) = \frac{N}{2}^{2}\,\frac{2kT}{\Delta_0}\tanh\left(\frac{\Delta_0}{2kT}\right)\omega \int \frac{e^2r^2}{3kT}\,\frac{\omega\tau}{1+\omega^2\tau^2}\,4\pi r^2 dr$$

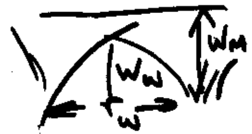
$\frac{N}{2}$ = no. of hopping pairs of electrons

Change integration variable $r \rightarrow W$

$$dW = \frac{2e^2}{\pi\epsilon\epsilon_0 r^2}\,dr$$

to find $\sigma(\omega) = \frac{\pi^3}{3} N^2 \epsilon\epsilon_0 \frac{kT}{\Delta_0}\tanh\left(\frac{\Delta_0}{2kT}\right)\omega\, r_\omega^6$

where $r_\omega = \left(\frac{2e^2}{\pi\epsilon\epsilon_0}\right)\frac{1}{W_m - W_\omega}$



and $W_\omega = kT\ln\left(\frac{1}{\omega\tau_0}\right)$

$$(W_M - W_\omega)^{-6} \rightarrow \frac{1}{W_m^6}\left(\frac{1}{\omega\tau_0}\right)^{\beta}\exp\left[3\left(\frac{kT}{W_m}\right)^2\ln^2\left(\frac{1}{\omega\tau_0}\right)\right]$$

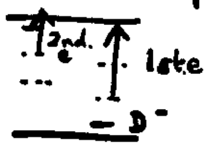
(exact to 2nd order)

$$\boxed{\sigma(\omega) \simeq \frac{\pi^3}{3}N^2\epsilon\epsilon_0\frac{kT}{\Delta_0}\tanh\left(\frac{\Delta_0}{2kT}\right)\left(\frac{2e^2}{\pi\epsilon\epsilon_0 W_m}\right)^6\frac{\omega^s}{\tau_0^{\beta}}}$$

where $s = 1-\beta$

and $\beta = \frac{6kT}{W_m}$

Now $W_m \sim$ band gap B



$\therefore \sigma(\omega) \propto B^{-6}$

$s = 1 - \frac{6kT}{B}$

$= 0.85$ for $B = 1eV$ } at RT
$= 0.93$ for $B = 2eV$

Plot of $\ln[\sigma(\omega)/[e^5/N^2]]$ vs $\ln B$ should have slope of -6

(see slide – slope $= -6.3$)

$\sigma(\omega)$ vs $\sigma(0)$ – see vu-graph

RANDOM curve assumes N constant
– data for films

PAIRED curve
– data for glasses

IVAPs $G(r) = 4\pi N r^2 \exp\left(-\frac{4\pi N r^3}{3}\right) \exp\left(\frac{e^2}{4\pi\epsilon\epsilon_0 k T_g r}\right)$

T_g = glass transition temp.

