

# **Characterization of Conductivity: Basic Properties and Challenges**

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# Conductivity

$$\sigma = en\mu_n + ep\mu_p$$

e : elementary charge  
n: electron density  
p: hole density  
 $\mu_n$ : electron mobility  
 $\mu_p$ : hole mobility

# Outline

- 1) Introduction
- 2) Defects in Diamond
- 3) Deep Trapping Lifetime, Schubweg and Mobility
- 4)  $\mu\tau$ -Products as a Function of Nitrogen Content
- 5) Properties of Poly-Crystalline CVD Diamond
- 6) Spectrally Resolved Photoconductivity
- 7) Contact Properties
- 8) Summary

# 1. Introduction: Comparison Sheet

*Physical characteristics of Si and major WBG semiconductors*

Property	Si	GaAs	6H-SiC	4H-SiC	GaN	Diamond
Bandgap, $E_g$ (eV)	1.12	1.43	3.03	3.26	3.45	5.45
Dielectric Constant, $\epsilon_r$	11.9	13.1	9.66	10.1	9	5.5
Electric breakdown field , $E_C$ (MV/cm)	0.3	0.4	2.4	2	0.2	5.6
Electron mobility, $\mu_n$ (cm <sup>2</sup> /Vs)	1,500	8,500	370	720	1,250	4,500
Hole mobility, $\mu_p$ (cm <sup>2</sup> /Vs)	600	400	101	115	850	3,800
Thermal conductivity, $\lambda$ (W/cmK)	1.5	0.46	4.9	4.9	1.3	22
Saturation electron drift velocity, $v_{sat}$ (x10 <sup>7</sup> cm/s)	1	2	2	2	2.2	2.7

# Diamond

## Available:

- natural
- High pressure high temperature (HTHP)
- CVD diamond

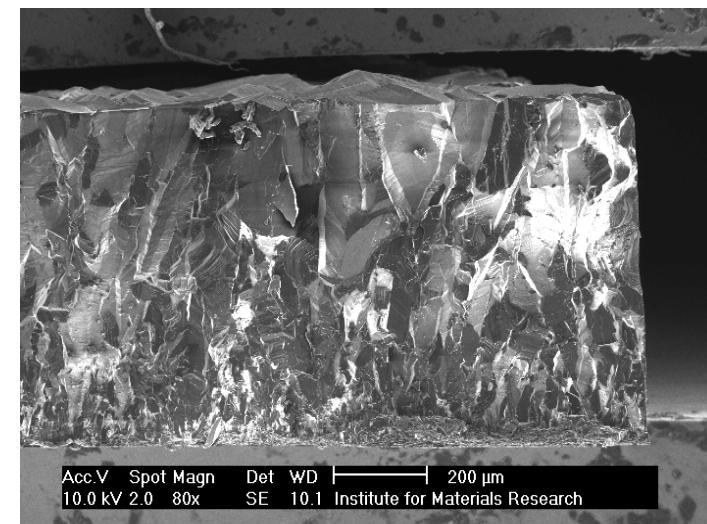
## Morphology:

- single-crystalline
- poly-crystalline
- nano-crystalline
- ultra-nano-crystalline

*Single Crystalline Diamond  
4 mm x 4 mm*



*Poly-Crystalline CVD Diamond*



# Electron Mobilities

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

Isberg et al.,: Time-of-flight in undoped CVD diamond  
( Science 297, p. 1670 (2002): **4500** cm<sup>2</sup>/Vs)

Nava: Time-of-flight on natural undoped diamond

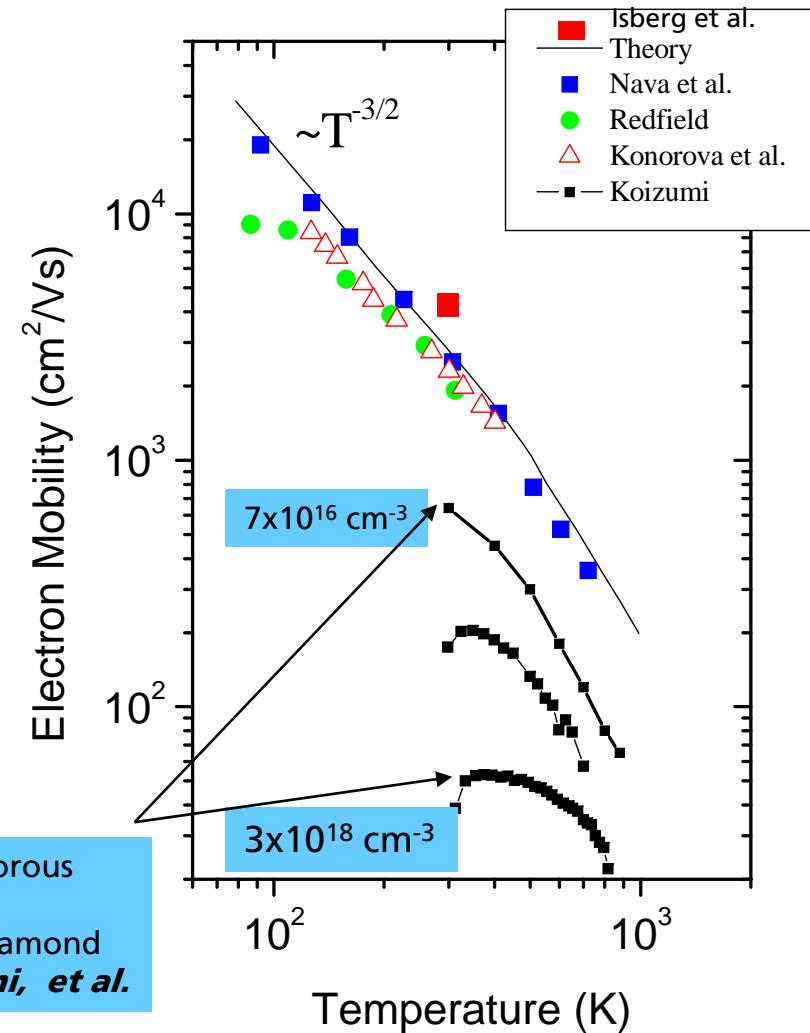
Konorova: Hall effect

Redfield: Hall effect

Koizumi et al.: Hall effect on Phosphorus doped diamond

RT-mobility: 725 to 4500 cm<sup>2</sup>/Vs

Phosphorous  
Doped  
(111) Diamond  
**Koizumi, et al.**



# 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 cm<sup>2</sup>/Vs**)

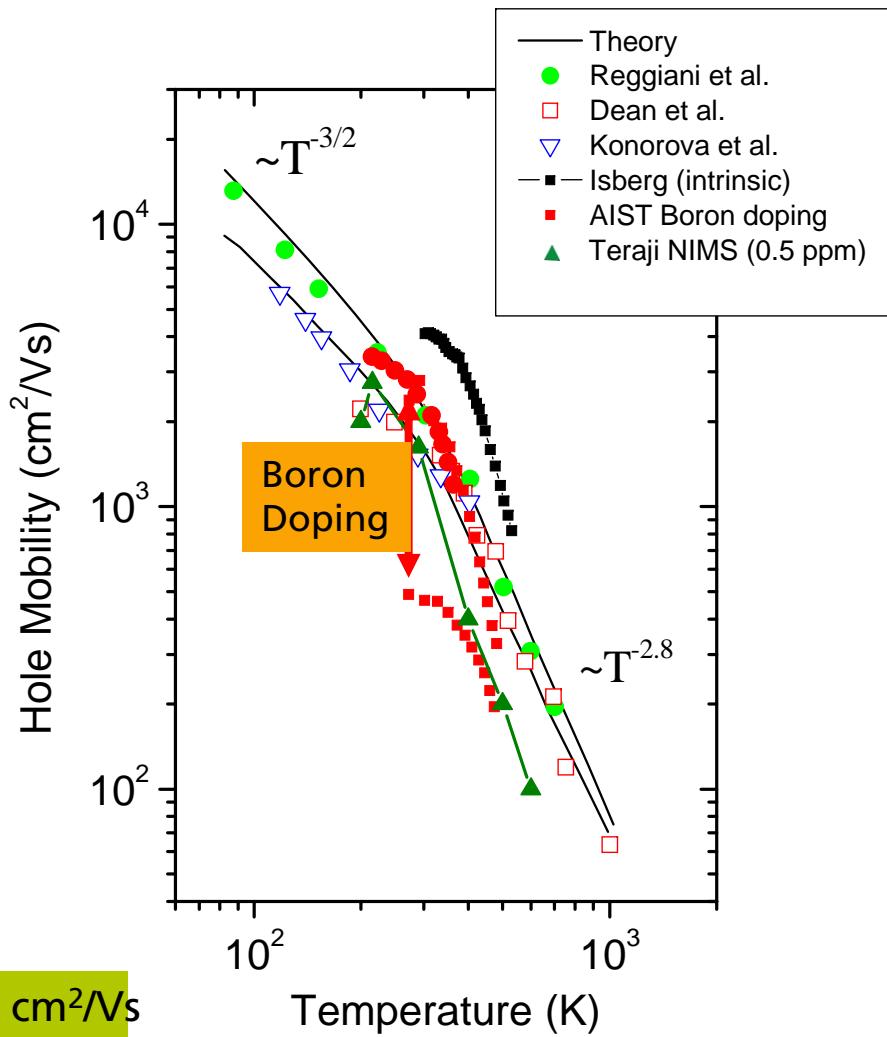
Reggiani: Time-of-flight on undoped natural diamond

Dean and Konorova: Hall Mobilities

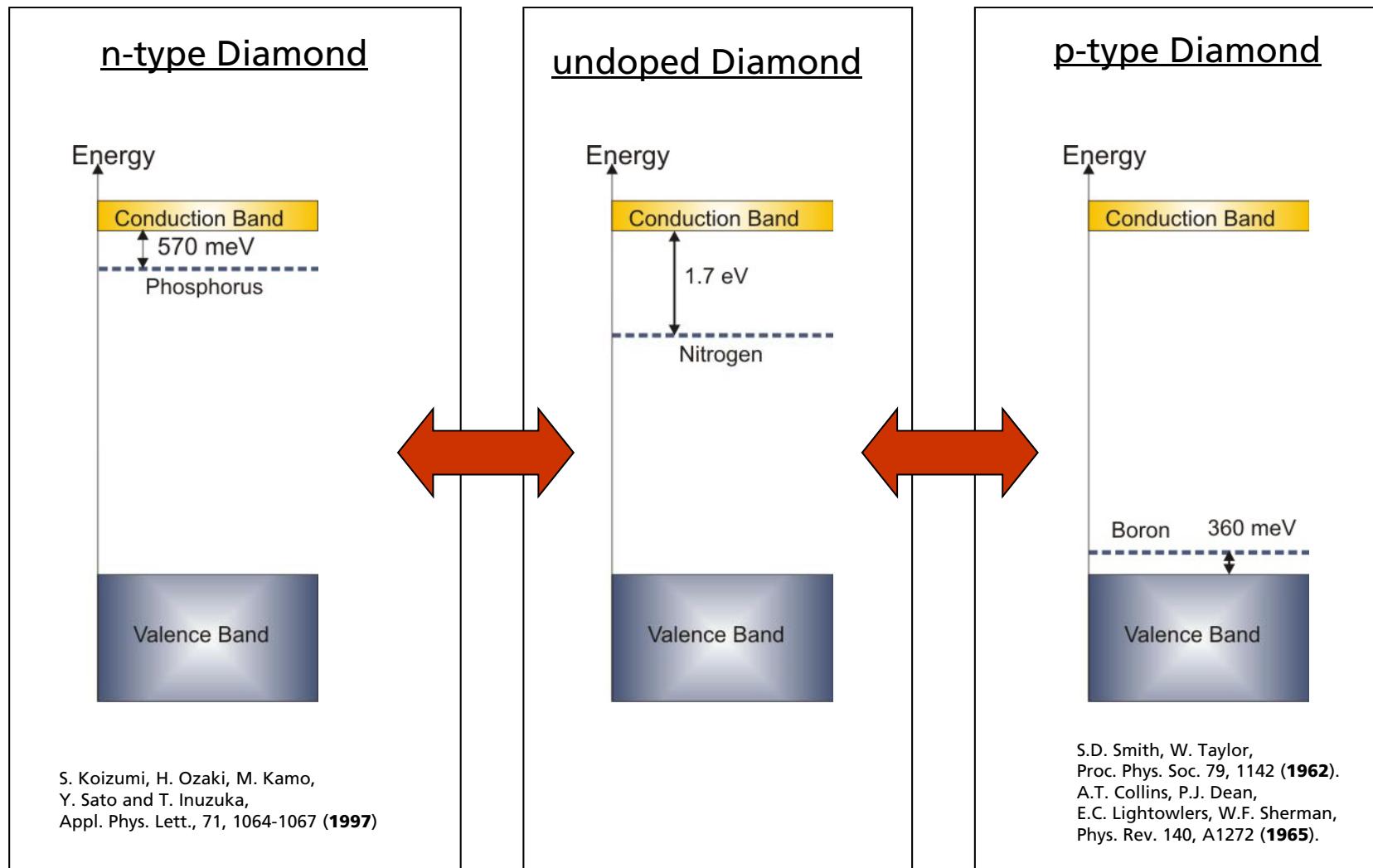
Okushi et al. AIST: Hall effect on boron doped CVD diamond

