



Diamond Research Center

*National Institute of
Advanced Industrial Science and Technology*

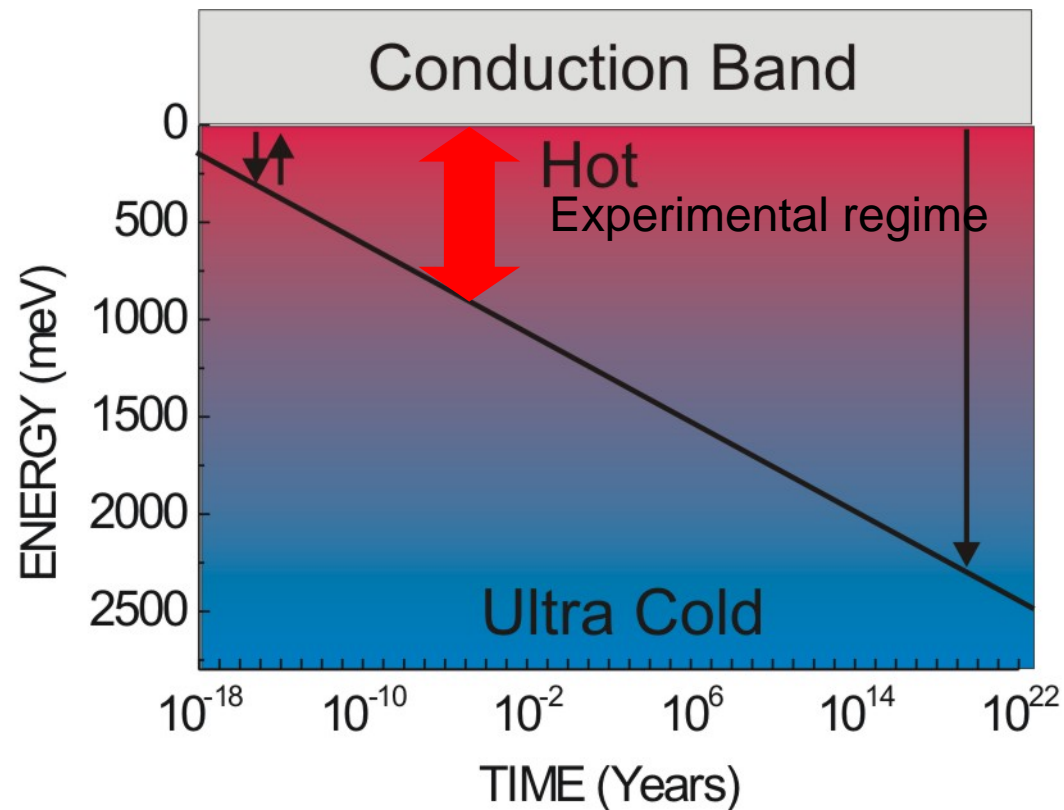


*Low Temperature
Optical and Electronic Properties
of
CVD Diamond
for Detector Applications*

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Diamond is ULTRA COLD



Assumptions: $T = 300 \text{ K}$, $\nu_0 = 10^{13} \text{ 1/s}$

Outline:

I) Optical properties

II) Electronic Properties:

Conductivity

Mobility

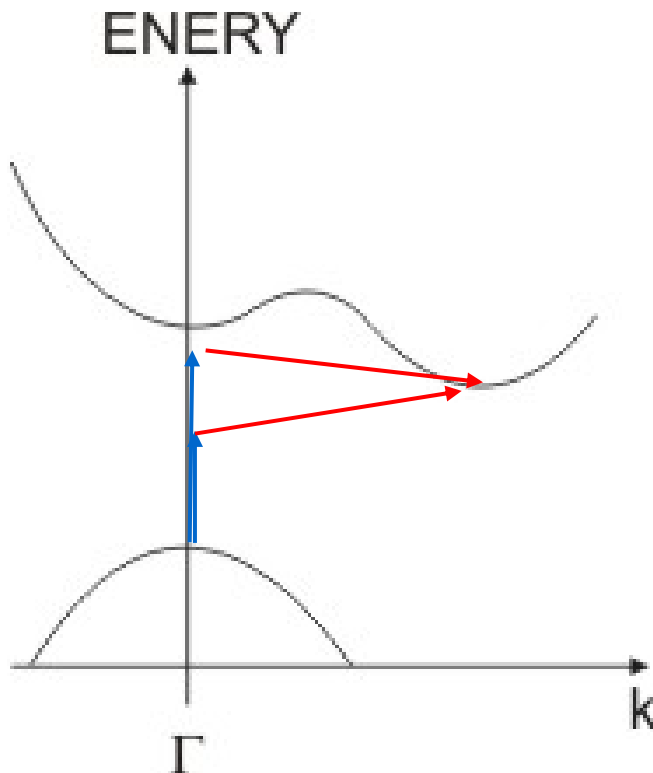
Drift Velocity in Diamond: Holes

Defects (H1 center)

Deep trapping of carriers



I. Optical Properties



Transition with phonon absorption ($h\nu > E_g - E_p$)

$$\alpha_a(h\nu) = \frac{A(h\nu - E_g + E_p)^2}{\exp\left(\frac{E_p}{kT}\right) - 1}$$

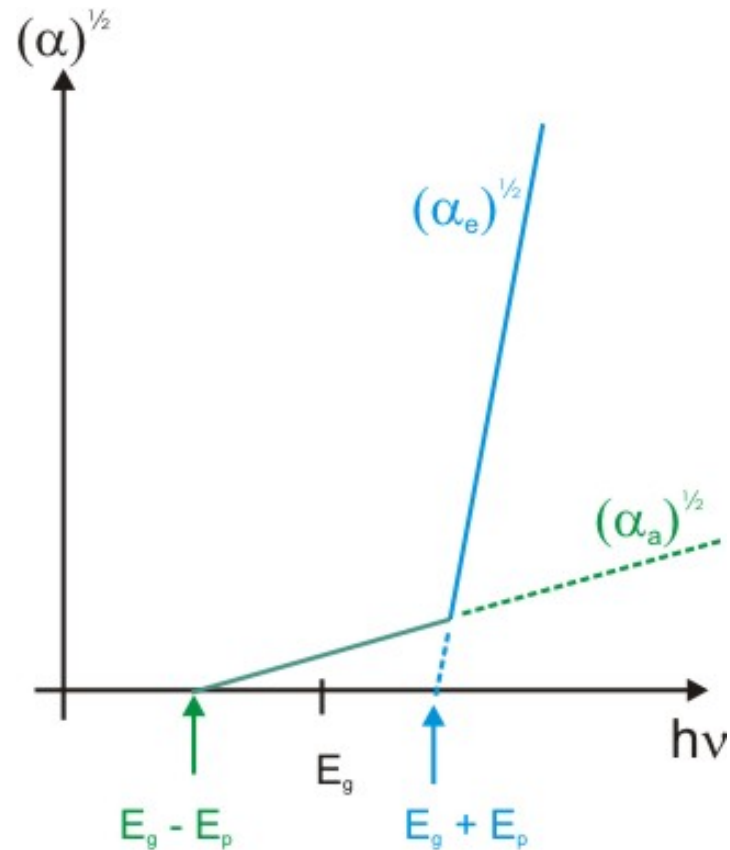
Transition with phonon emission ($h\nu > E_g + E_p$)

$$\alpha_e(h\nu) = \frac{A(h\nu - E_g - E_p)^2}{1 - \exp\left(-\frac{E_p}{kT}\right)}$$

For $h\nu > E_g + E_p$ both absorptions take place:

$$\alpha(h\nu) = \alpha_a(h\nu) + \alpha_e(h\nu)$$

Schematic Absorption



Several types of phonons involve:

- one longitudinal acoustic phonon
- Two transversal acoustic phonons

Temperature dependent absorption

thermal expansion of atoms
give rise to band gap decrease

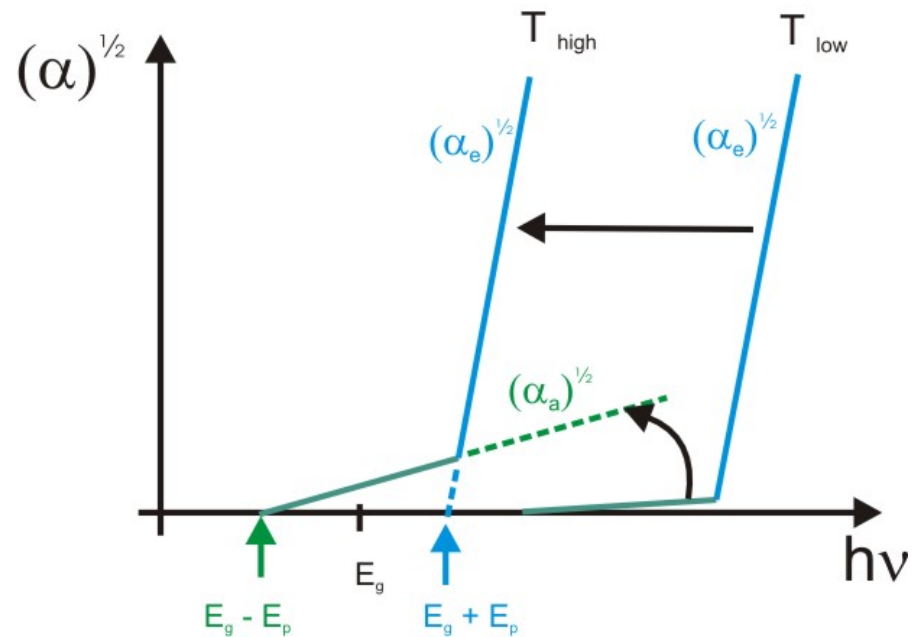
Diamond parameter

$$E_g(T) = E_g(T=0) - \frac{\alpha T^2}{T + \beta}$$

$$E_g(T=0) = 5.48$$

$$\alpha = -1.979$$

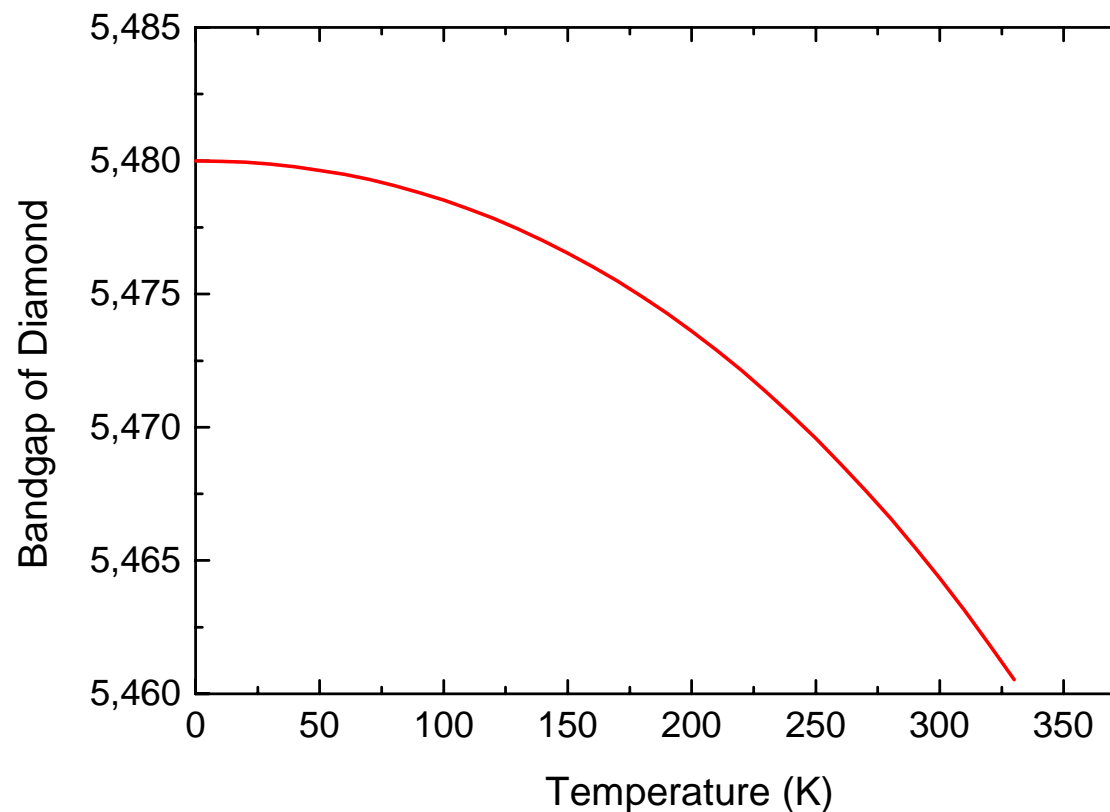
$$\beta = -1437$$



Temperature dependent variation of the band gap of Diamond

From 0 K to 300 K:

$$\Delta E = 15 \text{ meV}$$



Near band edge absorption

Phonon coupling with excitons:

LO = 163 meV

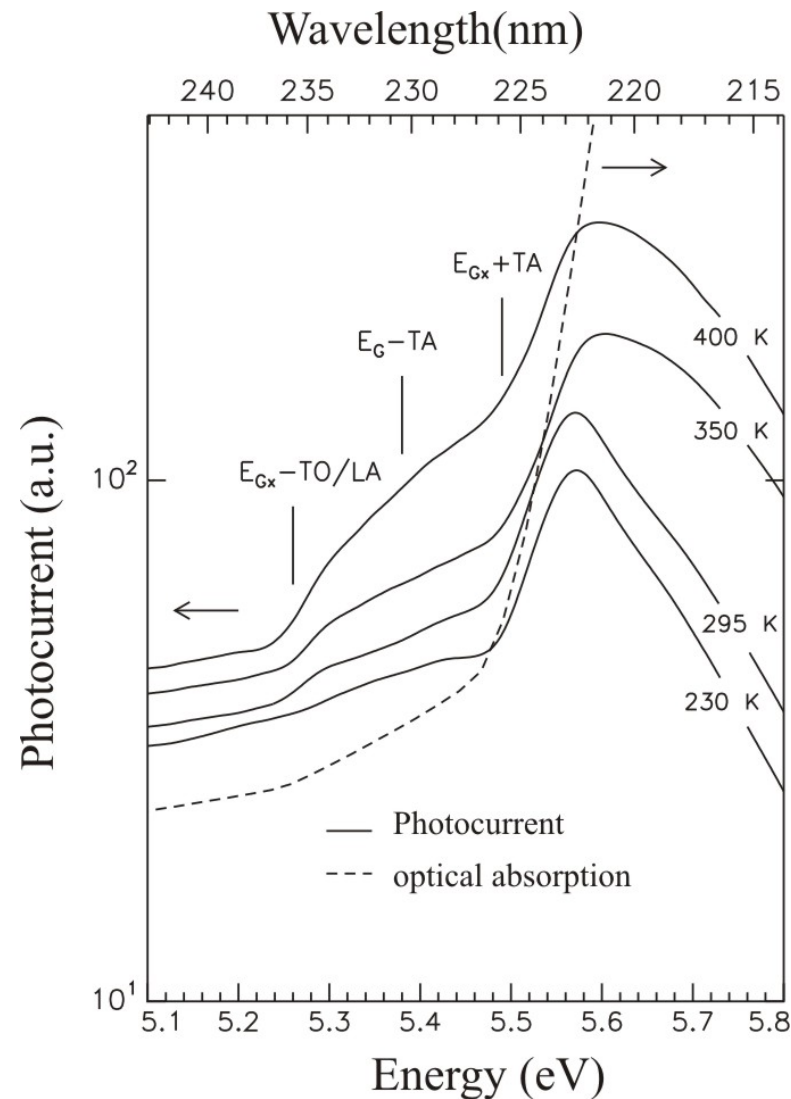
TA = 87 meV

TO = 141 meV

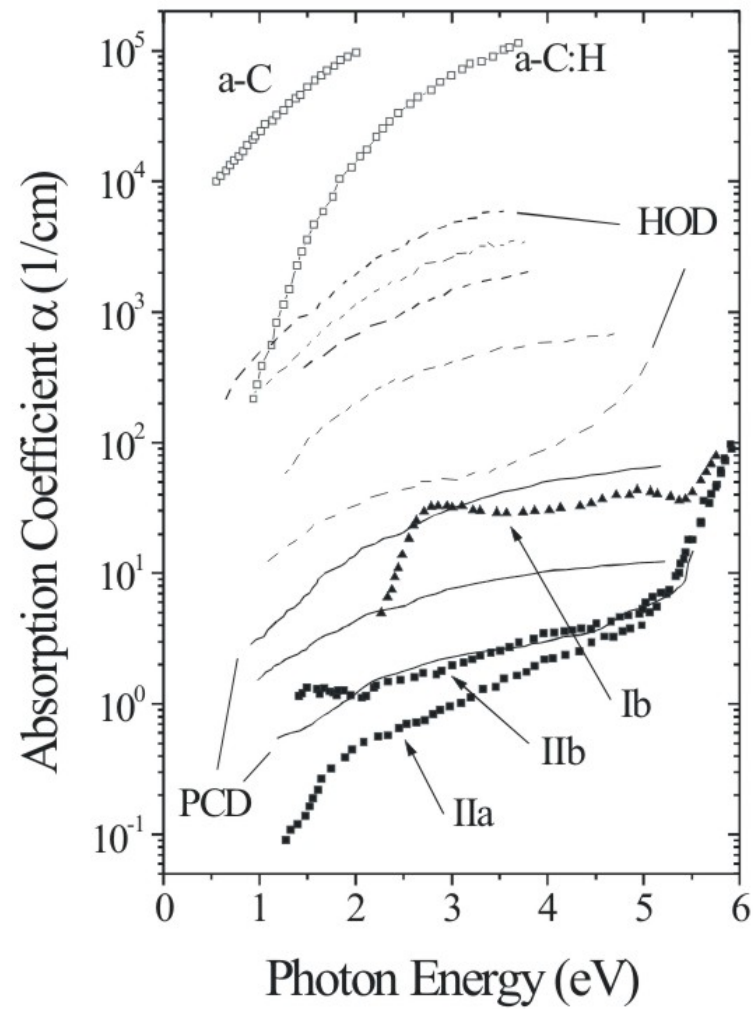
R. Sauer, in „Thin Film Diamond,
Elsevier 2003