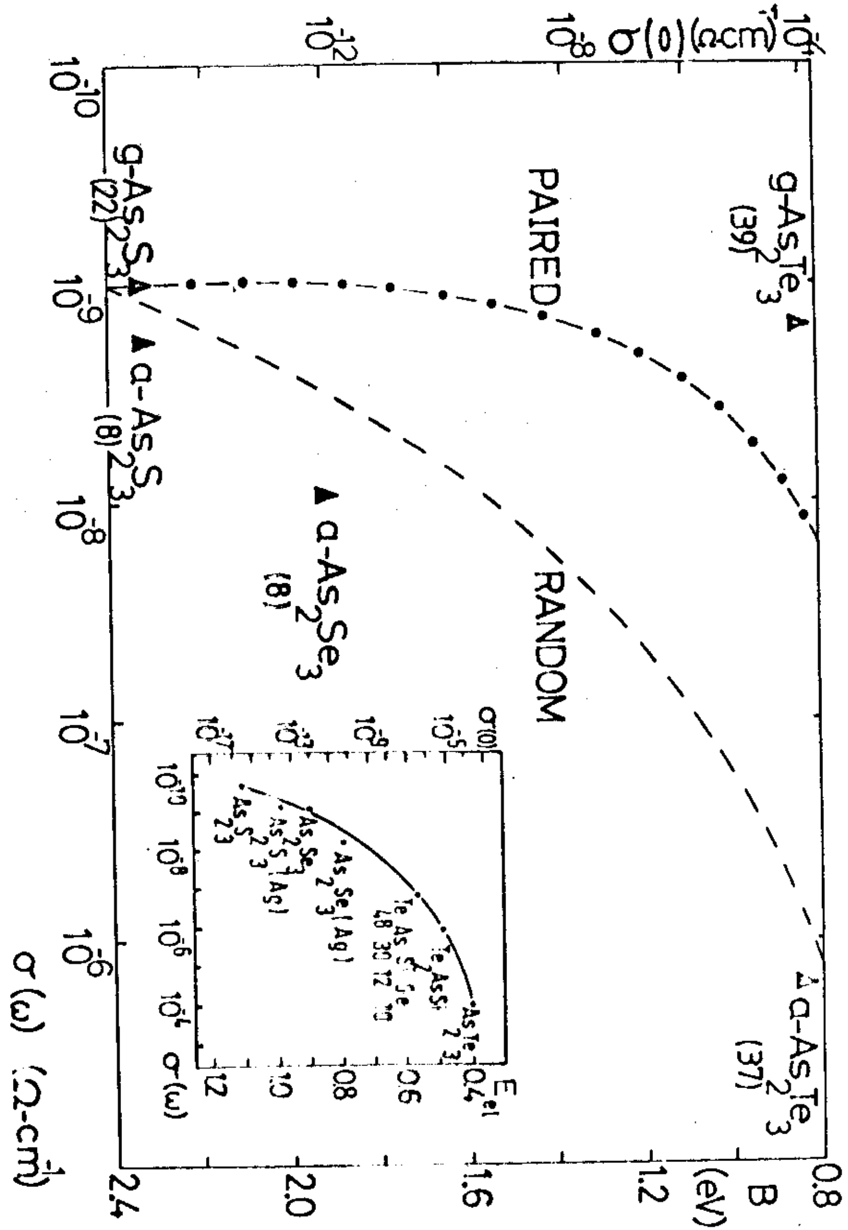
($r_{min} = 4.5$ Å) $s = 1 - \beta + \delta$, $\delta = \frac{T}{8T_g}$