**Teraji, Hall effect on (001) 0.5 ppm: 1620 cm<sup>2</sup>/Vs at 290 K**

Room temperature mobility: 500 to 3800 cm<sup>2</sup>/Vs



# Doping of Diamond for Electronic Applications

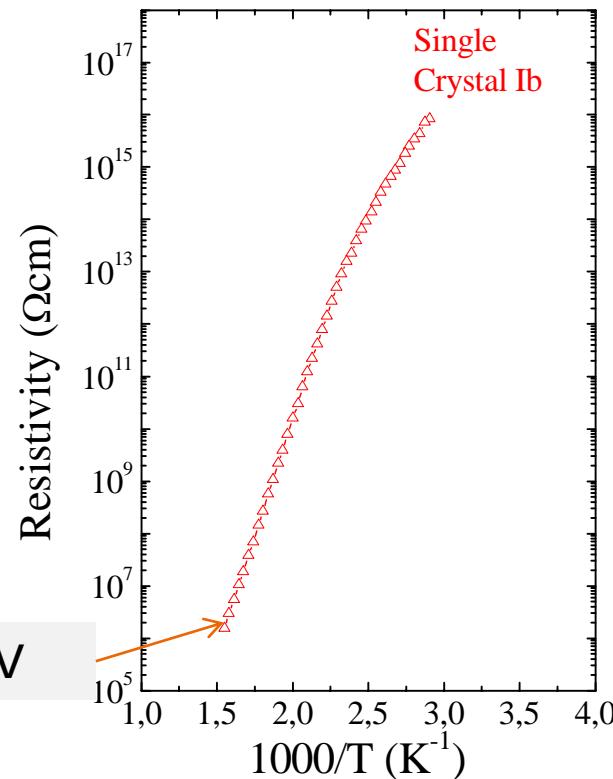


# Thermal Activated Resistivity of Undoped Diamond

$$\sigma = e \mu(T) n_0 e^{-E_{act}/kT}$$

$E_{act} \text{ ca. } 1.7 \text{ eV}$

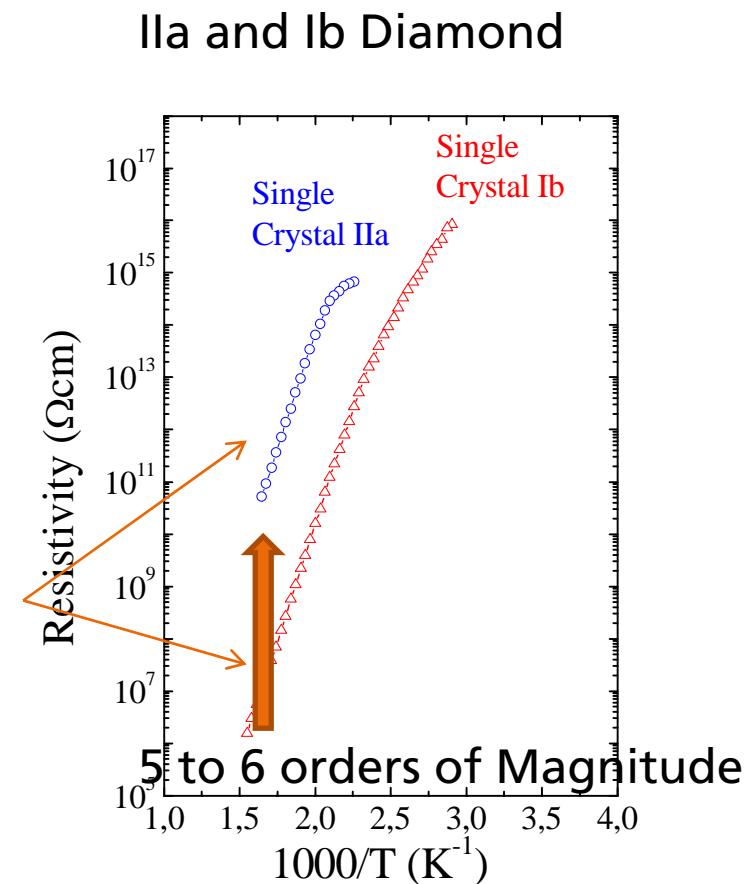
Ib-Diamond



# Thermal Activated Resistivity of Undoped Diamond

$$\sigma = e \mu(T) n_0 e^{-E_{act}/kT}$$

$E_{act}$  ca. 1.7 eV

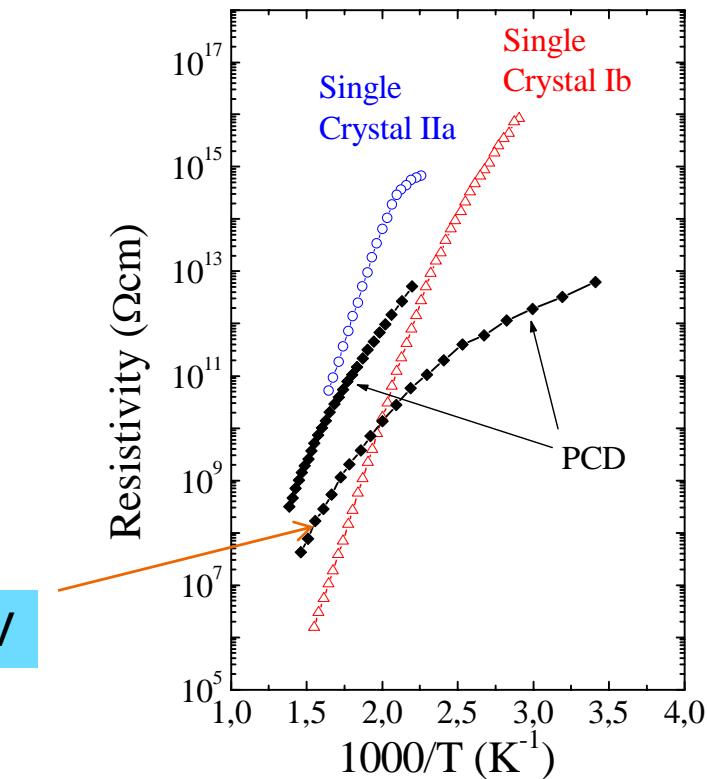


# Thermal Activated Resistivity of Undoped Diamond

$$\sigma = e \mu(T) n_0 e^{-E_{act}/kT}$$

$E_{act}$  ca. 1 eV

Polycrystalline CVD Diamond

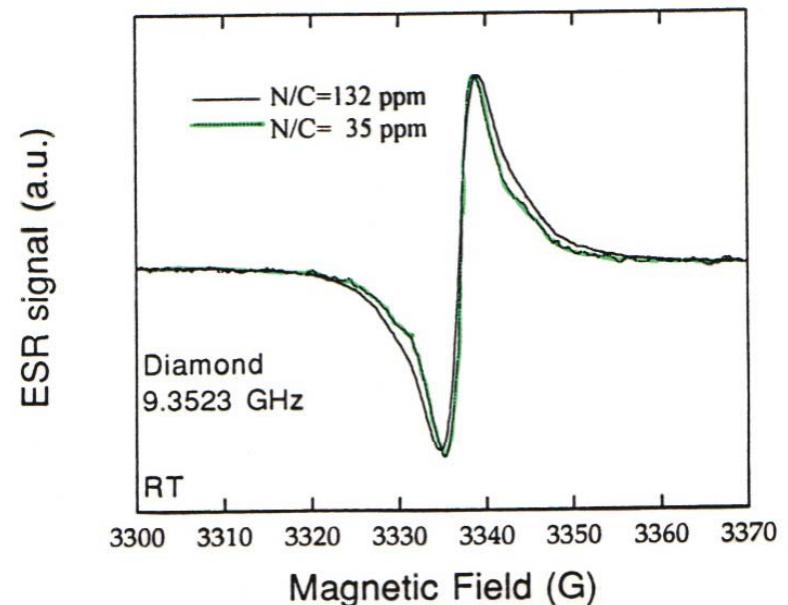
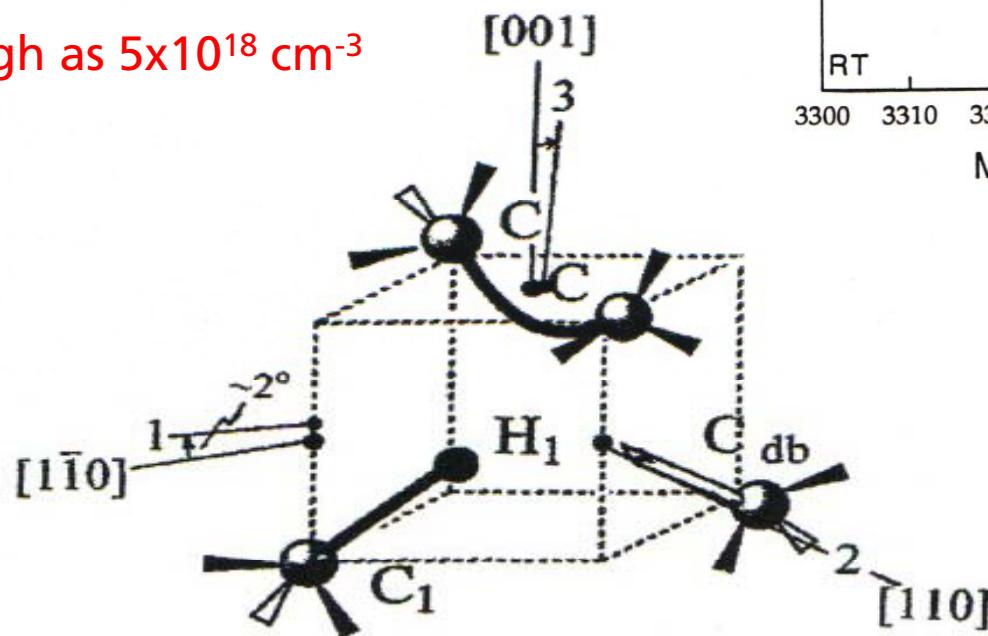


## 2. Defects in Diamond: H1 Center

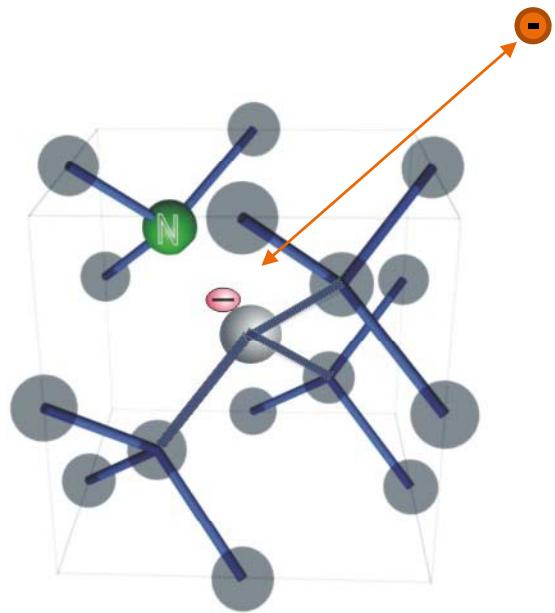
X. Zhou, G.D. Watkins et al. PRB 54 (1996) p. 7881

Homoepitaxial single crystalline diamond:

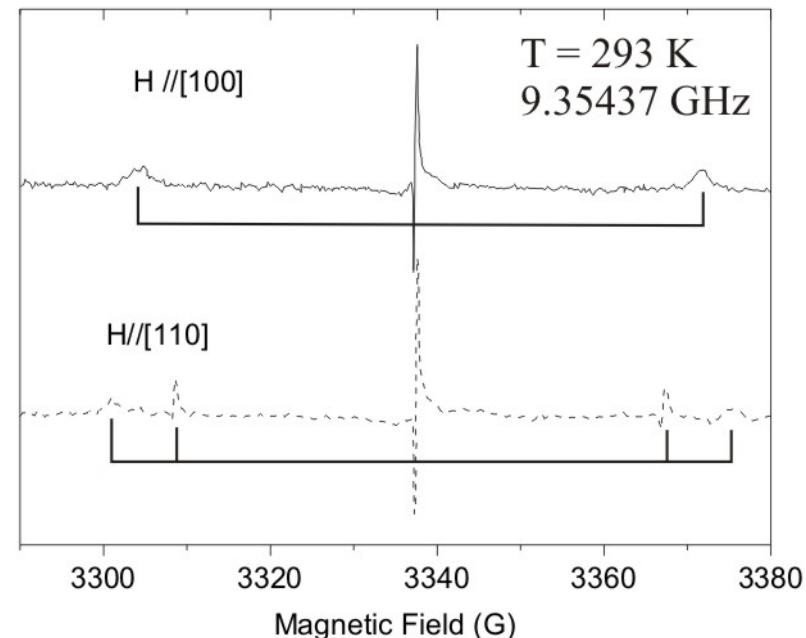
Density as high as  $5 \times 10^{18} \text{ cm}^{-3}$



# P1 Center (N-Dopant, g = 2.0024)



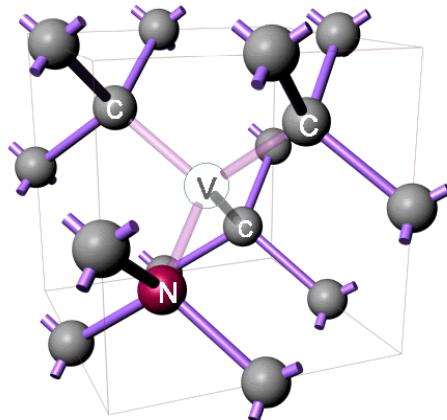
Capture Cross Section:  $10^{-14} \text{ cm}^{-2}$



EPR of substitutional nitrogen ( $g=2.0024$ ).  
Satellite position depends on magnetic field with respect to (111)-orientation