E_{Gx} = exciton threshold energies
(5.406 eV)

E_g = 5.467 eV



Typical absorption spectra



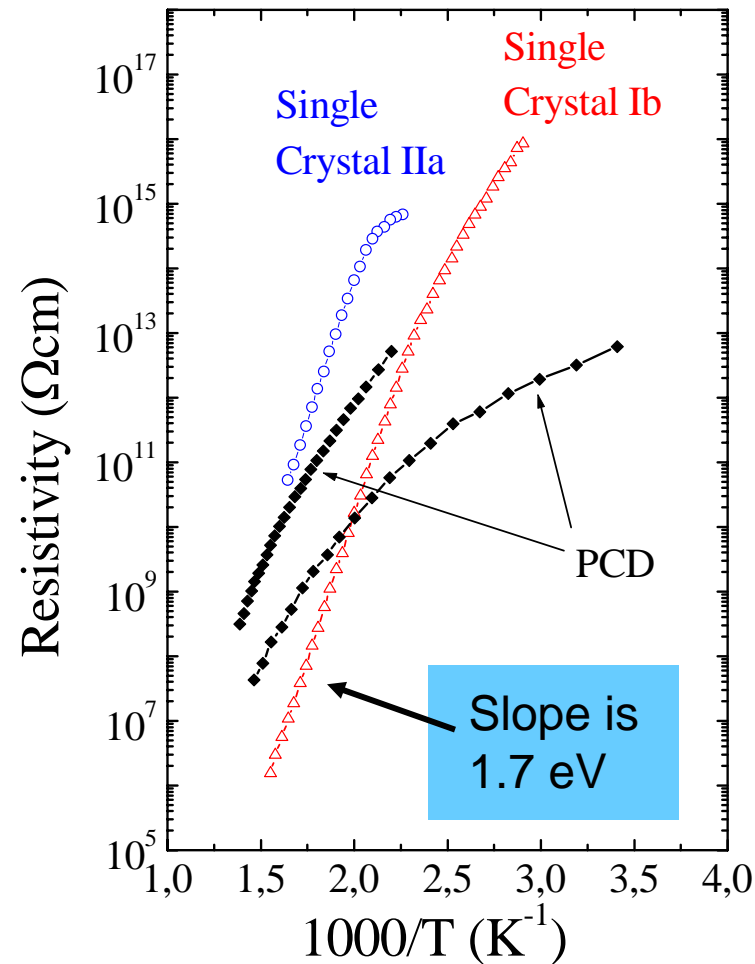


II. Electronic Properties: Conductivity

All undoped diamond layers
(Ib, IIa and CVD) are n-type:

Conductivity of CVD diamond
is governed by nitrogen
doping (P1-center):

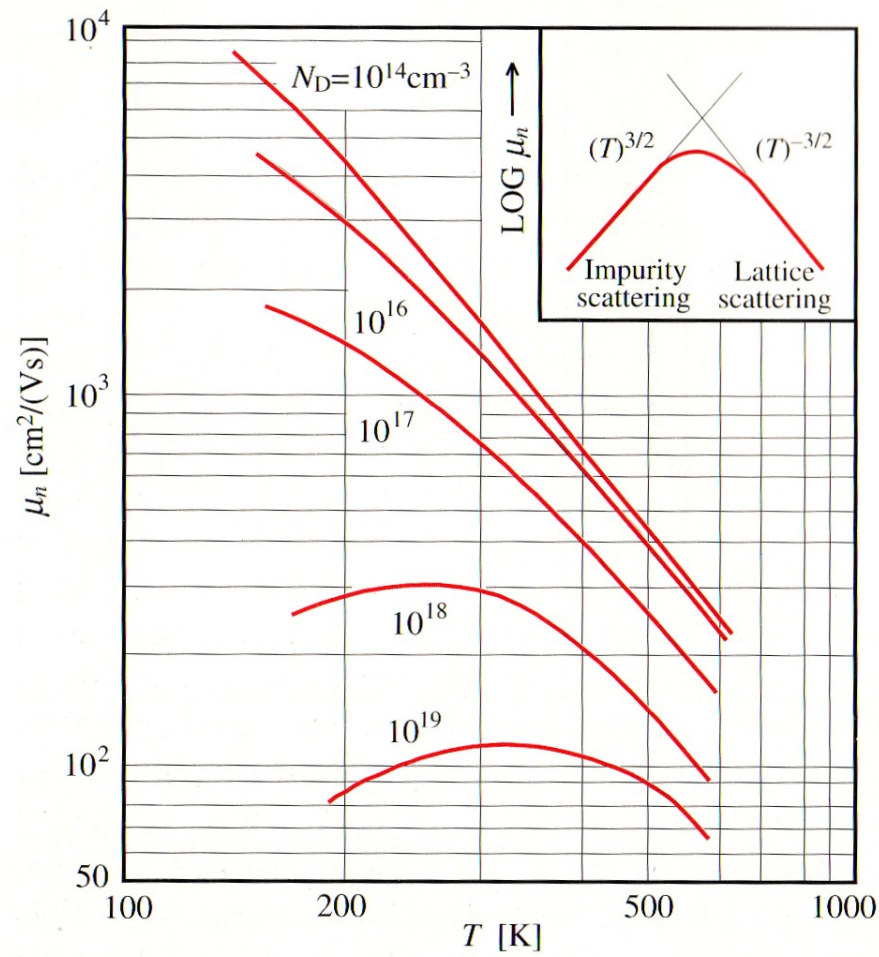
$$E_{\text{act}} = 1.7 \text{ eV}$$





Mobility

Textbook example:
Temperature dependent
mobility in n-type Si
(S.M. Sze: Semiconductor
Devices)



The band structure and the phonon bands in diamond

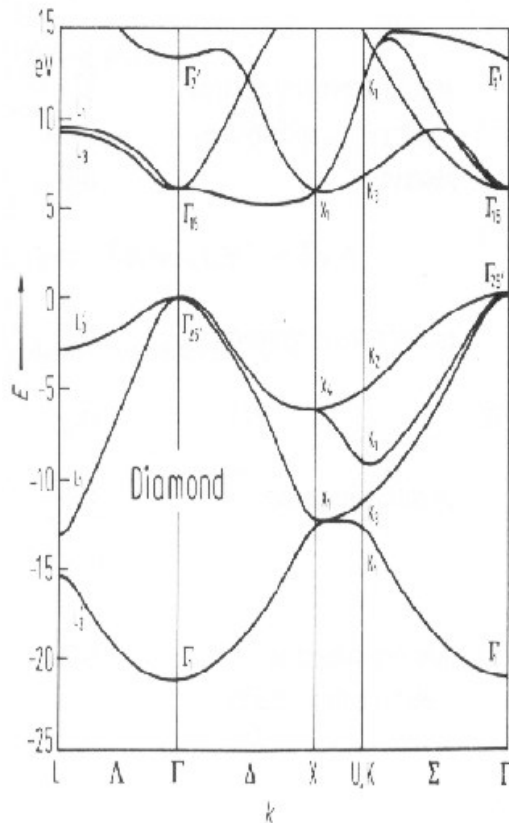
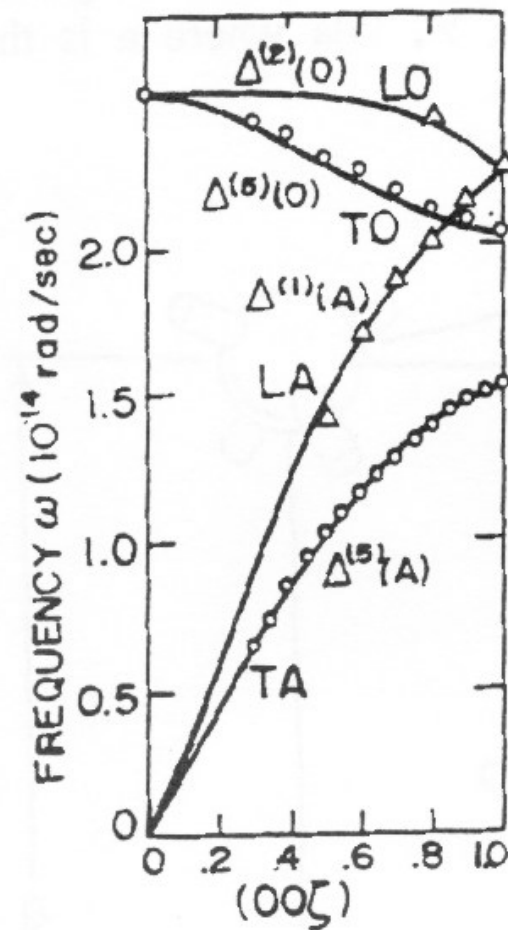


Fig. 1. Diamond. Band structure calculated by an ab initio LCAO method [84C].