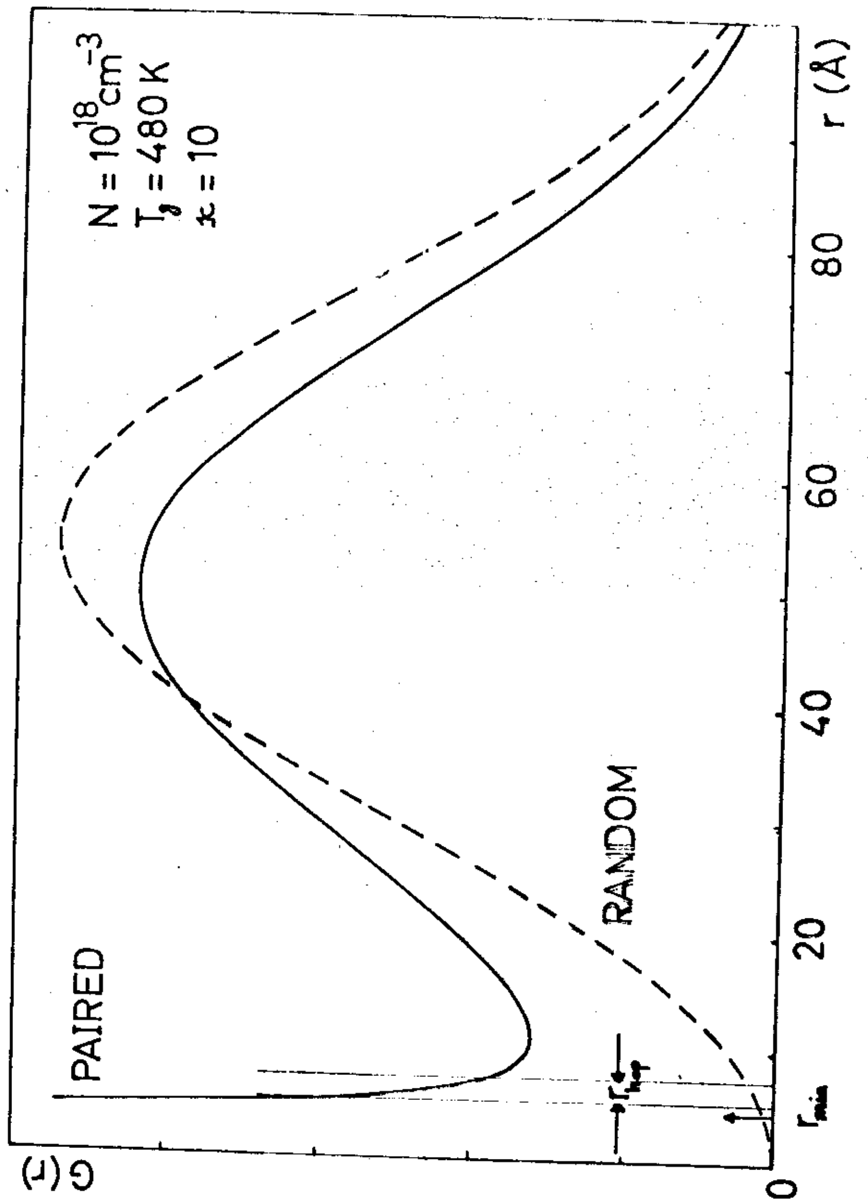
$s > 1$

(i) Shimakawa (Grenoble conference 1981 (1982 – J de Physique))