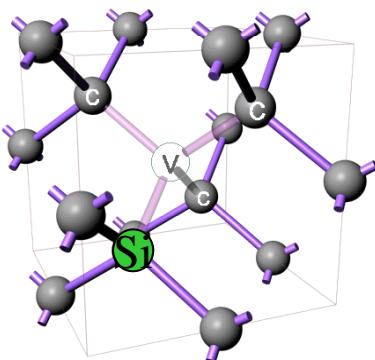
# Color Centers in Diamond

NV



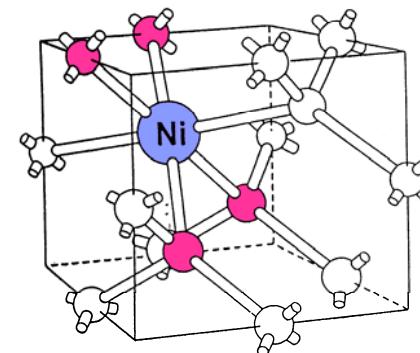
NV: 637 nm

SiV



SiV: 740 nm

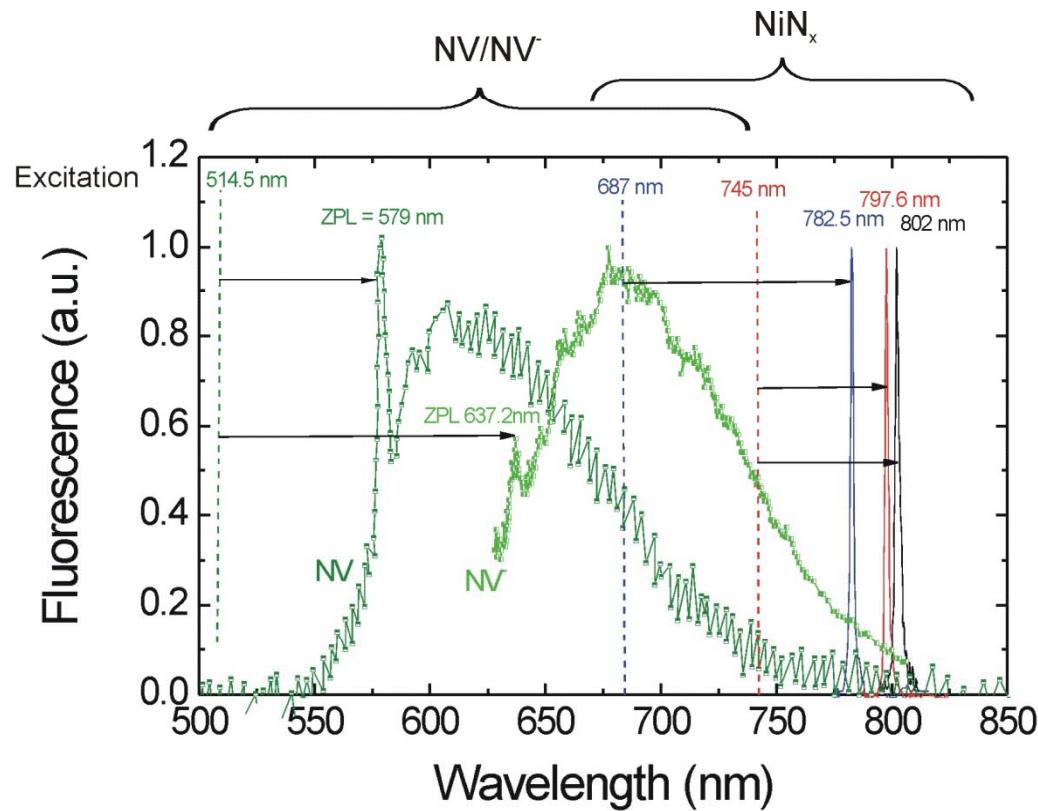
NE8



NiN<sub>x</sub>

around 800 nm

# Optical Excitation and Emission of NV and NiN<sub>x</sub>



The **NV centers** show two broad emission bands excited by 514.5 nm:

ZPL(1): 579 (neutral NV)  
ZPL(2): 637.2 nm (neg. charged NV<sup>-</sup>)

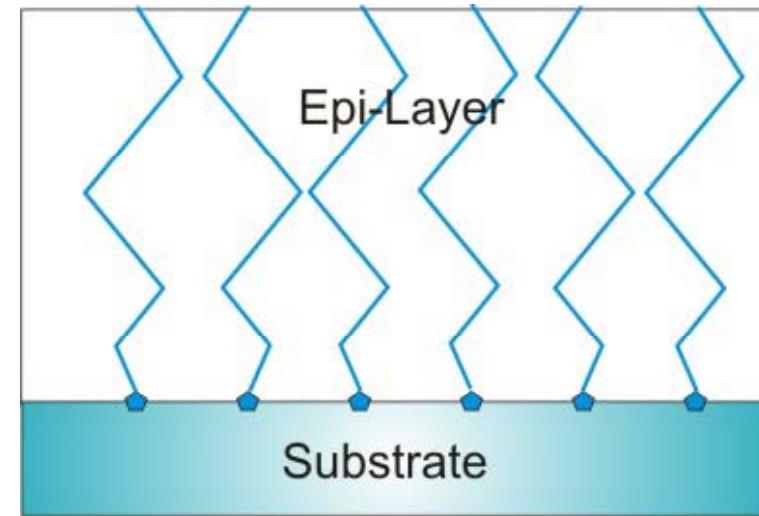
The **NiN<sub>x</sub> centers** show three very narrow (FWHM of 1.7 nm) emission lines excited by 687 nm and 745 nm:

782.5 nm  
797.6 nm  
802.0 nm

This shift is caused by slightly different arrangements of this Center (need to be characterized).

# Dislocations

- Lattice distortion
  - Grow from substrate into epi-layer
  - Killer of high voltage devices
- 
- Minimization:
    - soft etching of substrate before growth , to remove distortions



### 3. Deep Trapping Lifetime, Schubweg and Mobility

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

$$v_{th} = 10^7 \text{ cm/s}$$

$$\sigma_{cross} = 10^{-14} \text{ cm}^2$$

$$N_D = 10^{18} \text{ cm}^{-3}, 10^{17} \text{ cm}^{-3}, 10^{16} \text{ cm}^{-3}$$

Deep Trapping Livetime

$$\tau_1 = 10^{-11} \text{ s}$$

$$\tau_2 = 10^{-10} \text{ s}$$

$$\tau_3 = 10^{-9} \text{ s}$$

Schubweg:

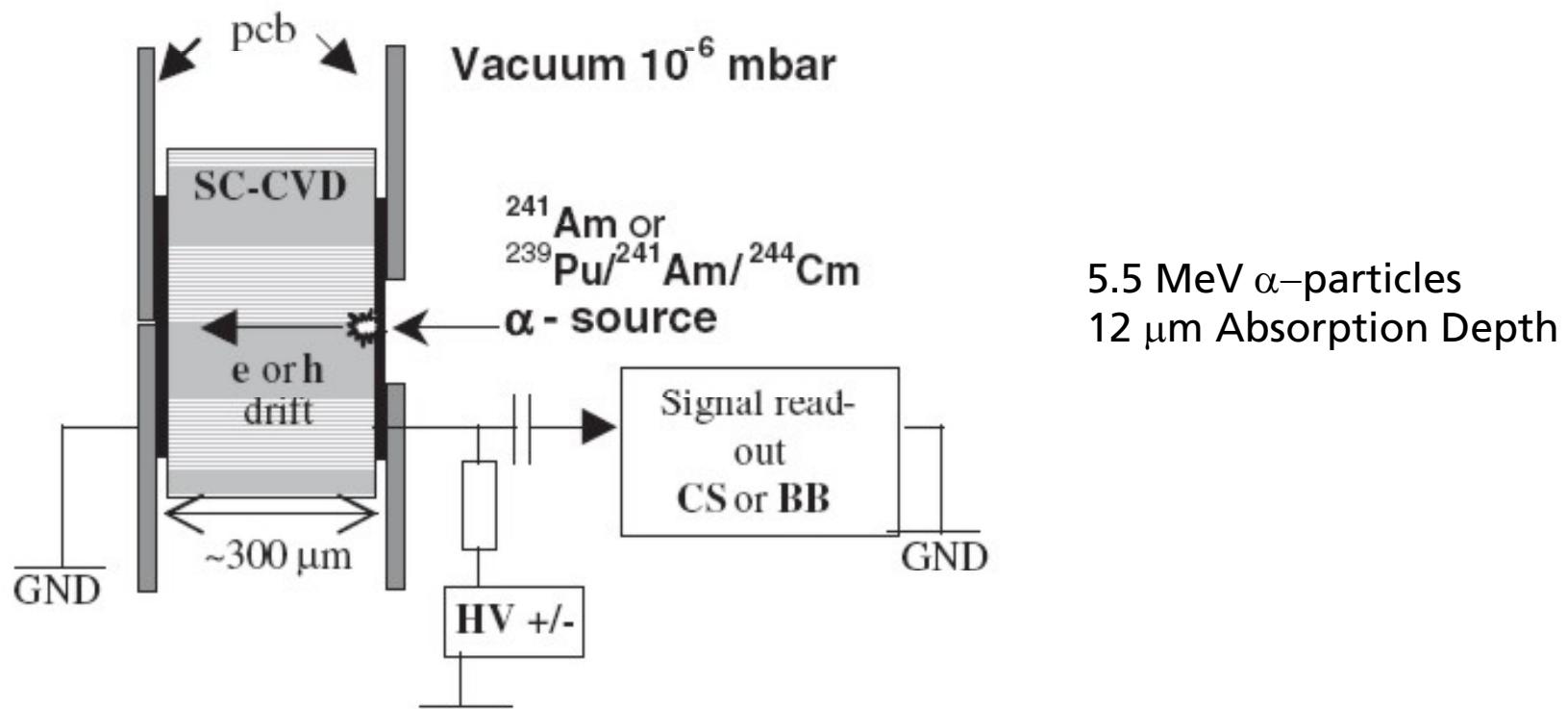
$$s = F \mu \tau$$

For  $F = 10^4 \text{ V/cm}$  and  $\mu = 10^3 \text{ cm}^2/\text{Vs}$ :  $s = 10^{-4} \text{ cm}, 10^{-3} \text{ cm}, 10^{-2} \text{ cm}$

$\mu \tau$  Products:  $10^{-8} \text{ cm}^2/\text{V}, 10^{-7} \text{ cm}^2/\text{V}$  and  $10^{-6} \text{ cm}^2/\text{V}$

# Time of flight set-up for $\alpha$ -particle detection

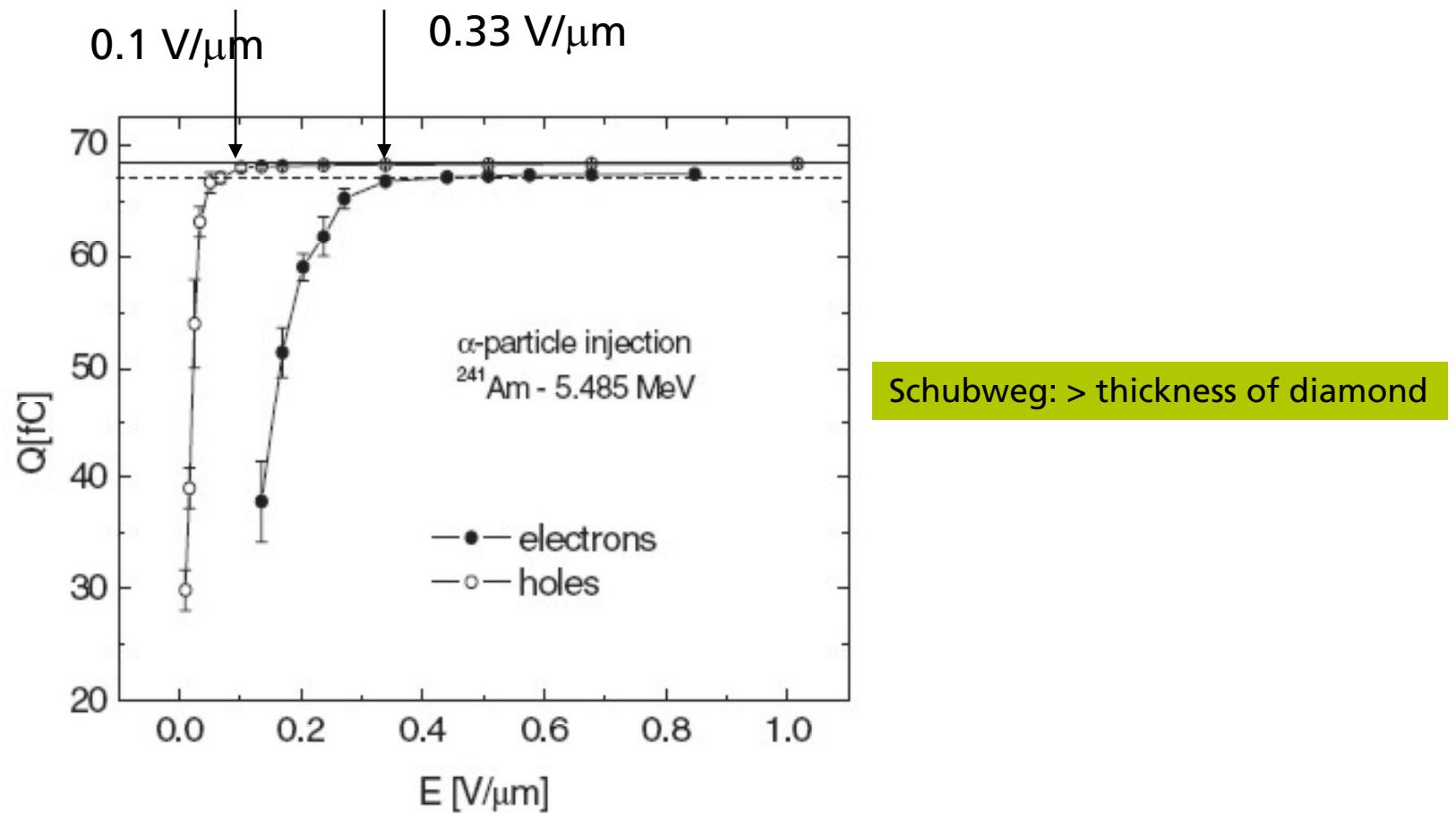
Source for  $\alpha$ -particle  $^{90}\text{Sr}$  or  $^{241}\text{Am}$



M. Pomorski et al., phys. stat. sol.(a) 202, 2199-2205 (2005)

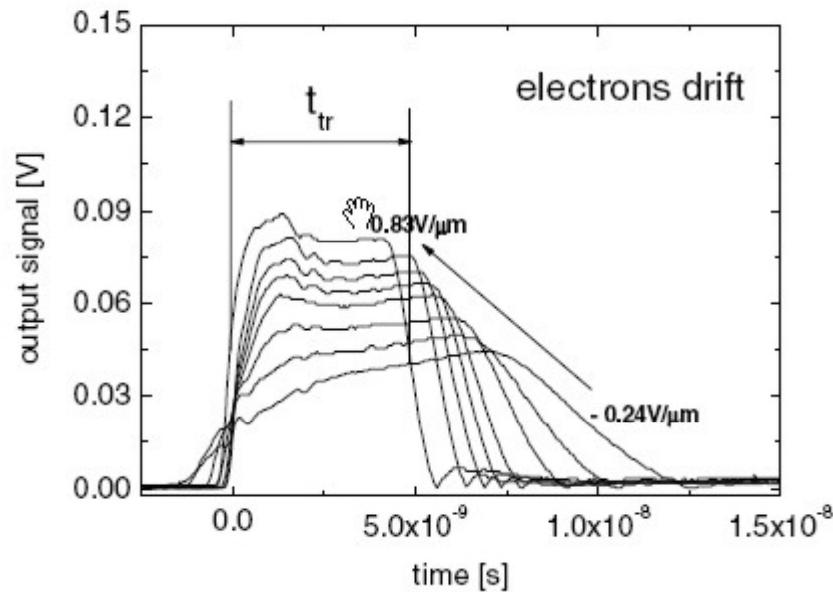
# 300 $\mu\text{m}$ SC Diamond (e6)

Collection efficiency of holes better than of electrons: but good!