Hole Mobilities

$T^{-3/2}$: acoustic phonon scattering

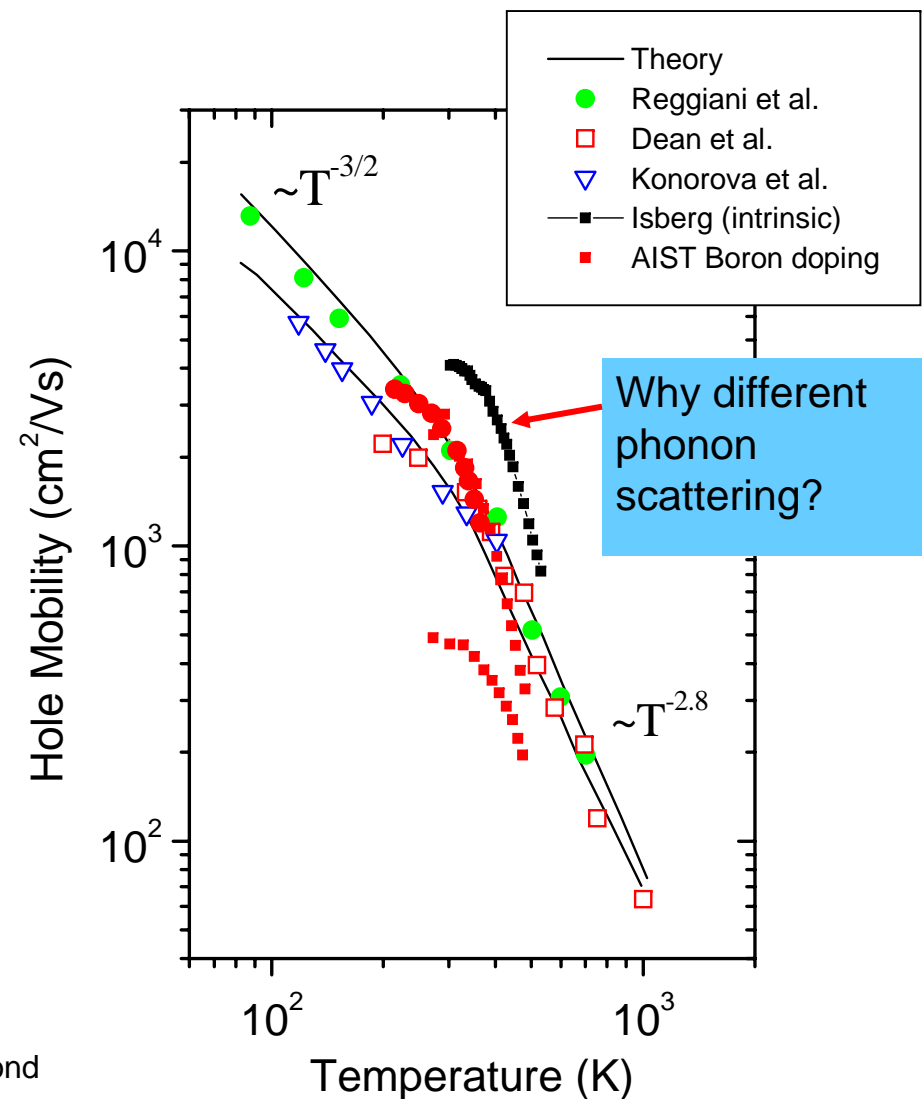
$T^{-2.8}$: optical phonon scattering

Isberg et al. : time-of-flight on undoped CVD diamond
(Science 297, p. 1670 (2002): 3800 cm²/Vs)

Reggiani: Time-of-flight on undoped natural diamond

Dean and Konorova: Hall Mobilities

Dr. Okushi et al. AIST: Hall effect on boron doped CVD diamond

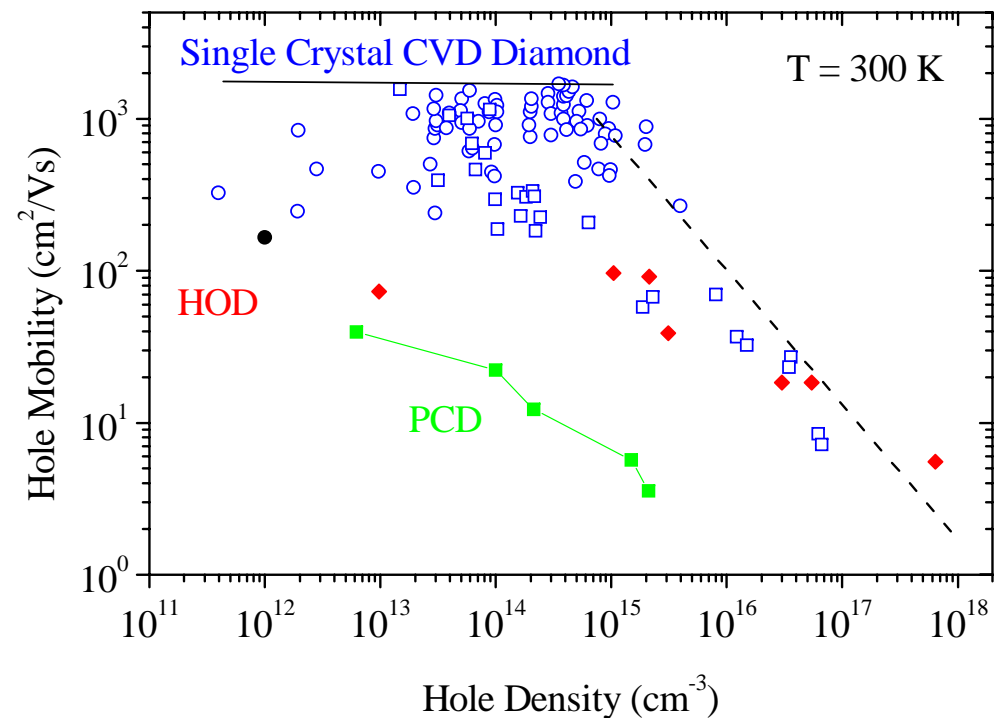




*CVD Hole Mobility Limitations:
Scattering due to residual impurities like Fe and Mo*

Scattering at ionized
impurities:

$$\mu \propto (m^*)^{1/2} \frac{T^{3/2}}{N_i}$$



Electron Mobilities in natural and P-doped Diamond:

$T^{-3/2}$: acoustic phonon scattering

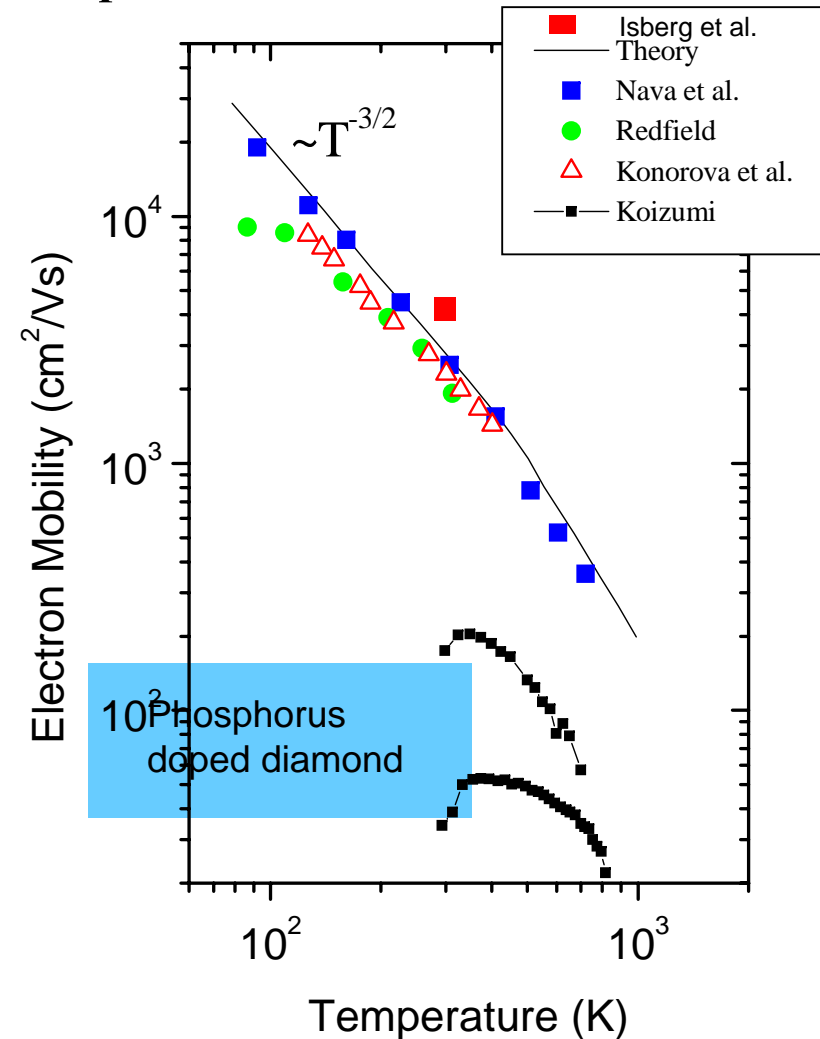
Isberg et al.: Time-of-flight in undoped CVD diamond
(Science 297, p. 1670 (2002): 4500 cm²/Vs)

Nava: Time-of-flight on natural undoped diamond

Konorova: Hall effect

Redfield: Hall effect

Koizumi et al.: Hall effect on Phosphorus doped diamond



$$\tau_e = \tau_m$$



The saturation velocity limitation:

Energy relaxation

$$\frac{d\Delta E}{dt} = eFv_s - \frac{E_{\text{phonon}}}{\tau_e}$$

Impuls relaxation

$$\frac{d(mv_s)}{dt} = eF - \frac{mv_s}{\tau_m}$$

For steady state conditions:

$$\frac{d\Delta E}{dt} = \frac{d(mv_s)}{dt} = 0$$

For only on scattering process
(one phonon)

$$\tau_e = \tau_m$$

Saturation velocity:

$$v_s = \left(\frac{E_{\text{phonon}}}{m^*} \right)^{1/2}$$

$$v_s = 3.8 \times 10^7 \text{ cm/s}$$

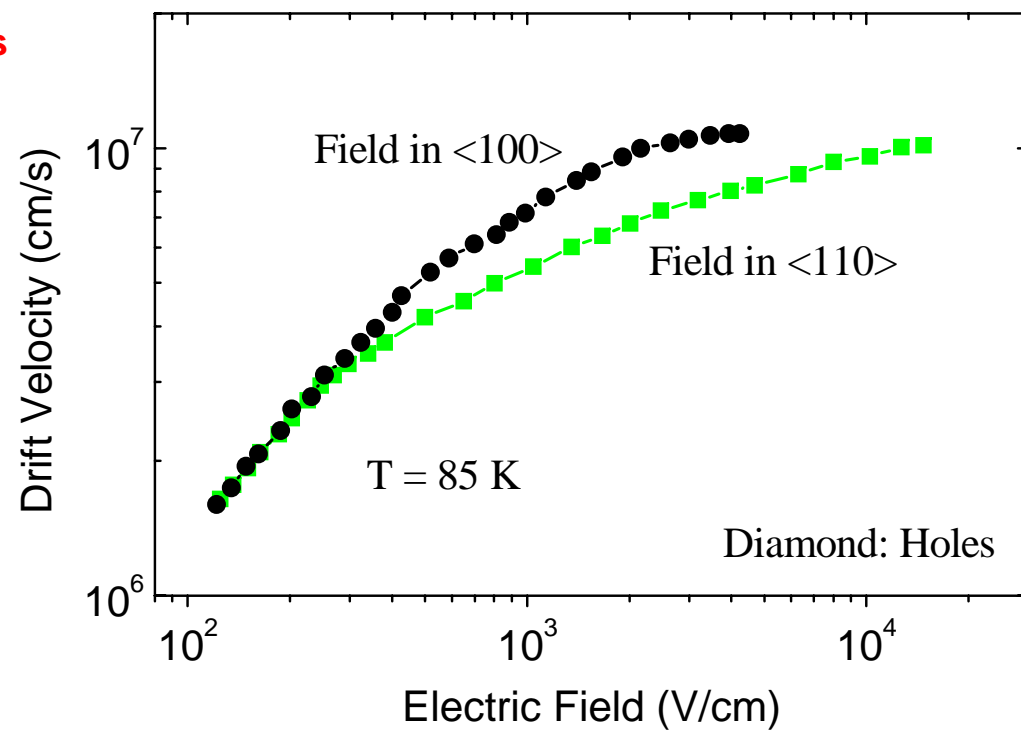
$$\text{for } 165 \text{ meV and } m = 0.2 m_0$$

Better:

$$v_{\text{sat}} = \left[\frac{8E_{\text{opticalphonon}}}{3\pi m^*} \right]^{1/2}$$

Drift Velocity in Diamond: Holes

Saturation hole velocity: **1.1×10^7 cm/s**

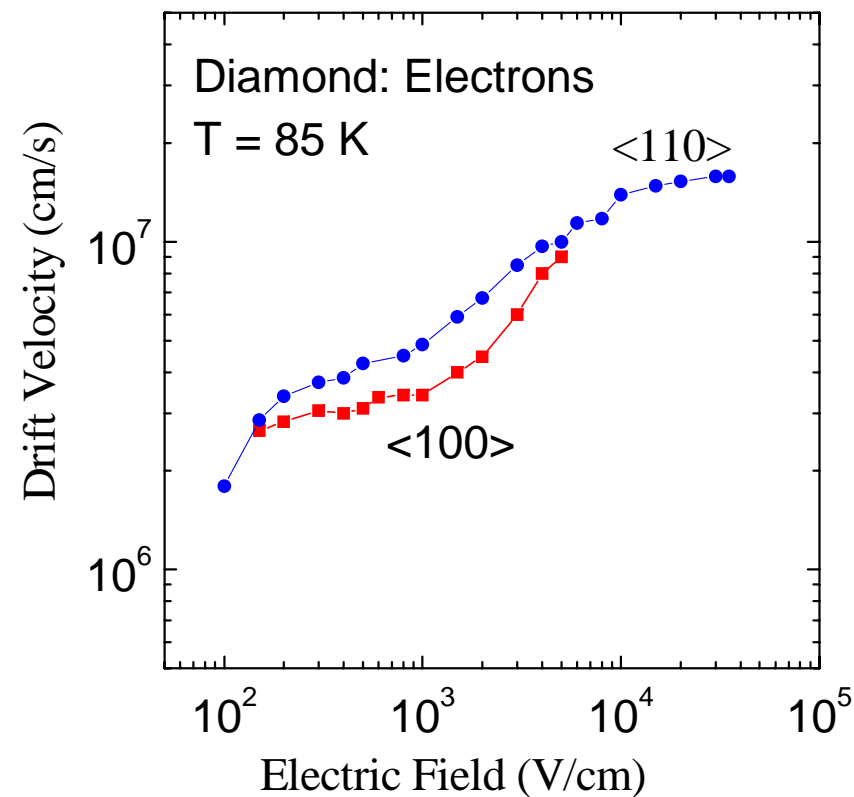


Reggiani et al, PRB 23 (1981) p. 3050

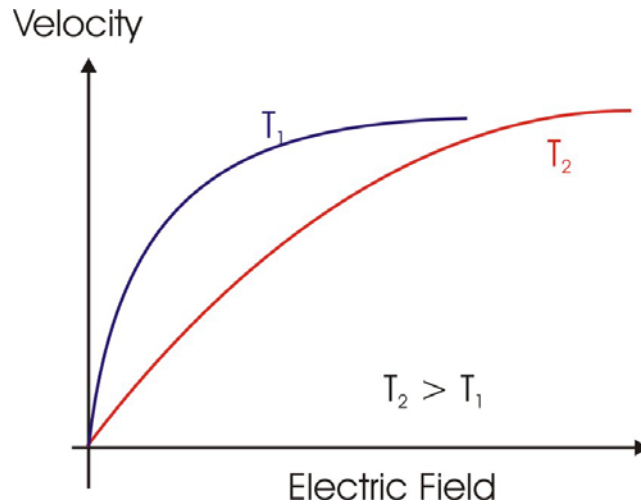
Drift Velocity in Diamond: Electrons

Saturated drift velocity: 1.5×10^7 cm/s

Anisotropy: multivalley band structure



Drift velocity



Drift velocity:

$$v_D = F\mu = F \frac{e}{m} \tau$$

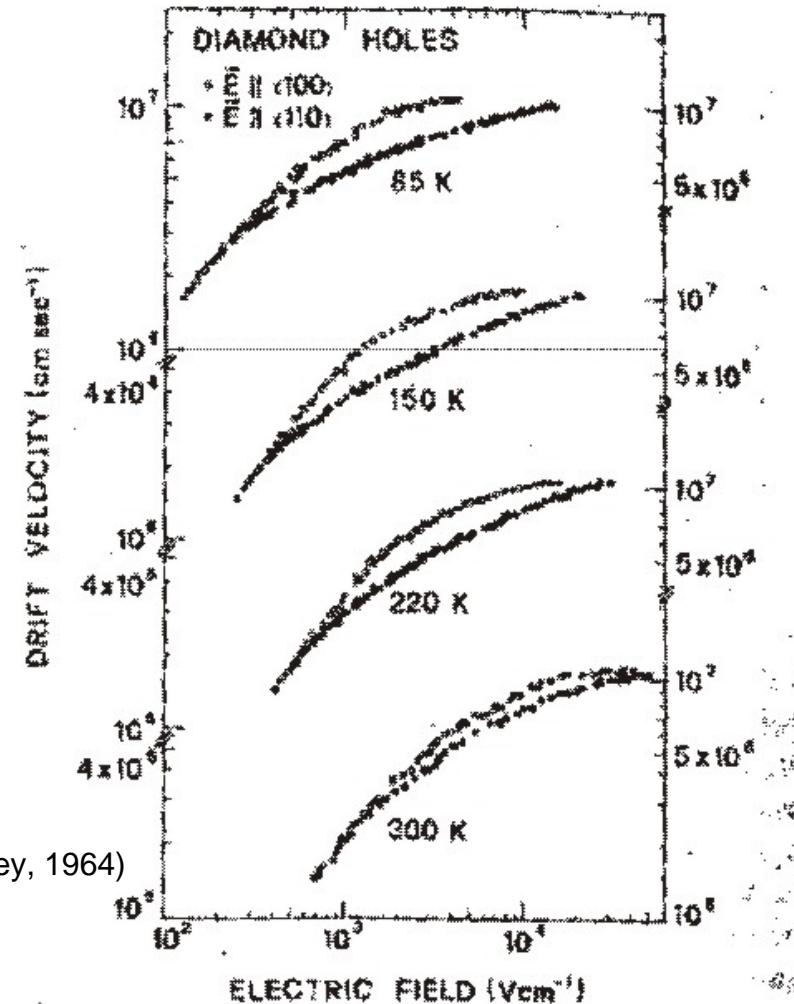
$$\tau = \tau_0 \left(\frac{\varepsilon}{kT} \right)^r$$

Scattering time:

J.L. Moll, Physics of Semiconductors (Wiley, 1964)

$r = -0.5$ acoustic deformation potential scattering

$r = +3/2$ ionized impurity scattering

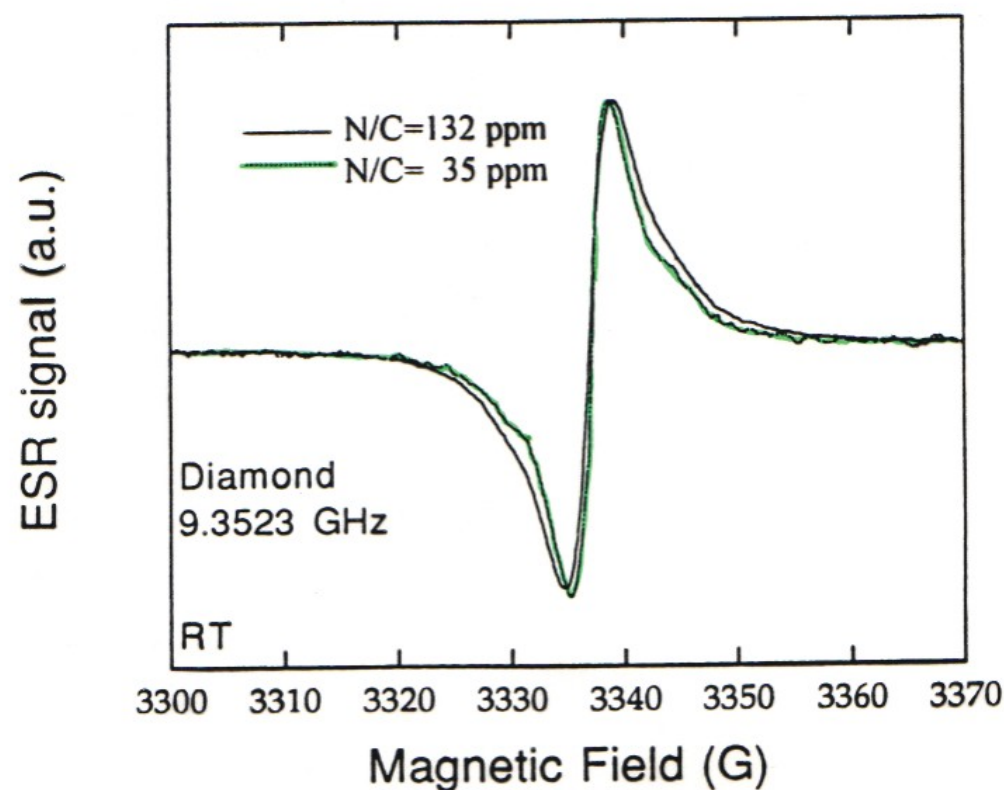


Reggiani et al, PRB 23 (1981) p. 3050

Defects: H1 Center $g = 2.0028$

Homoepitaxial single
crystalline diamond:

Typical Density: $5 \times 10^{18} \text{ cm}^{-3}$

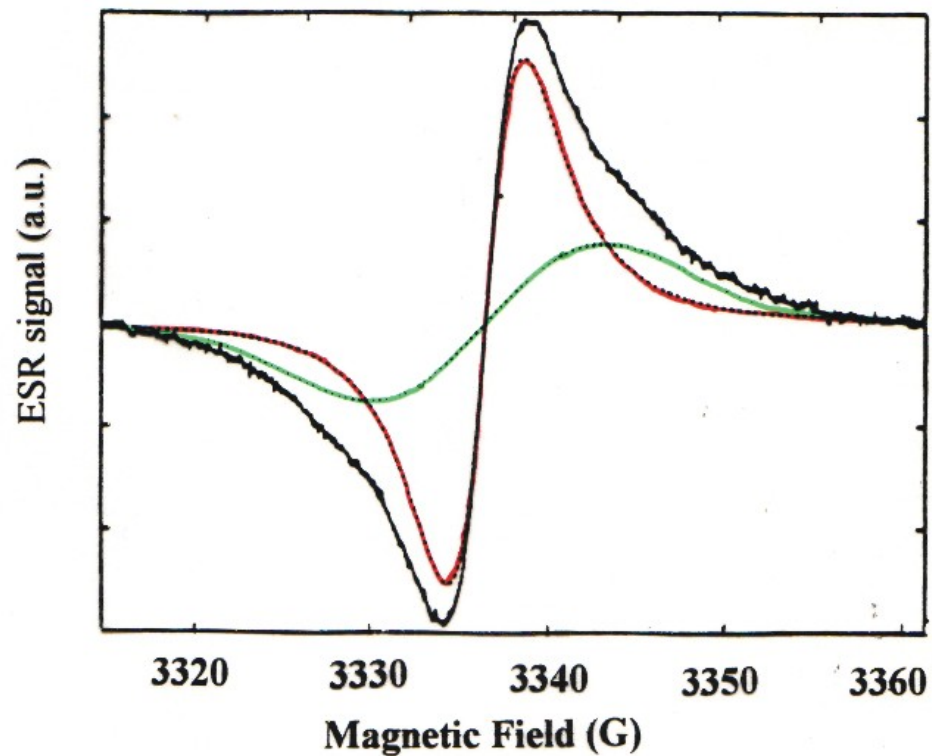


Zhou et al. PRB 54 (1996) p. 7881

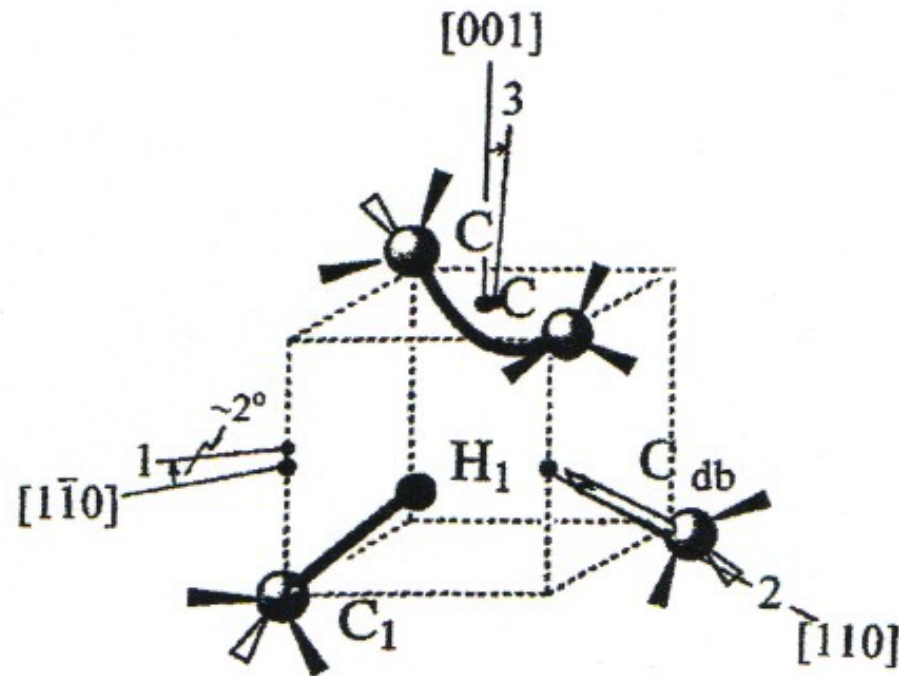
N. Mizuochi et al. DRM in print.



Carbon hyperfine interaction with Hydrogen
Distance: 1.9 to 2.3 Å



Defect Model: X. Zhou, G.D. Watkins et al. PRB 54 (1996) p. 7881





Deep trapping of carriers

Hecht equation:

$$Q(t) = Q_0 \frac{\mu\tau E}{L} \left[1 - \exp\left(-\frac{t}{\tau}\right) \right]$$

Deep trapping lifetime

$$\tau = \frac{1}{N_D v_{th} S_{cross}}$$

Capture cross section S_{cross} :

$$10^{-14} \text{ cm}^2 - 10^{-15} \text{ cm}^2$$

Ionized Impurities:

$$E(r) = \frac{1}{4\pi\epsilon_0\epsilon_r} \frac{1}{r^2}$$

ϵ_r in diamond much smaller!

$$\epsilon_r(\text{Diamond}) = 5.7$$

$$\epsilon_r(\text{Si}) = 11.9$$

Temperature dependent capture cross sections for 7 deep levels in GaAs and two in GaP (D.V. Lang)

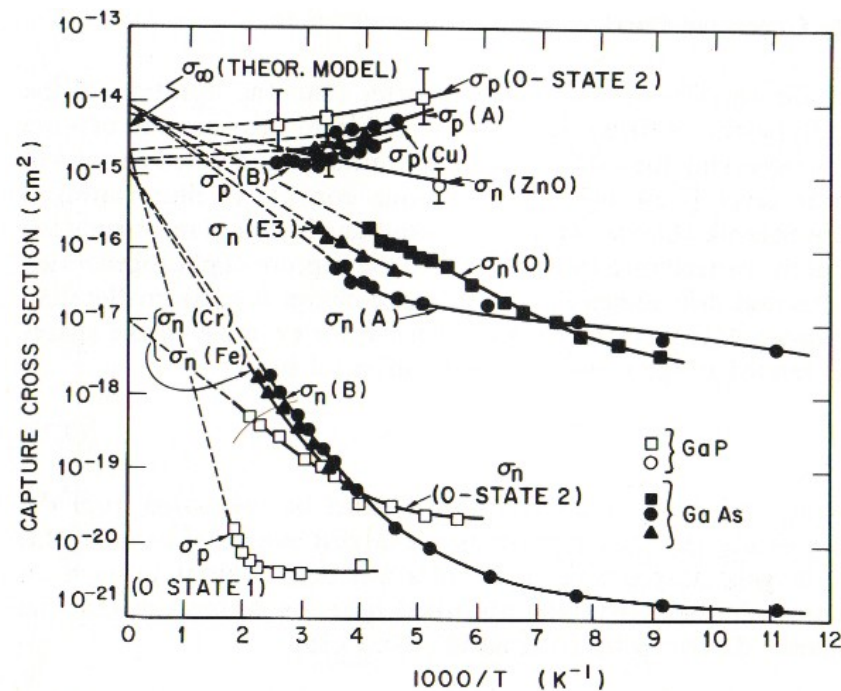
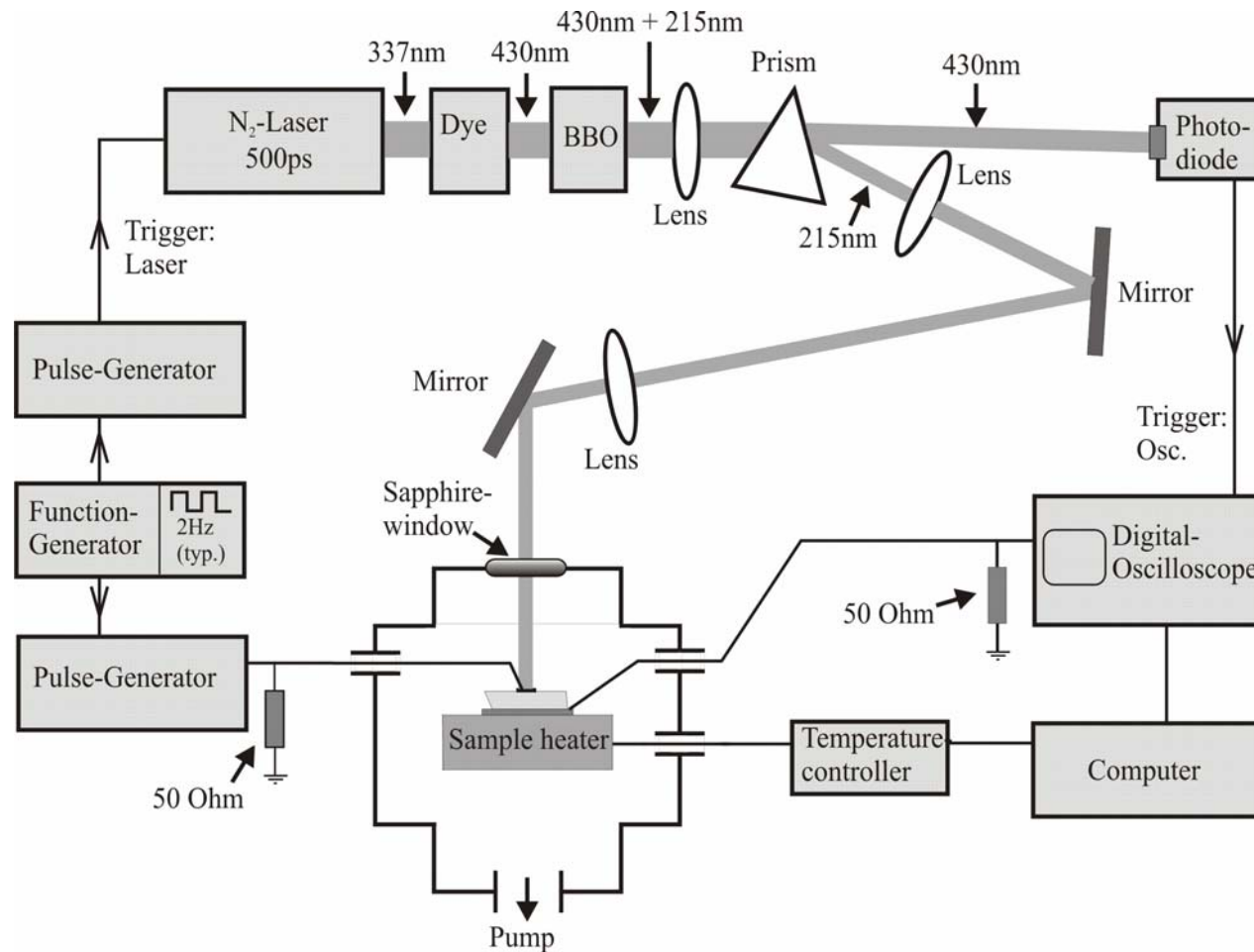