has extended this to case where D^0s are thermally created

(ii) Long + Balkan (Phil Mag B41 287 1980)
– a-Ge   – a-Si:H





④ Defects in Group-V materials

As, P, Sb

a-Ge	a-Si:H	a-Se
a-Si	>Si–H	a-As_2Se_3
a-III-Vs	>Si<H	a-SiO_2
4-fold rigid	→	essentially 2-fold flexible
v.b. sp^3 bonds		lone-pair non-bonding
defects dangling bonds ←.		charged paired defects
+ve U	-ve U ?	VAP IVAP −ve U
$T^{1/4}$	No $T^{1/4}$	No $T^{1/4}$
ESR	No ESR	No ESR
$\sigma(\omega)$ QMT?		$\sigma(\omega)$ CBH

Defects in Group-V materials

1 Davis in Topics in Applied Physics Vol 36 "Amorphous Semiconductors" (Ed) M.H. Brodsky 1979

2 Elliott + Davis J Phys C 12 2577 (1979)

3 Davis J Phys Soc Japan 49 1139 (1980)

4 Davis J de Physique 42 C4-855 (1981)

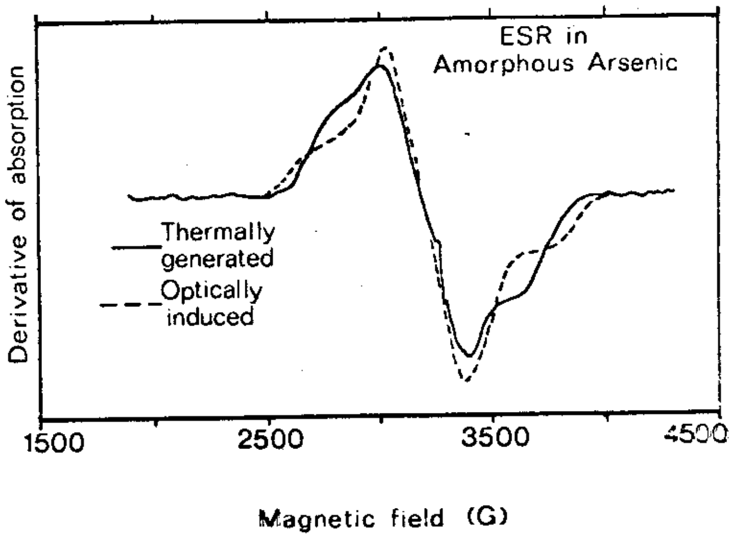
5 Fasol + Davis " C4-571

6 Depinna + Cavenett Solid State Comm. 40 813 (1981)

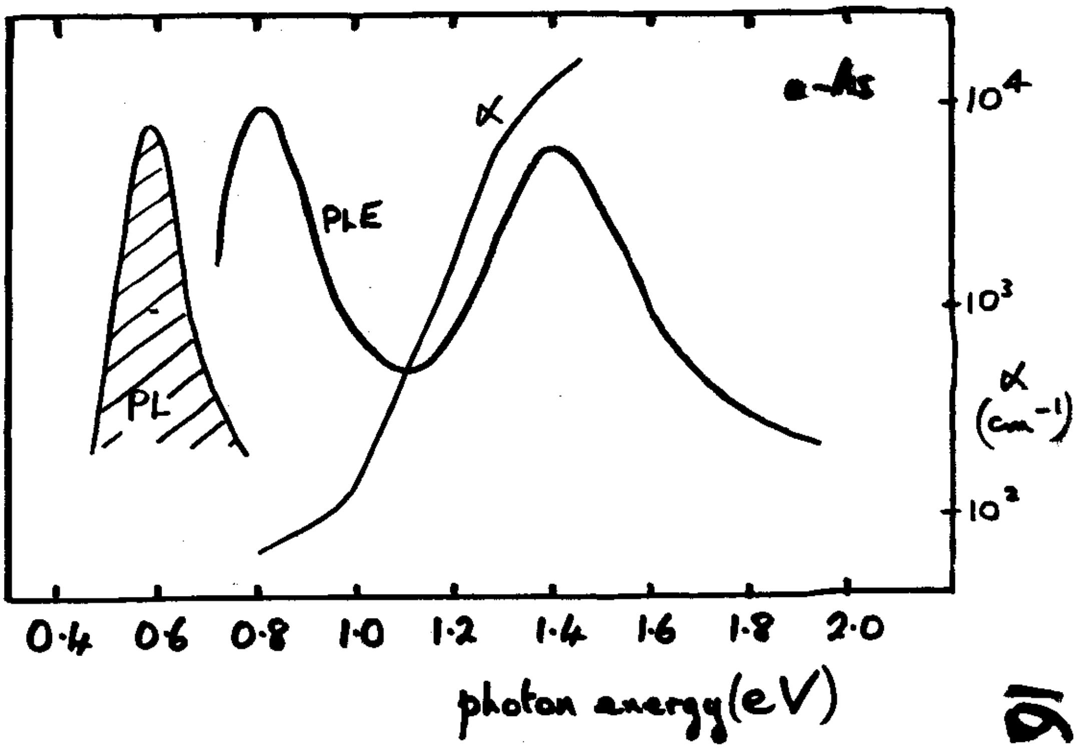
7. Pollard + Joannopoulos Phys Rev B19 4217 (1979) B21 760 (1980)

8 O'Reilly Phil Mag B43 579 (1981)

9. Kastner + Fritzsche Phil Mag B37 199 (1978)


ESR in
Amorphous Arsenic
Derivative of absorption
Thermally
generated
Optically
induced
1500
2500
3500
4500
Magnetic field (G)

15


a-As
α
PLE
PL
10^4
10^3
10^2
α
(cm^{-1})
0·4
0·6
0·8
1·0
1·2
1·4
1·6
1·8
2·0
photon energy(eV)