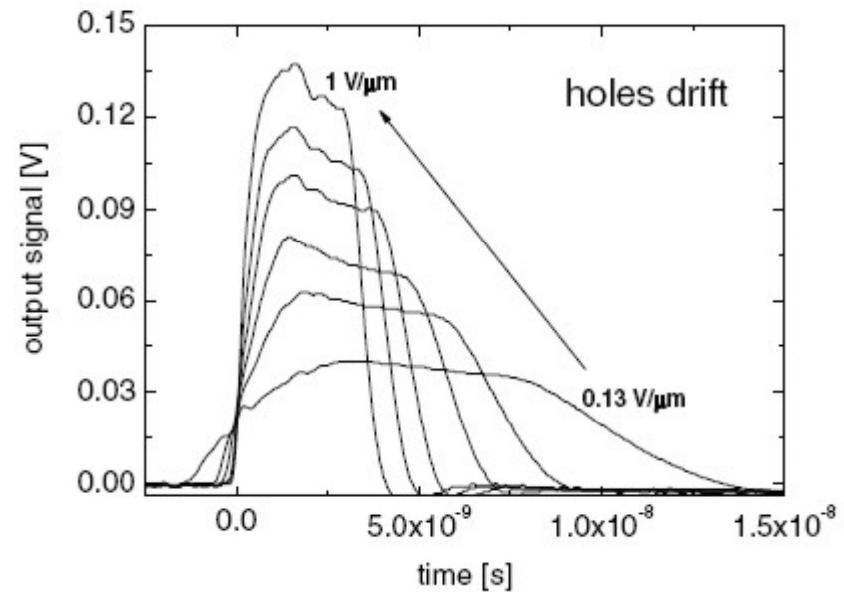


M. Pomorski et al., phys. stat. sol.(a) 202, 2199-2205 (2005)

# Time of Flight Signals



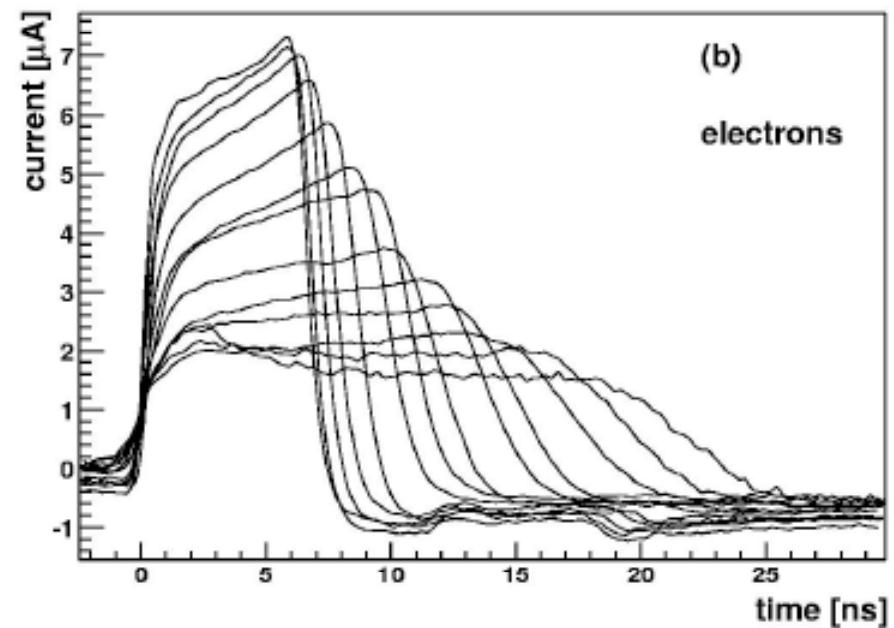
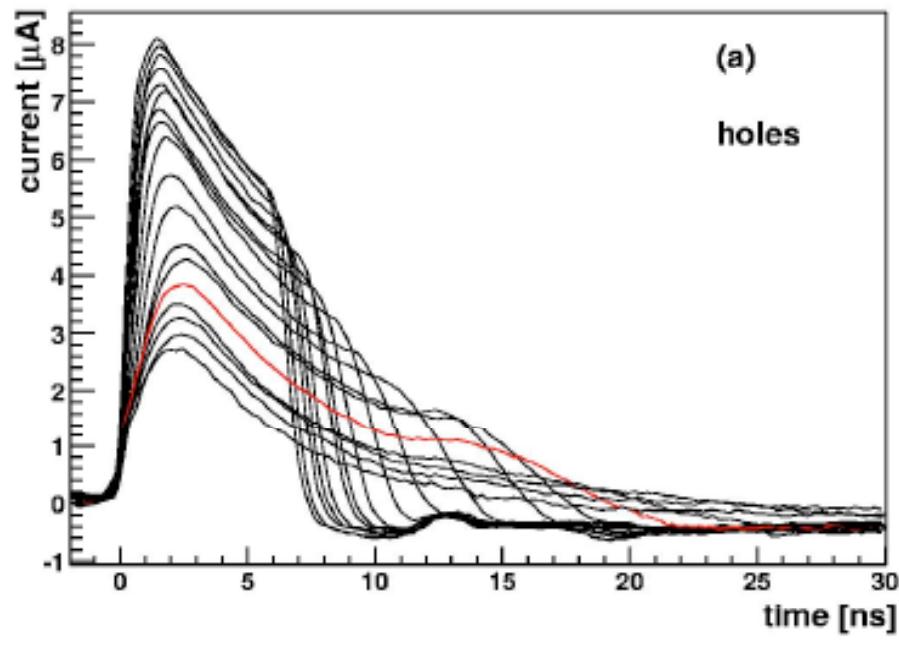
**Fig. 7** Electron-drift signals at different electric fields:  $0.24, -0.27, -0.34, -0.44, -0.51, -0.58, 0.68, -0.83$  V/μm.



**Fig. 8** Hole-drift signals at different electric fields:  $E = 0.18, 0.24, 0.34, 0.51, 0.68, 1$  V/μm.

M. Pomorski et al., phys. stat. sol.(a) 202, 2199-2205 (2005)

# TOF by Pernegger et al.



H. Pernegger, CERN, RD42 coll. Meeting May 2004

# Result Summary

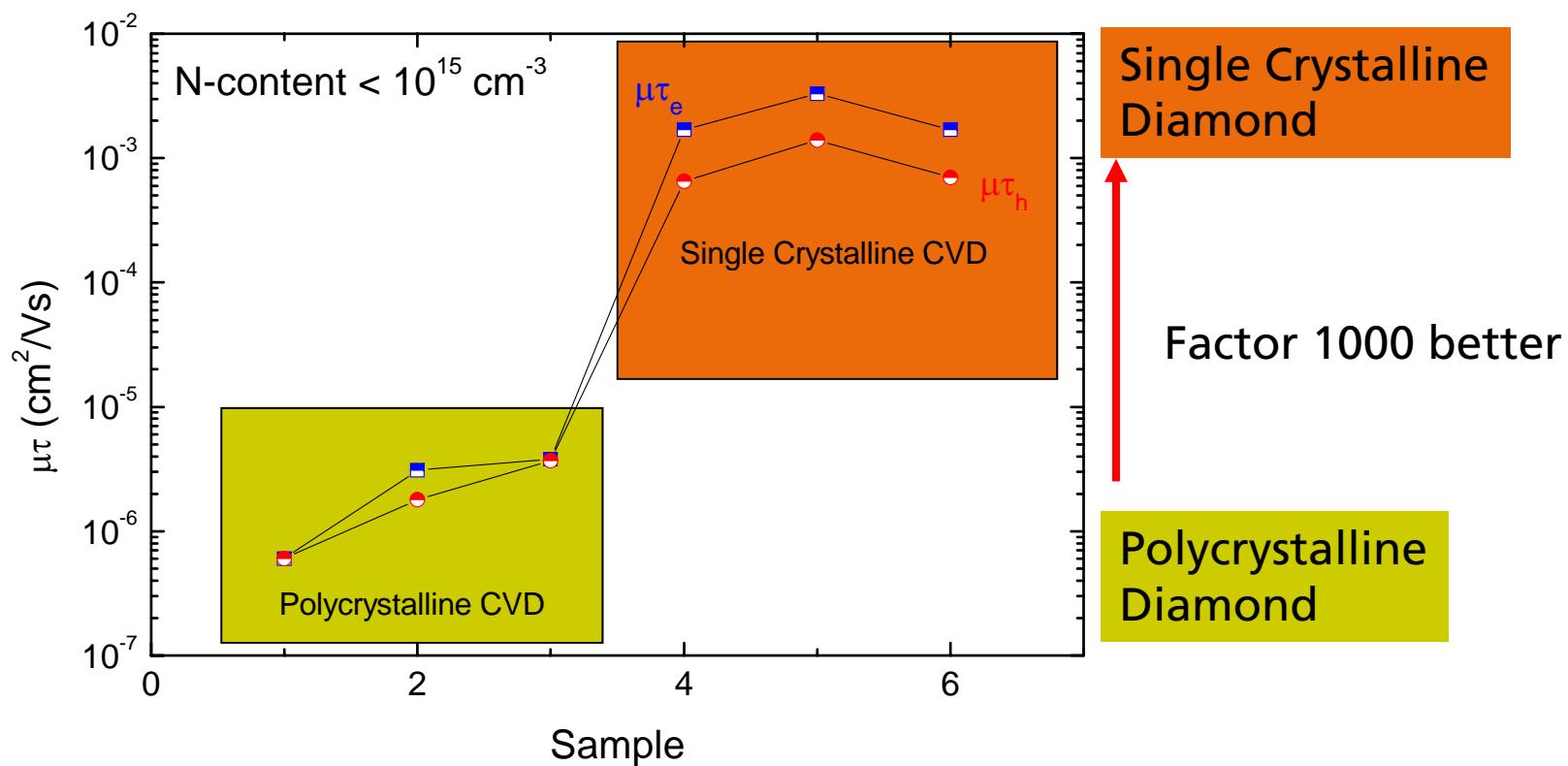
M. Pomorski et al., phys. stat. sol.(a) 202, 2199-2205 (2005)

	$\mu_0$ – low field mobility [cm <sup>2</sup> /Vs]	$v_s$ – saturation velocity [cm/s]	$\tau$ – life time [ns]
electrons	$2071 \pm 212$	$0.85 \pm 0.08 \times 10^7$	$174 \pm 15$
holes	$2630 \pm 123$	$1.34 \pm 0.05 \times 10^7$	$968 \pm 230$

Excellent Properties, but not 4500 and 3800 cm<sup>2</sup>/Vs  
Saturation velocity of electrons <  $1.5 \times 10^7$  cm/s  
Electon properties are not as good as holes!