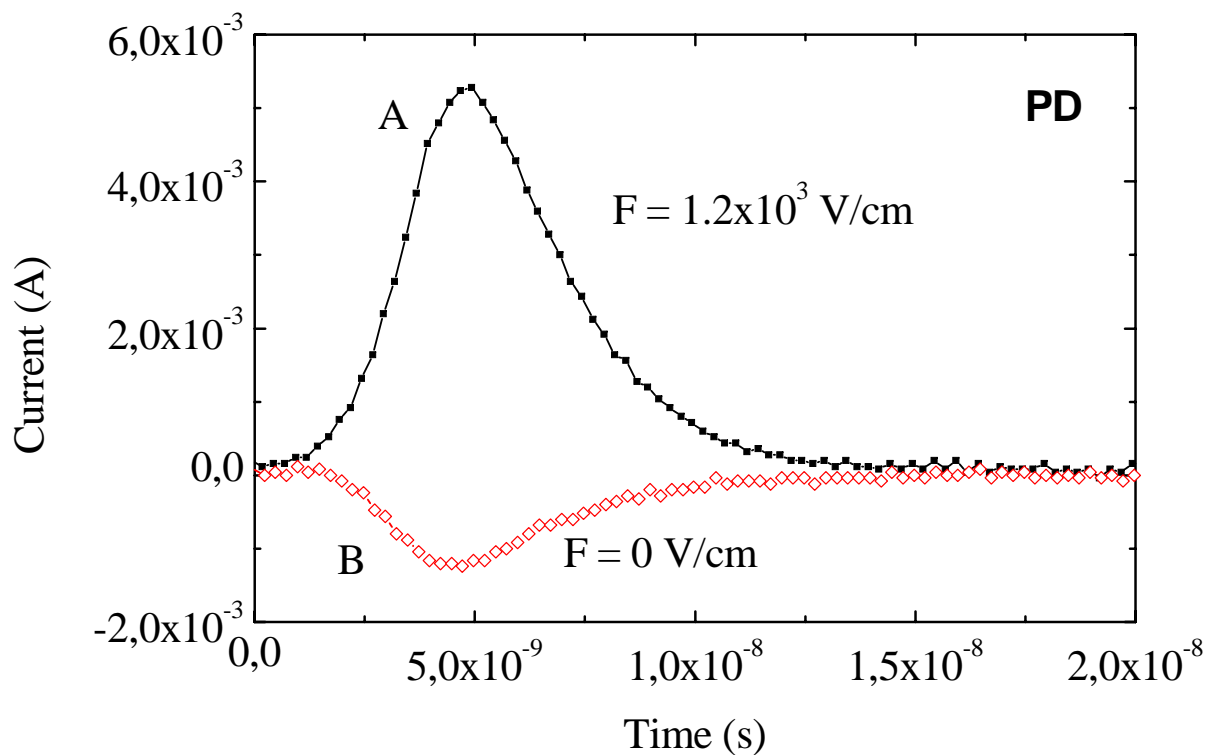
Fig. 3.21. Capture cross section (denoted here by σ) as a function of inverse temperature for seven deep levels in GaAs and two in GaP

Time-of-flight setup



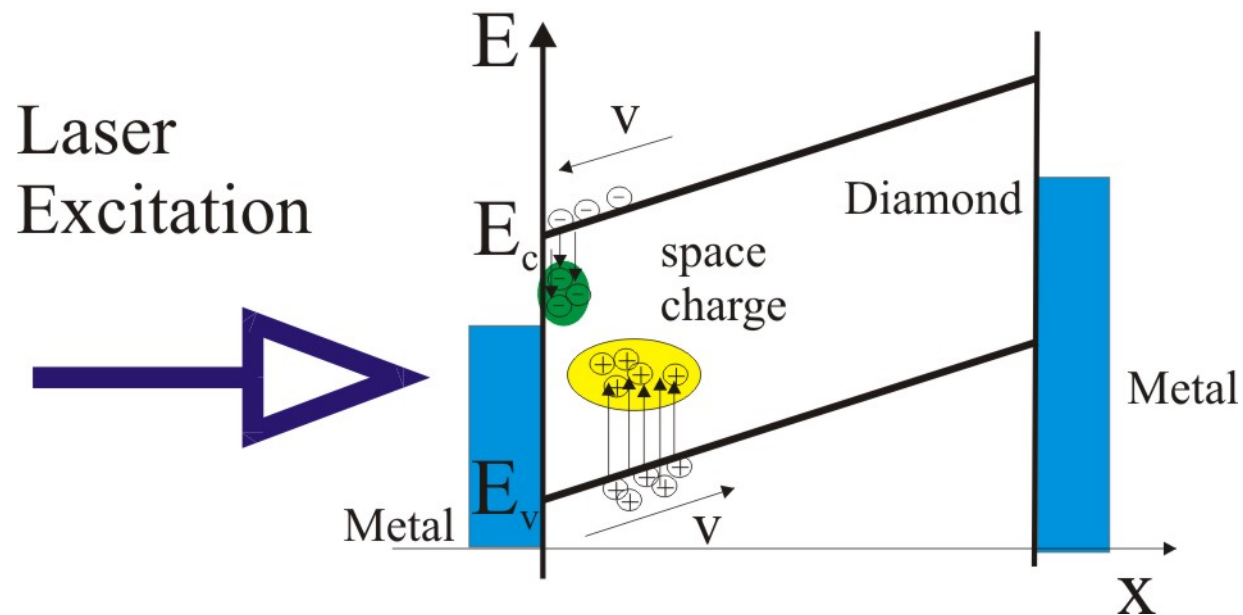


Deep trapping of carriers (electrons and holes) in undoped CVD diamond



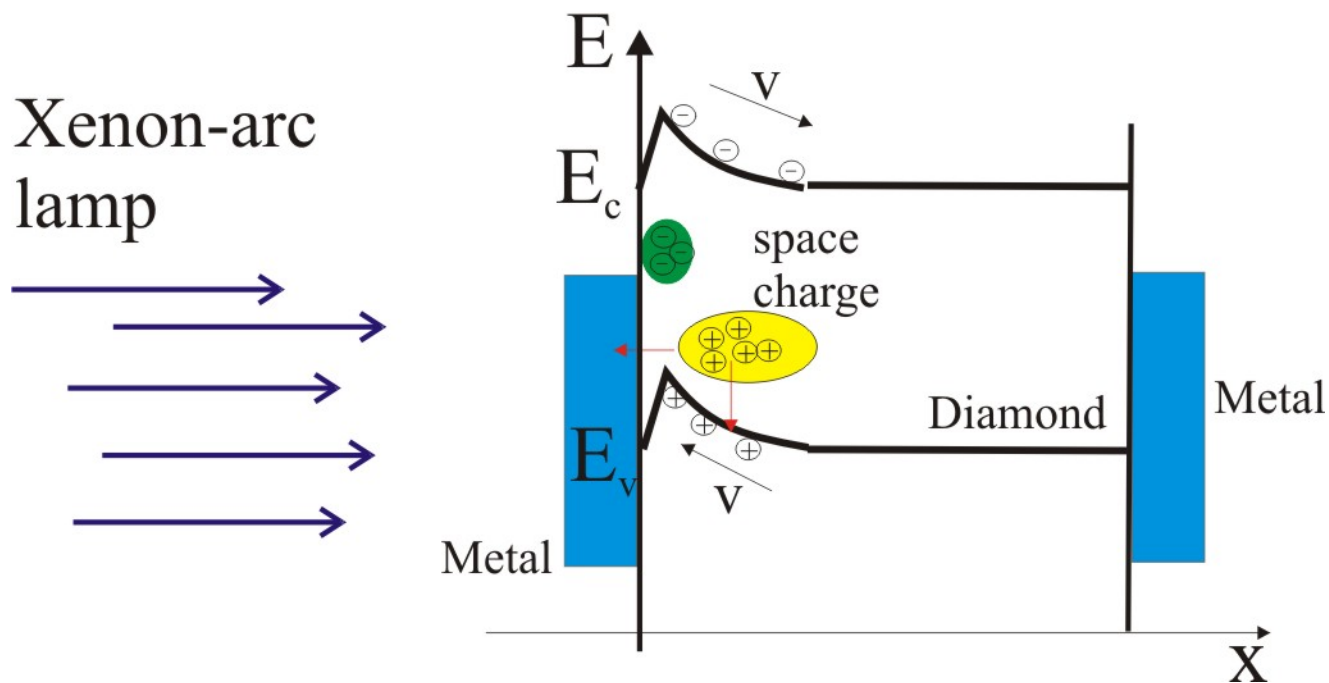
Model:

pos. applied el. field



After laser exposure the internal field is reversed, giving rise to a current in opposite direction

short circuit illumination



The same features for electrons and holes: Traps or defect, which can be occupied by electrons and holes!