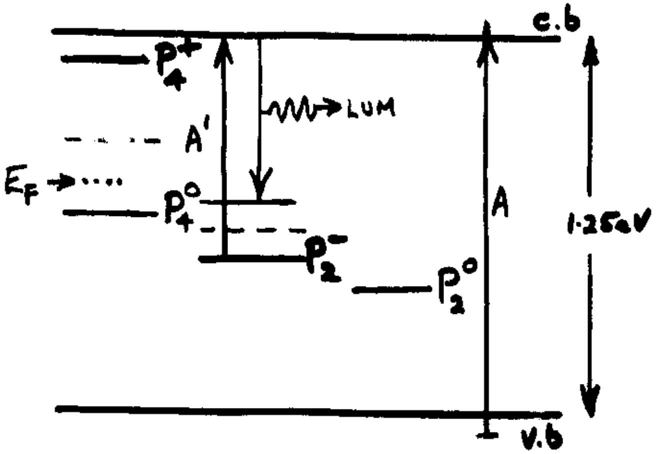
16

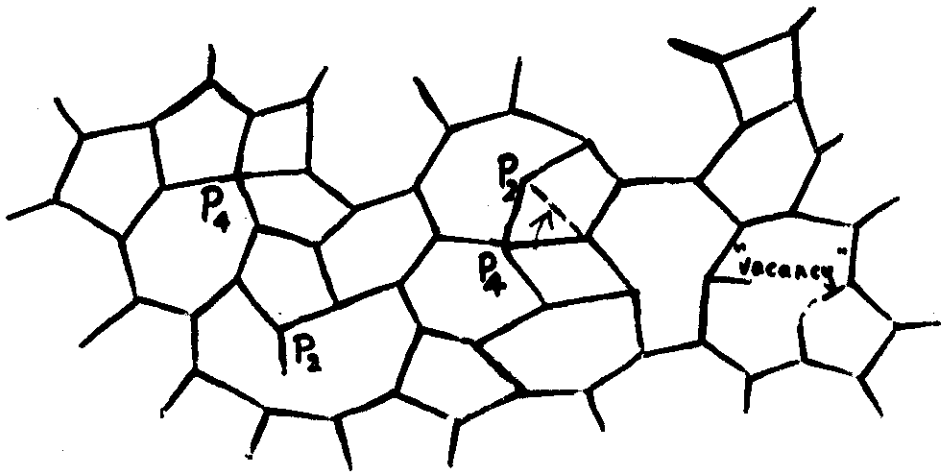
charge state

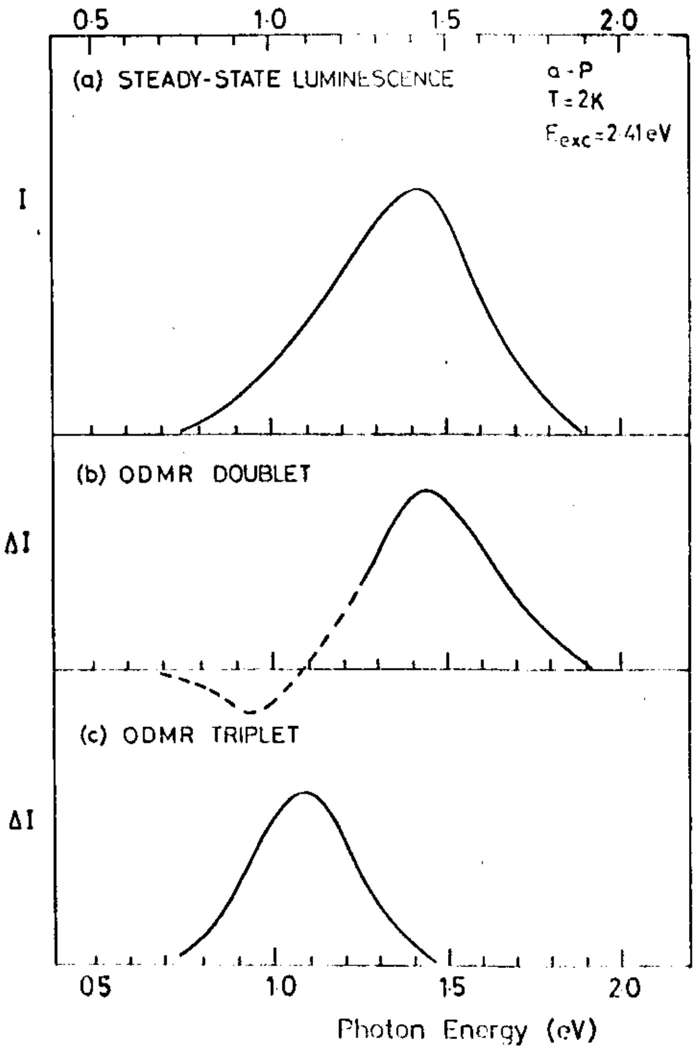
P_4^0

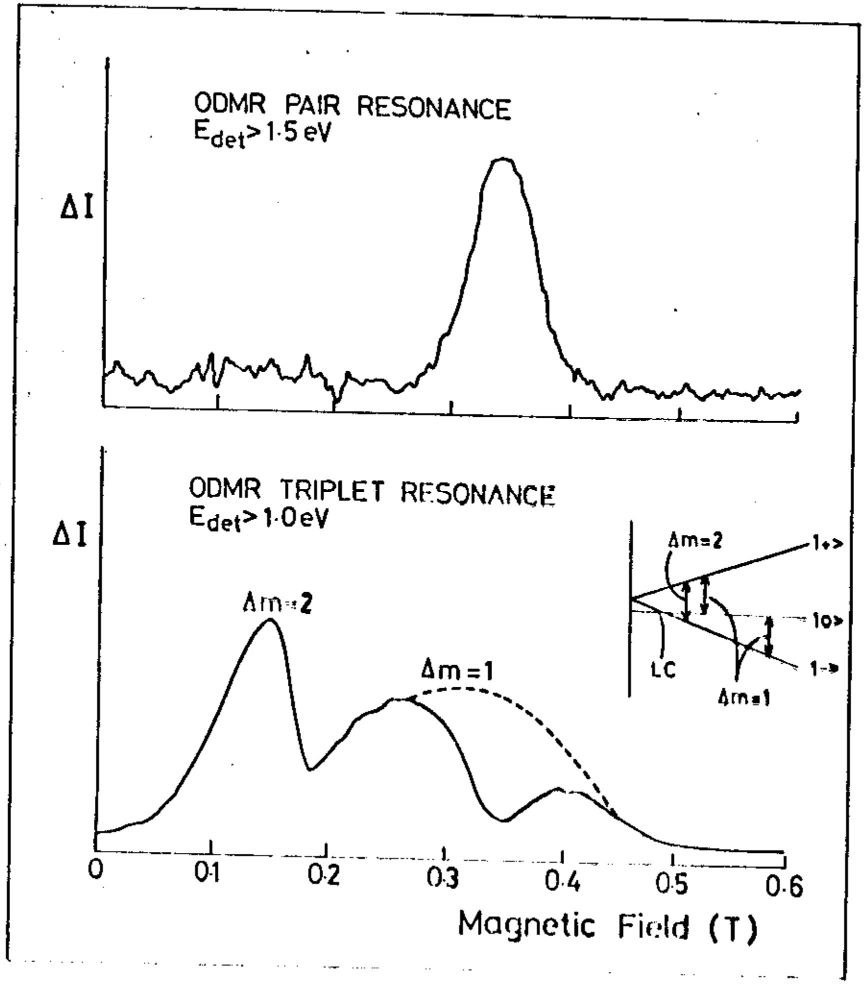
coordination

pnictide









Analogy with chalcs

$$2\,{}_{p}P_2^{0} \rightarrow {}_{p}P_2^{-} + {}_{sp}P_4^{+}$$

— probably not exothermic because of large hybridisation energy ~0.8eV required