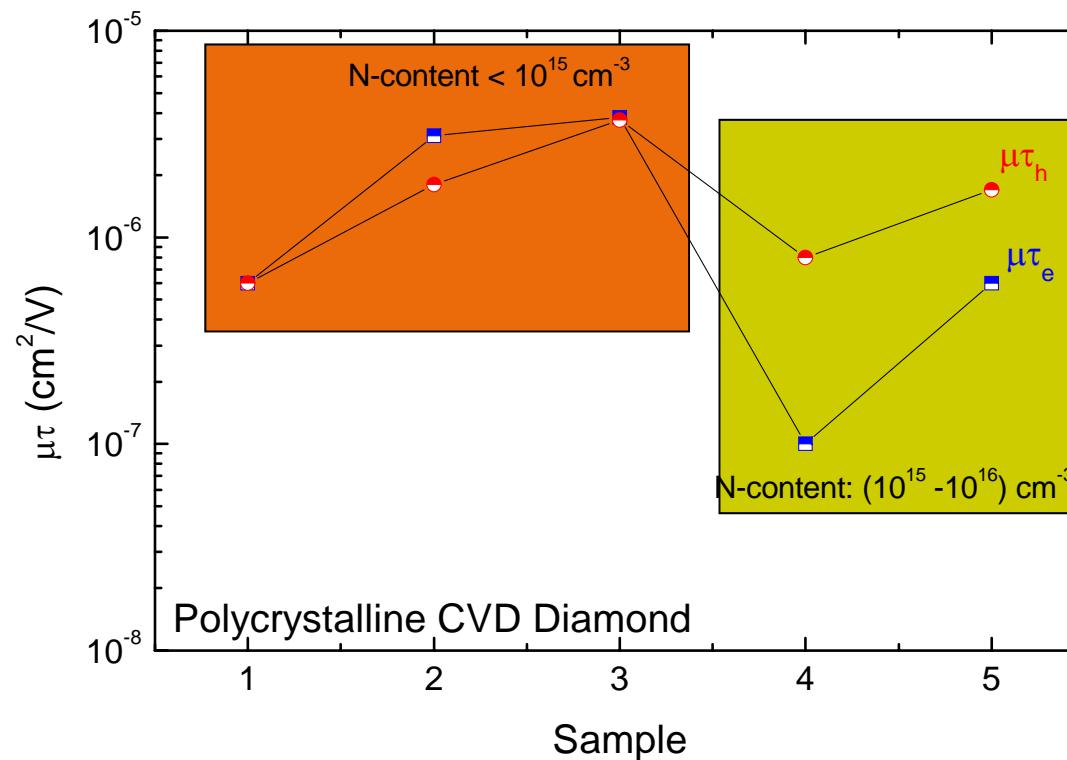
## 4. $\mu\tau$ –Product as Function of Morphology and Nitrogen

$$\begin{aligned}\mu\tau = 10^{-5} \text{ cm}^2/\text{V} &\rightarrow 10^{15} \text{ cm}^{-3} \text{ Nitrogen} \\ \mu\tau = 10^{-4} \text{ cm}^2/\text{V} &\rightarrow 10^{14} \text{ cm}^{-3} \text{ Nitrogen} \\ \mu\tau = 10^{-3} \text{ cm}^2/\text{V} &\rightarrow 10^{13} \text{ cm}^{-3} \text{ Nitrogen}\end{aligned}$$



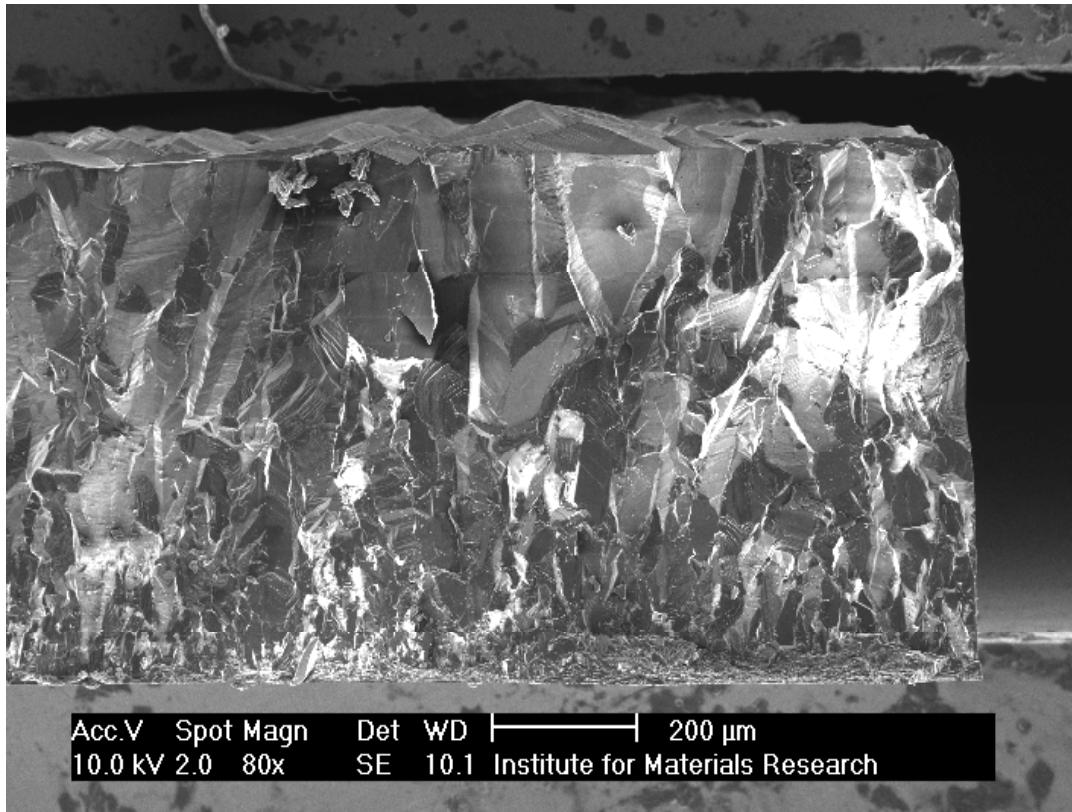
# $\mu\tau$ -Product as Function of Nitrogen Content

Nitrogen not important (Isberg!!!!)



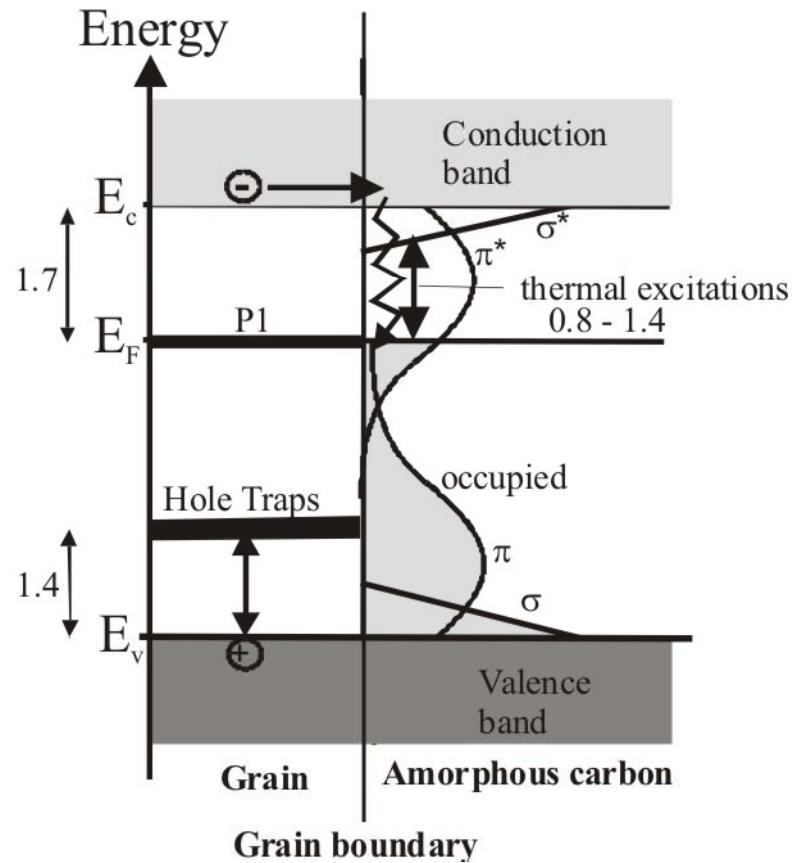
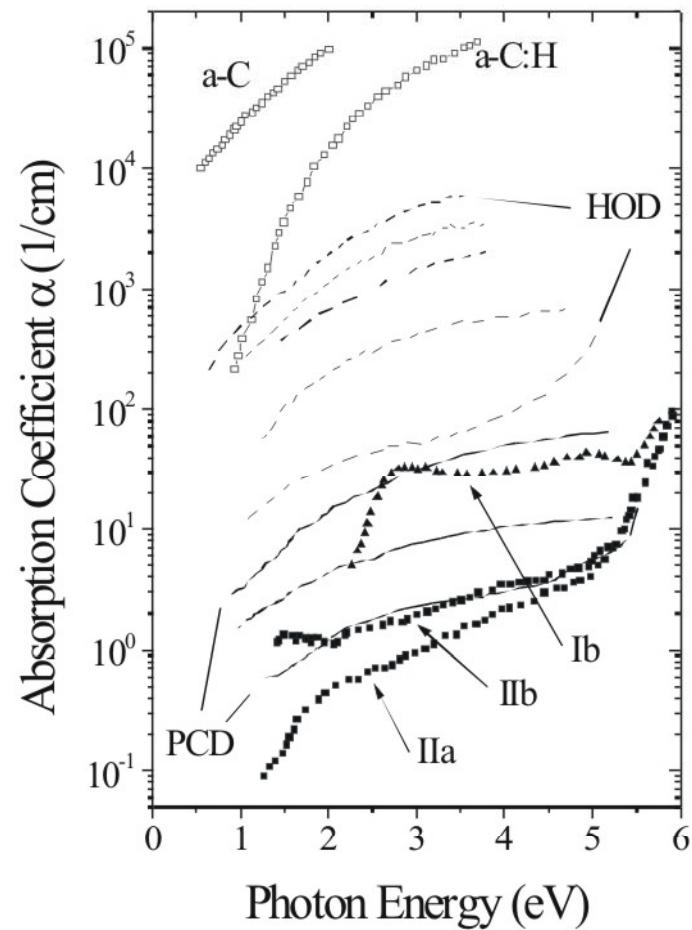
J. Isberg et al., Diam. Rel. Mat. 13 (2004) 872.

## 5. Properties of Poly-Crystalline CVD Diamond

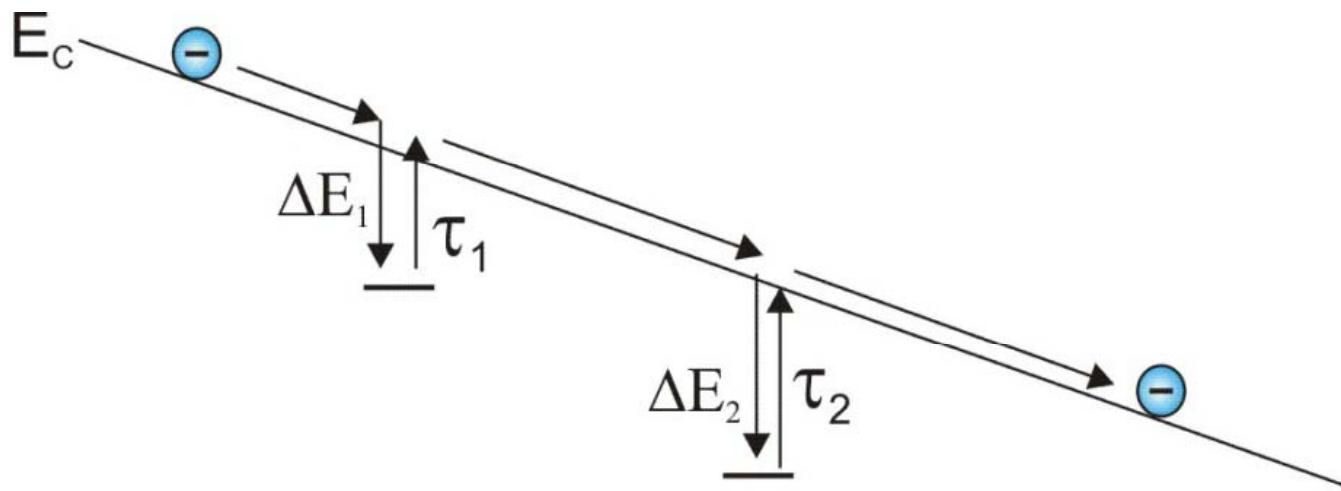


Acc.V Spot Magn Det WD 200 μm  
10.0 kV 2.0 80x SE 10.1 Institute for Materials Research