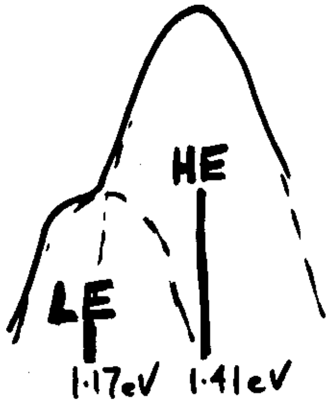
However in certain configurations might be favourable but in which case back reaction easy — weak temp. dependent dark esr signal (NRL)?

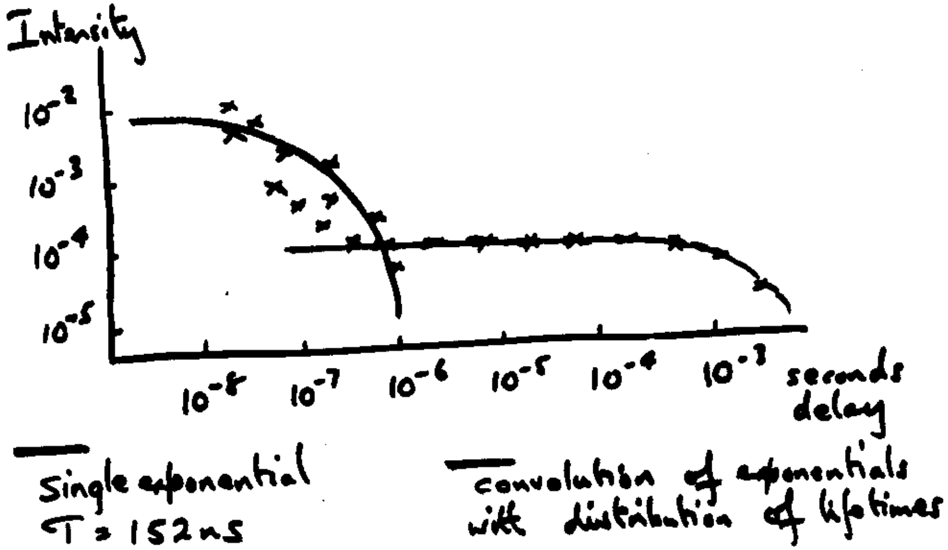
However another route is

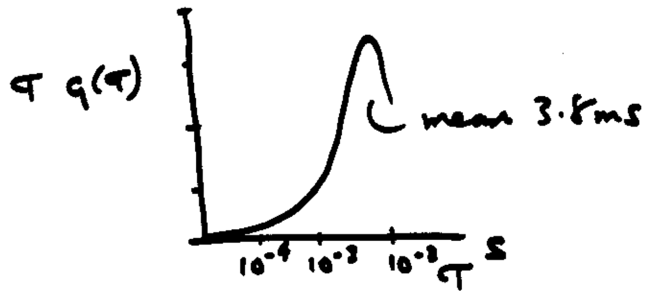
$$_{p}P_2^{0} + {}_{sp}P_3^{0} \rightarrow {}_{p}P_3^{0} + {}_{sp}P_4^{0}$$

(forced by topological constraints)

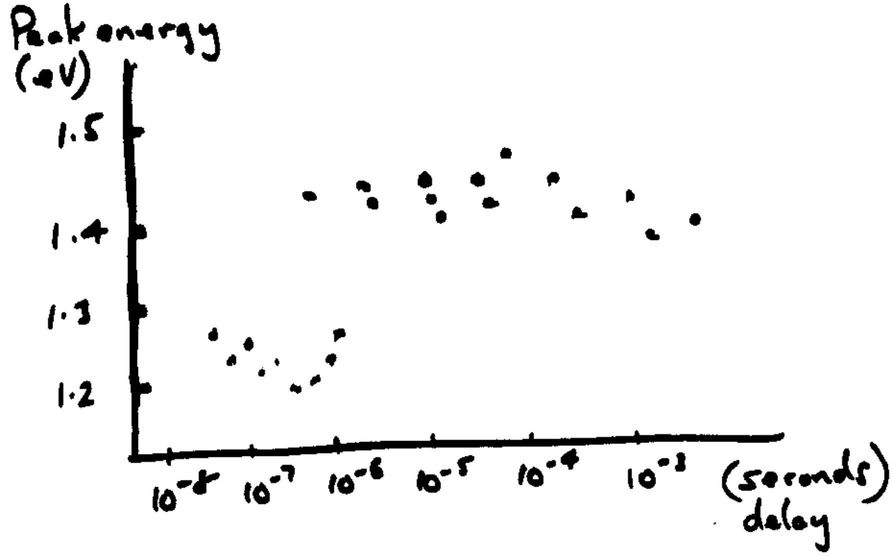
$$2\,{}_{sp}P_4^{0} \rightarrow {}_{p}P_2^{-} + {}_{sp}P_4^{+}$$

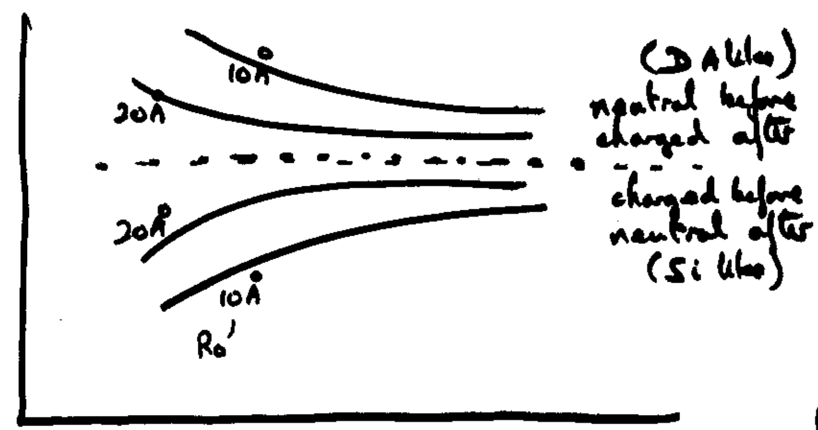




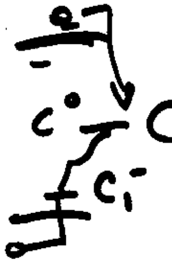


TIME-RESOLVED SPECTROSCOPY ON a-P



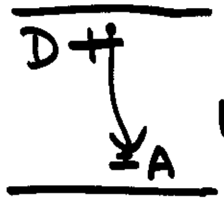


r



Coulomb terms $E = \frac{e^2}{4\pi\epsilon\epsilon_0 r}$

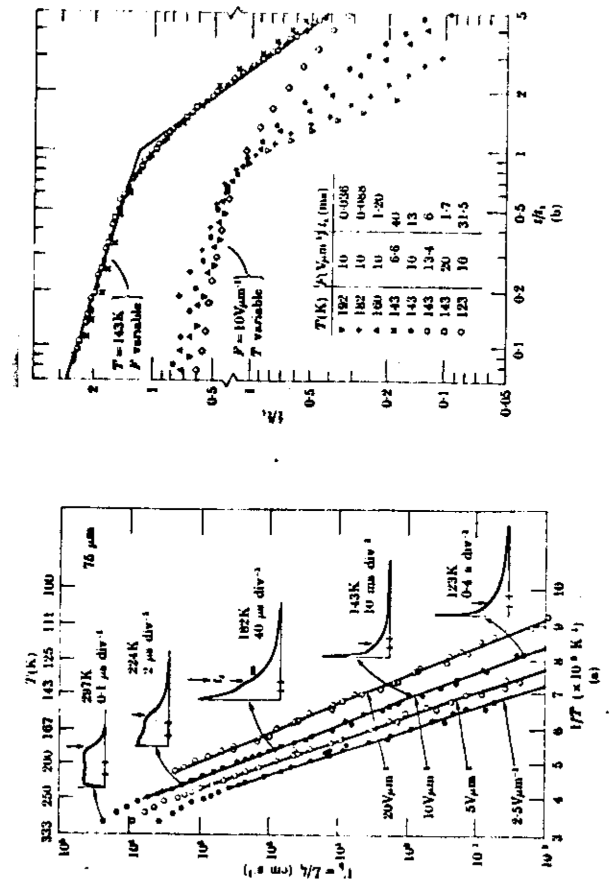
Radiative tunnelling $\tau = \tau_0 \exp(2r/R_0)$



DA rec^n

both neutral before rec^n

both charged after "



(a) Temperature dependence of hole drift velocity in amorphous selenium at various values of electric field. The shape of the current transients at various temperatures are illustrated; the arrows indicate transit times. (b) (p. 252) Current transients plotted on a log–log basis for various values of temperature and electric field F. The scales have been normalized to illustrate the scaling with respect to the transit time. (From Pfister 1976.)