# Density-of-State Distribution



# Charrier Propagation: Trapping and Emission Dominated

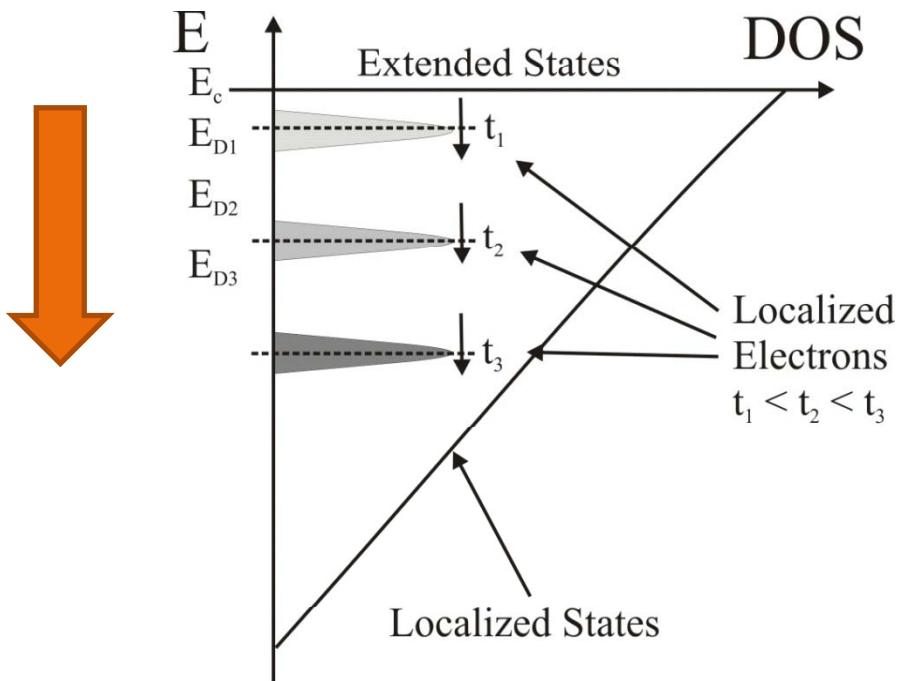


Trapping Time constant:  $\tau = \frac{1}{v_{th} N_D \sigma}$

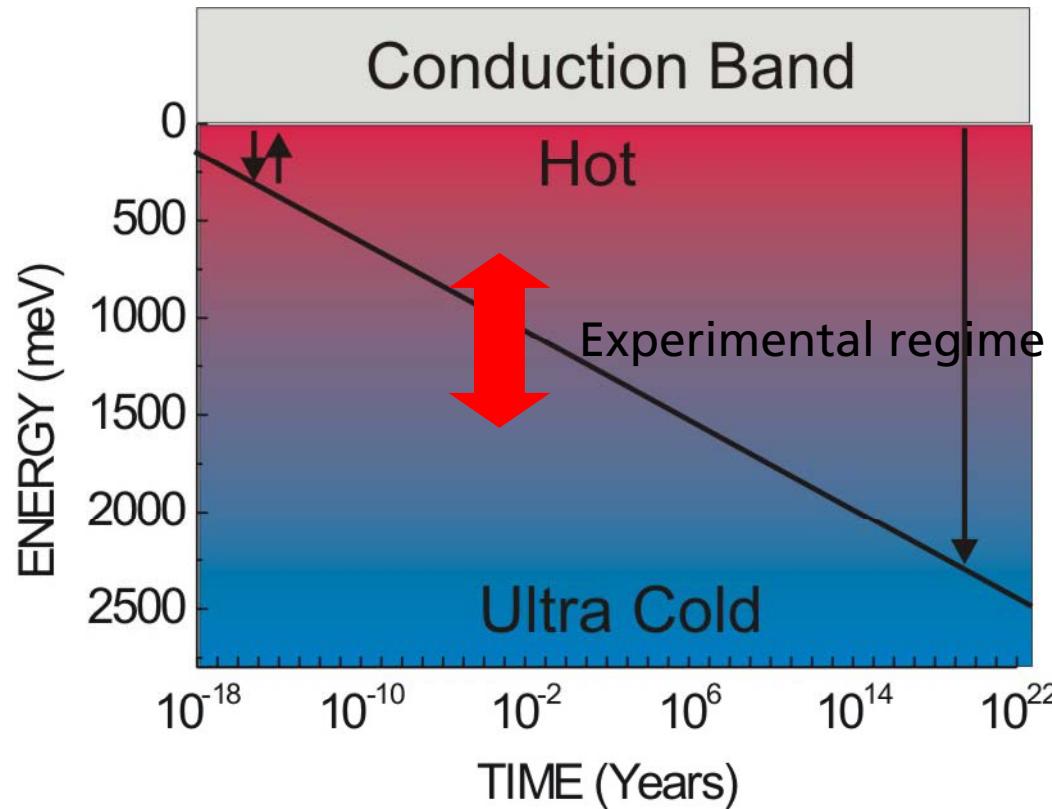
Re-Emission Time Constant  $\tau$ :  $v(E) \tau \geq 1 \rightarrow \tau(E) = \frac{1}{v_o} e^{\frac{\Delta E}{kT}}$

Where:  $v_o = 10^{12}$  to  $10^{13}$  1/s (Raman Frequency)

# Thermalization of Carriers into the DOS

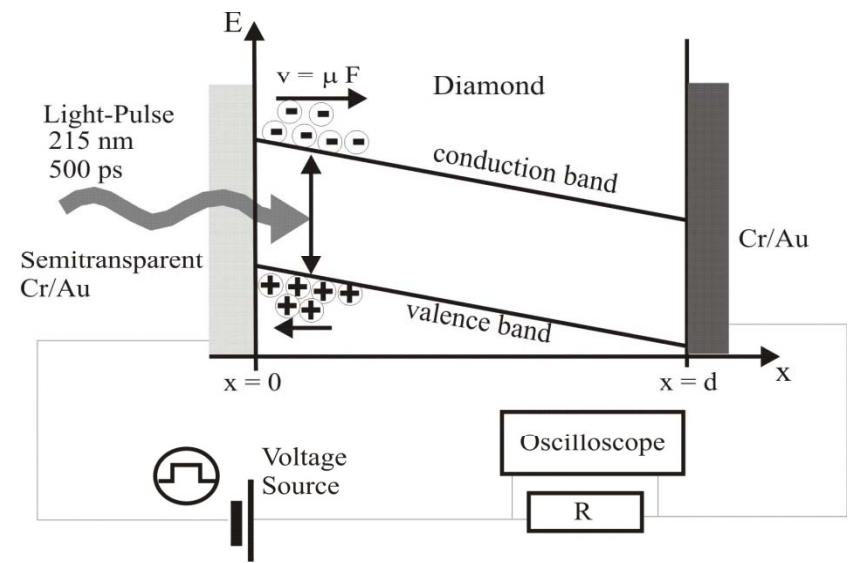
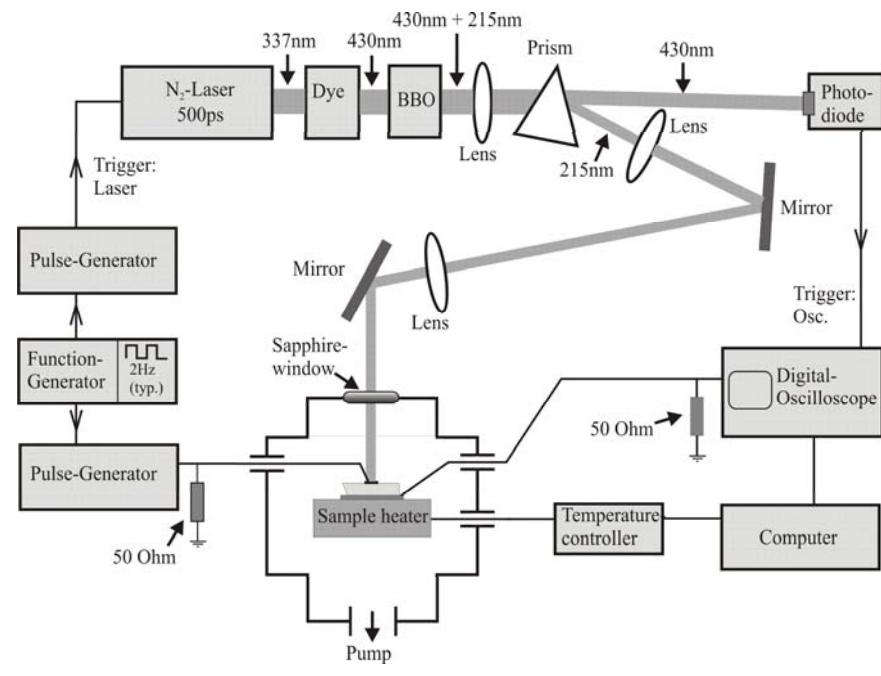


# Diamond is: ULTRA COLD



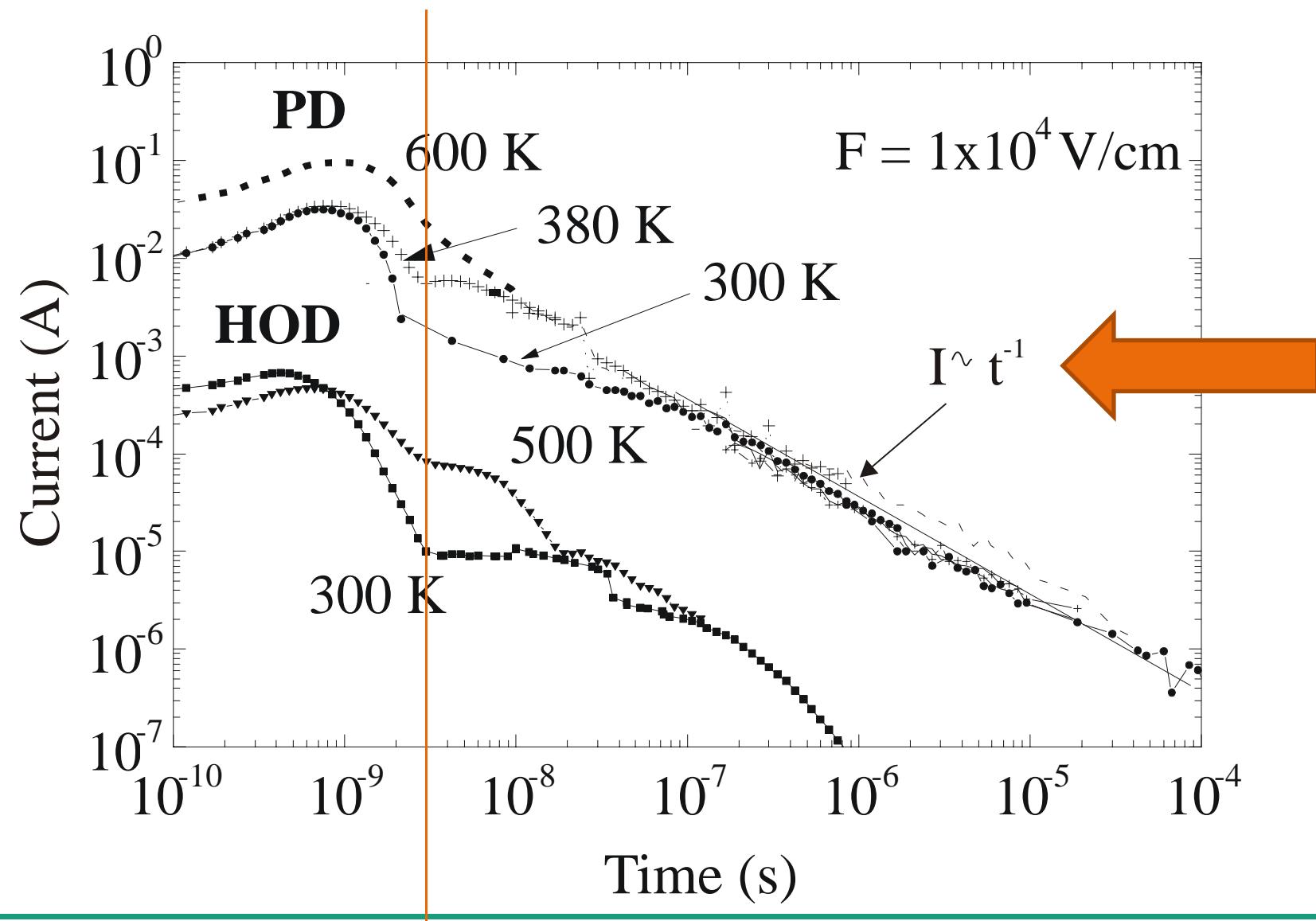
Assumptions:  $T = 300 \text{ K}$ ,  $v_o = 10^{13} \text{ 1/s}$