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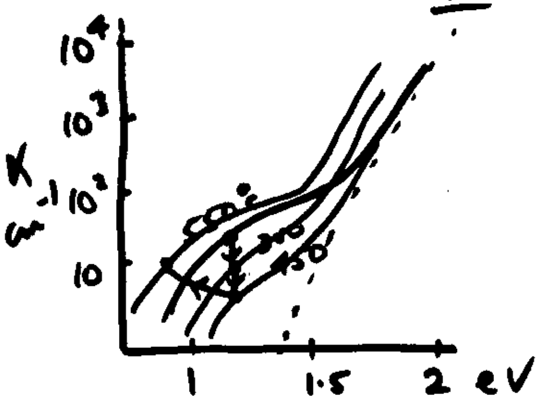
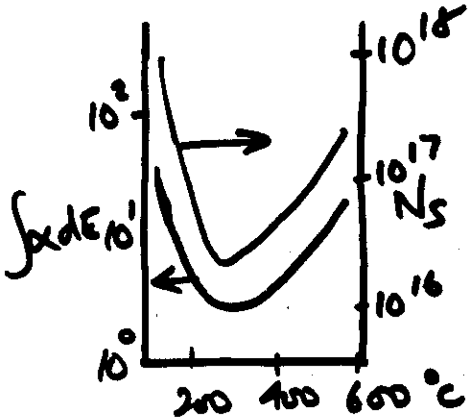
Yamasaki et al J. de Physique **42** C4-297 (1981)



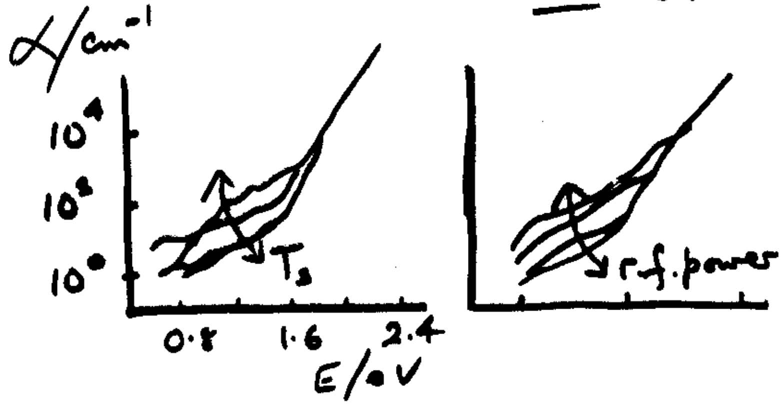
a-Si:H



<u>Photoacoustic spectroscopy</u>

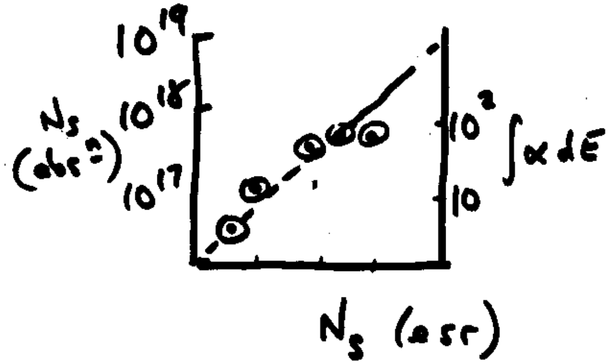
26

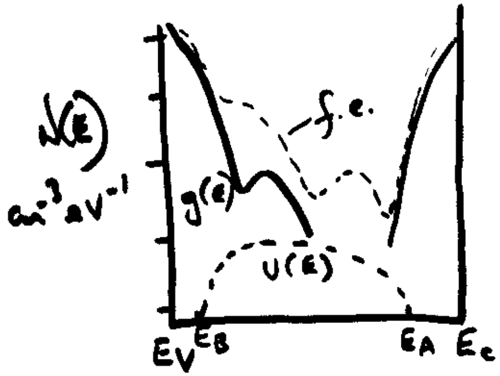
Jackson Amer J de Physique **42** C4-293 (1981)



Photothermal deflection spectroscopy PDS

(Abs^n ⇒ heating ⇒ change of n of adjacent thin layer of liquid — detected by probe beam





Schweitzer et al
J. de Physique
42 C4-827
(1981)