# TOF Set-Up

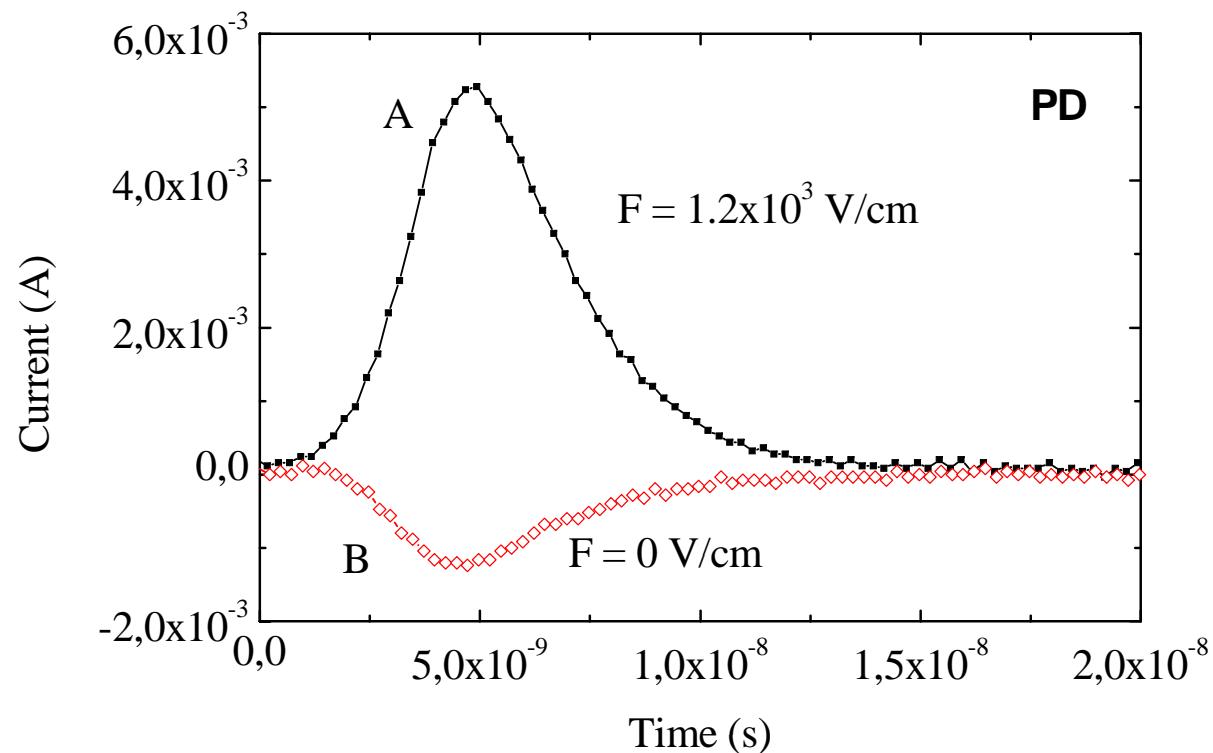


tof1.cdr

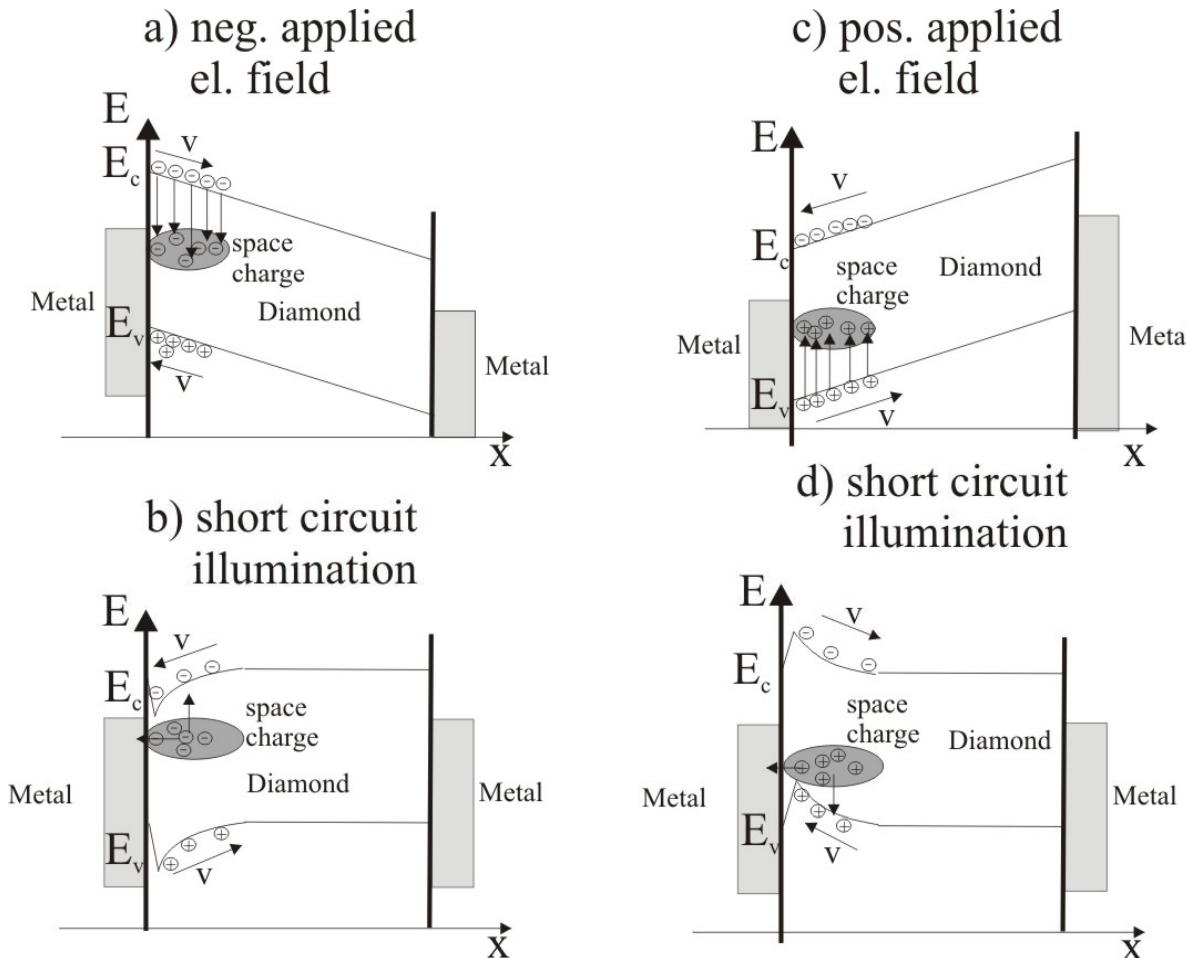
# TOF on PCD



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



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



## 6. Spectrally Resolved Photoconductivity

$$\frac{j_{ph}(hv)}{\Phi_o(hv)} \approx \tau_n \alpha(hv)$$

where:

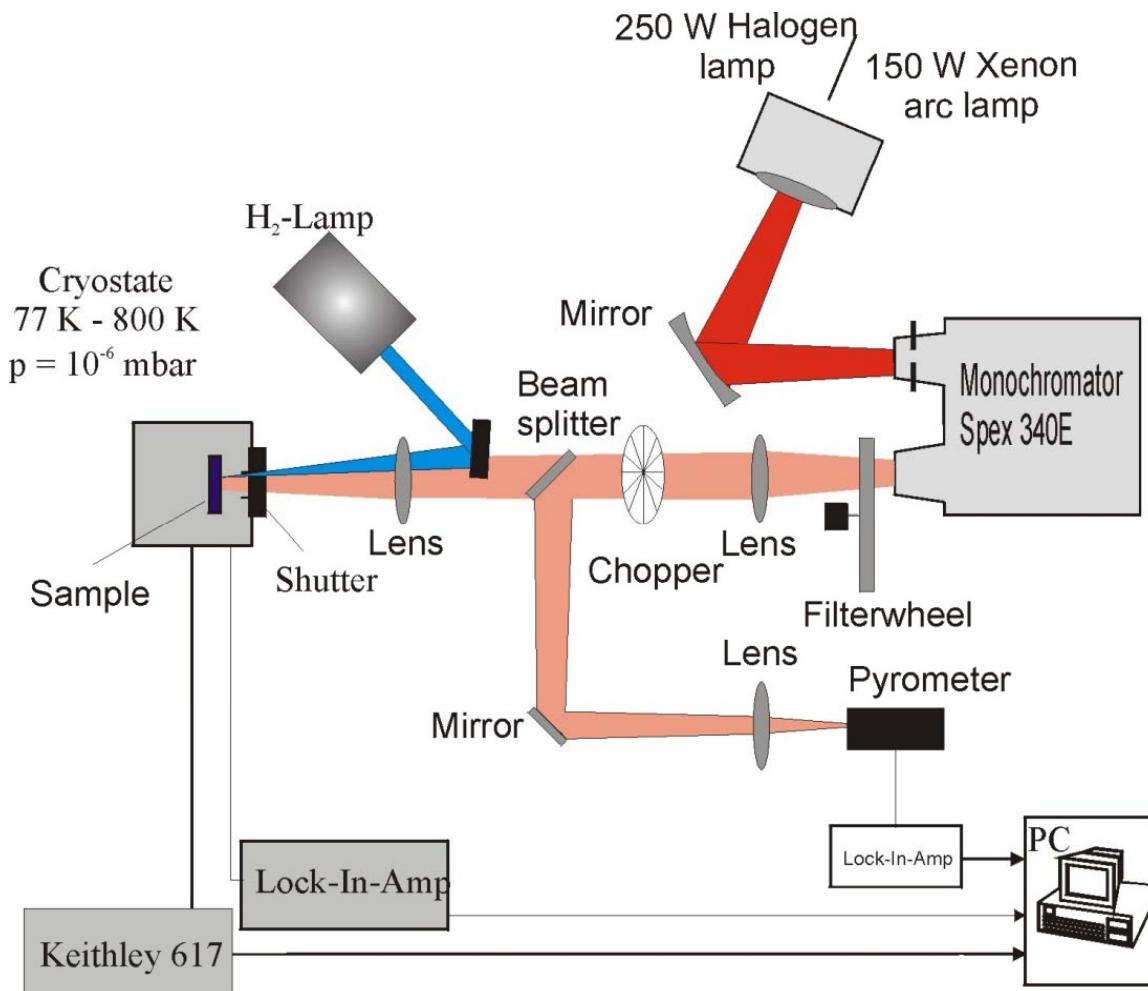
$j_{ph}$  : photo-current

$\Phi_o$  : photon flux

$\tau_n$  = lifetime

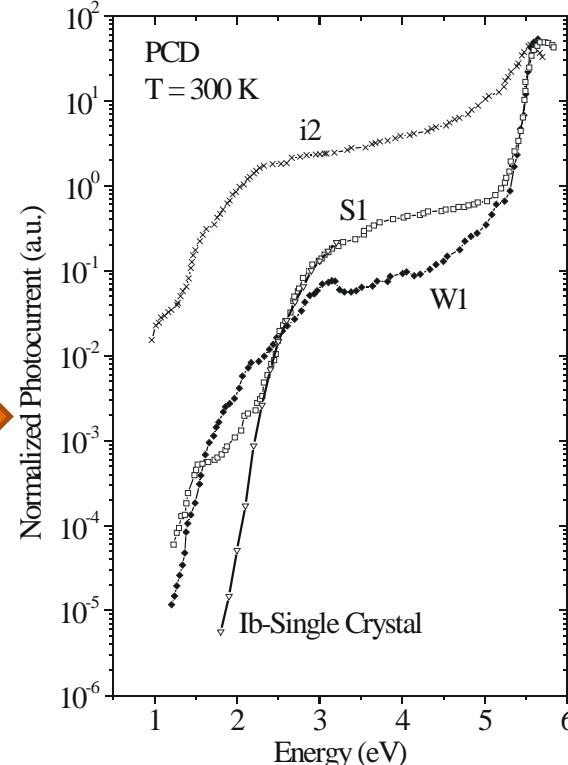
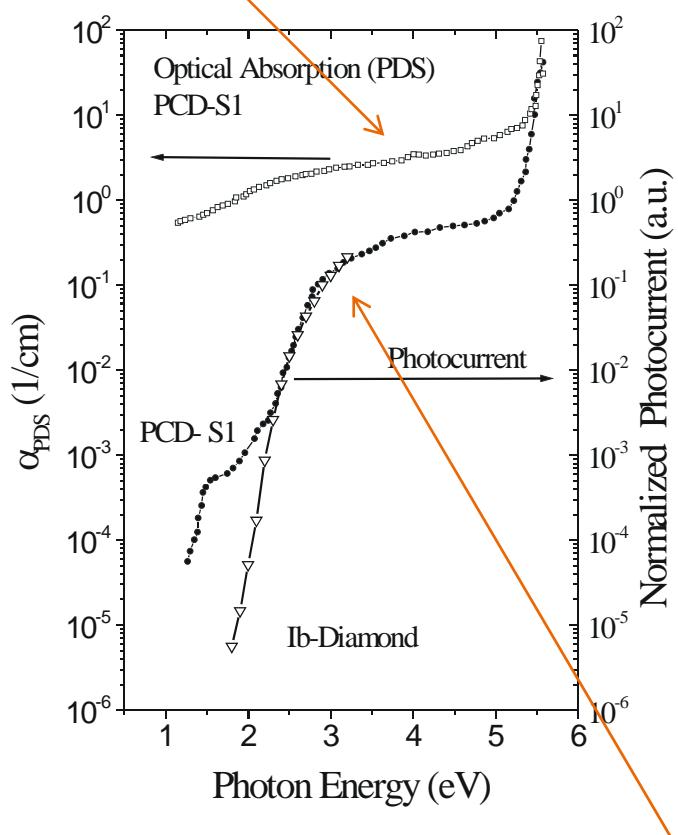
$\alpha(hv)$ = absorption coefficient

# Set-Up



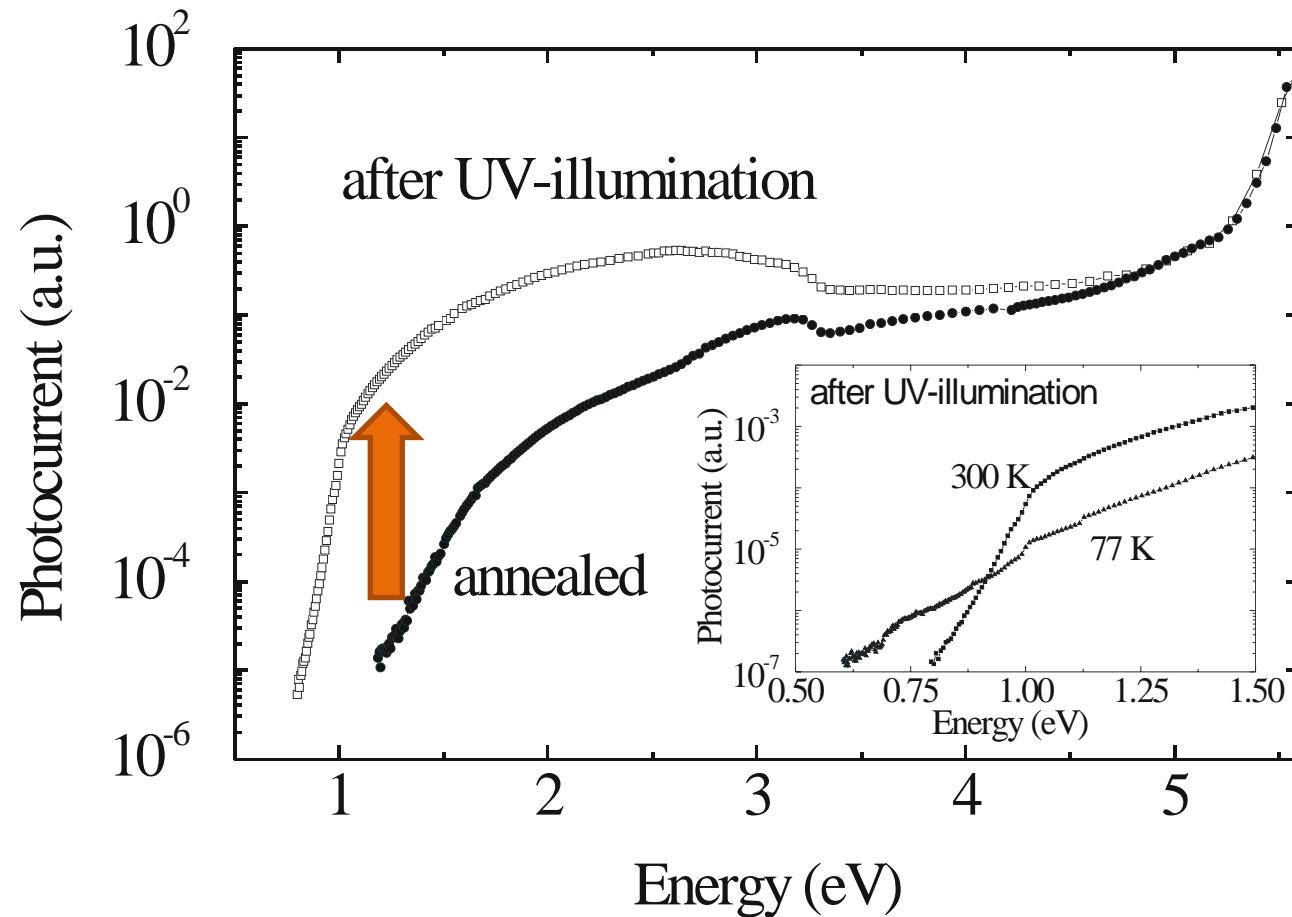
# Spectrally Resolved PC and PTD Spectroscopy

all carriers

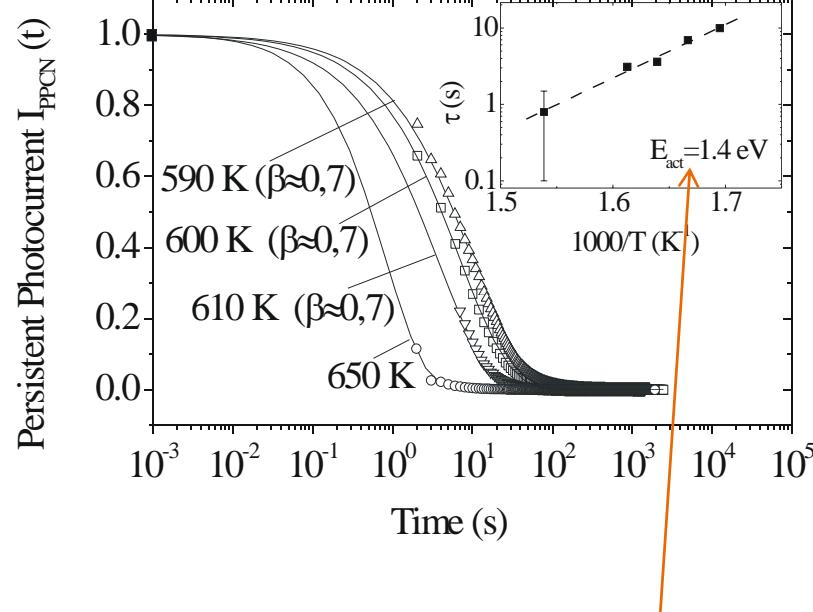
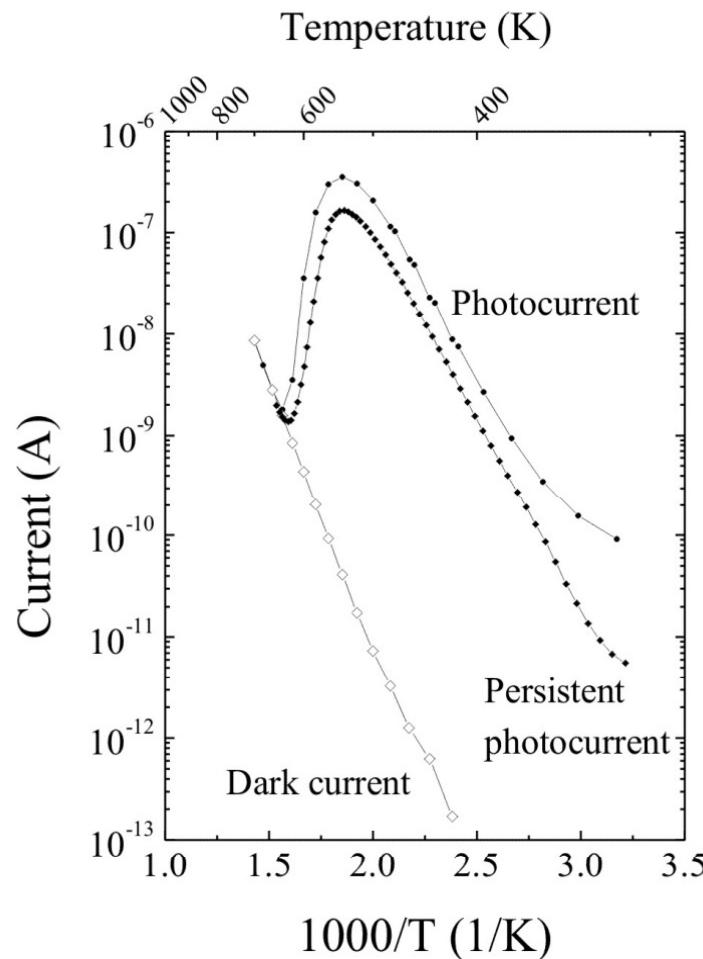


mobile carriers

# Spectrally Resolved PC:

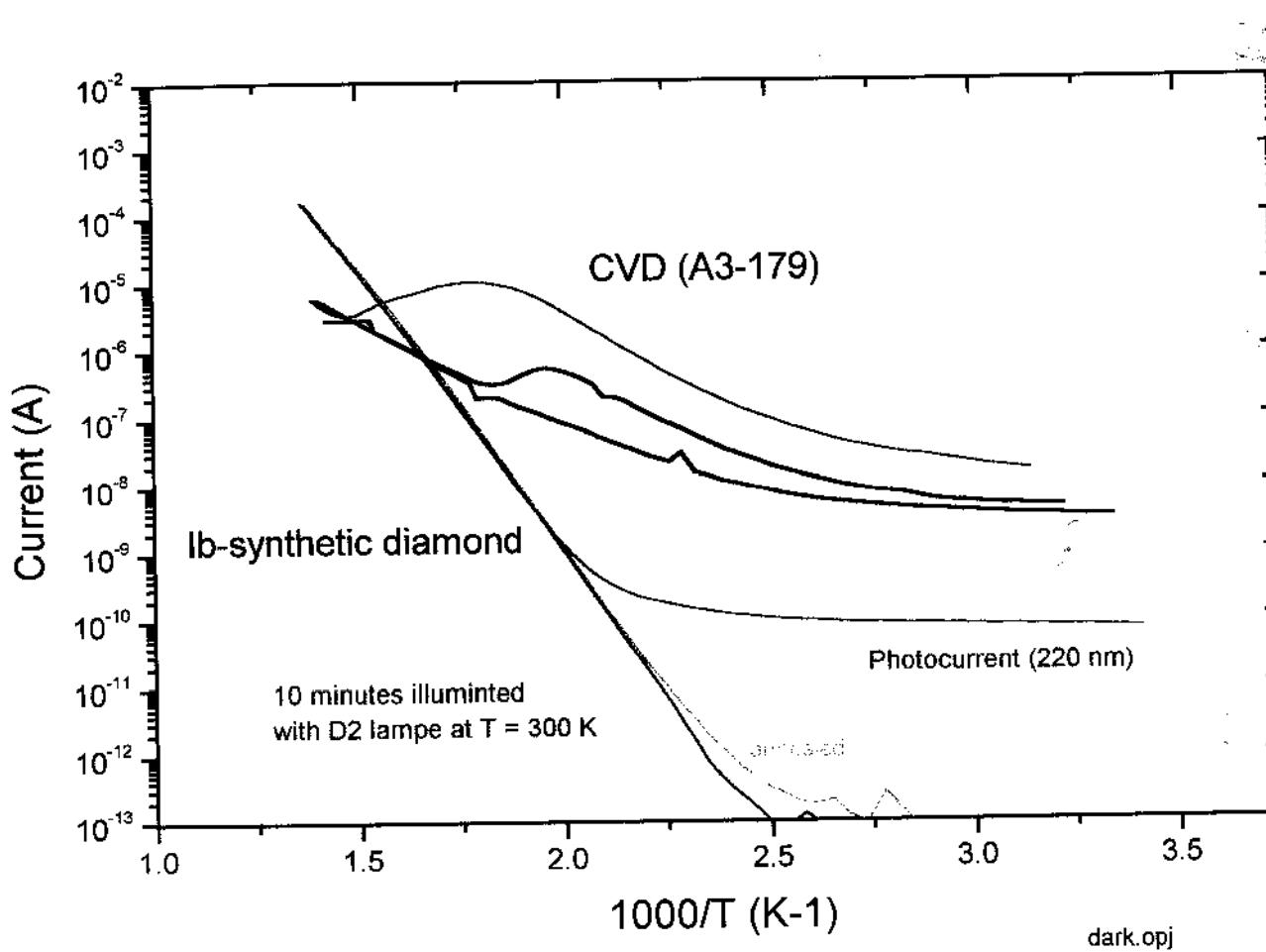


# Thermally Stimulated Currents

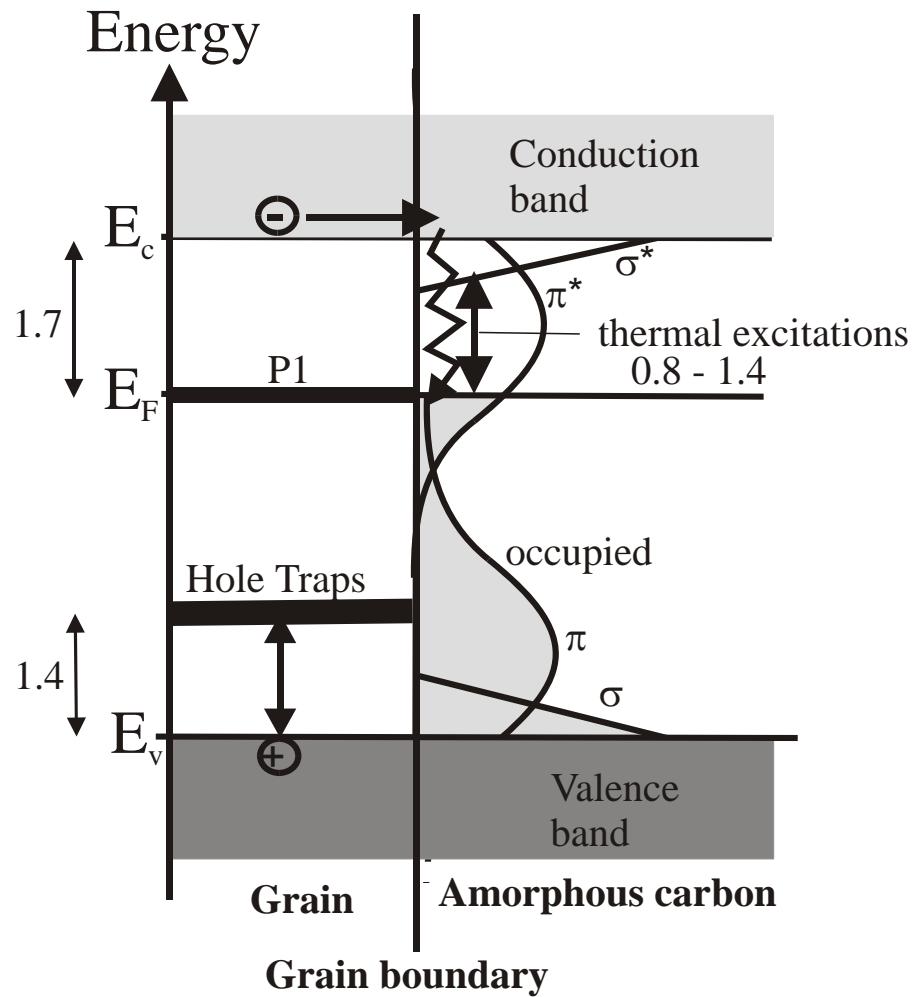


Annealing Out Energy: 1.4 eV

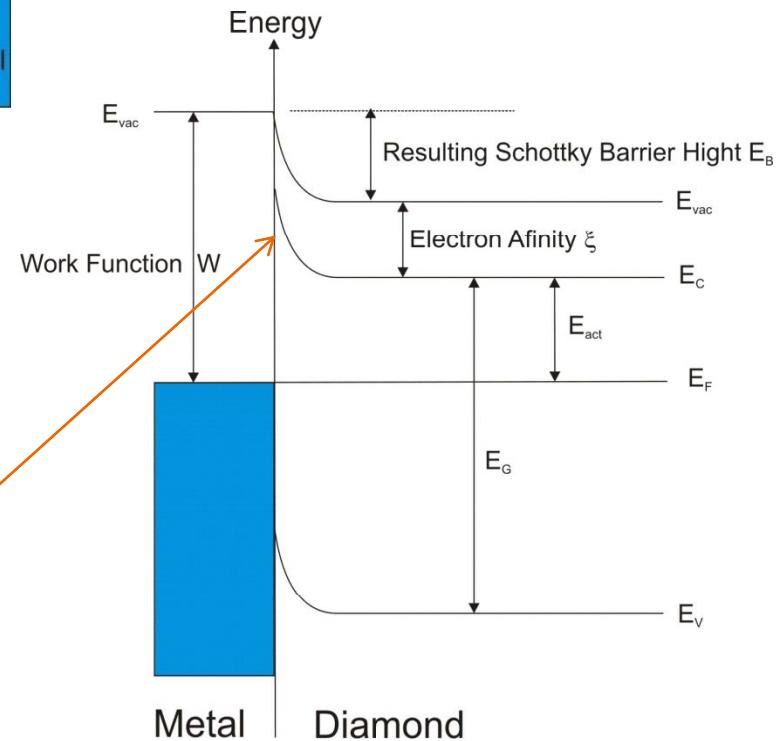
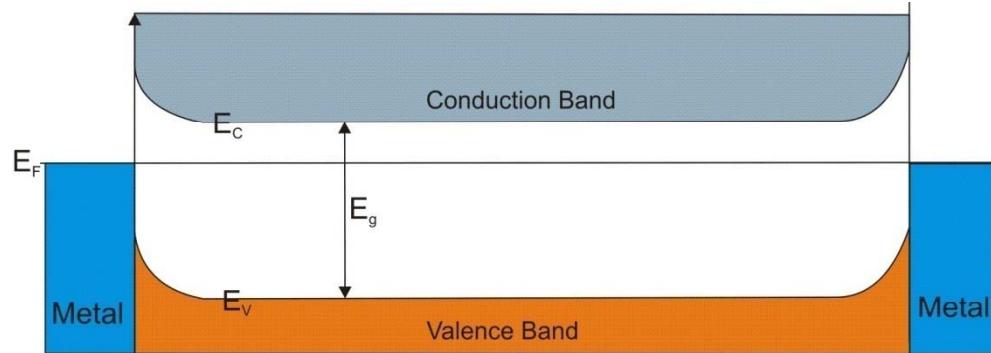
# Thermally Stimulated Currents in PCD and Single CD



# Model:

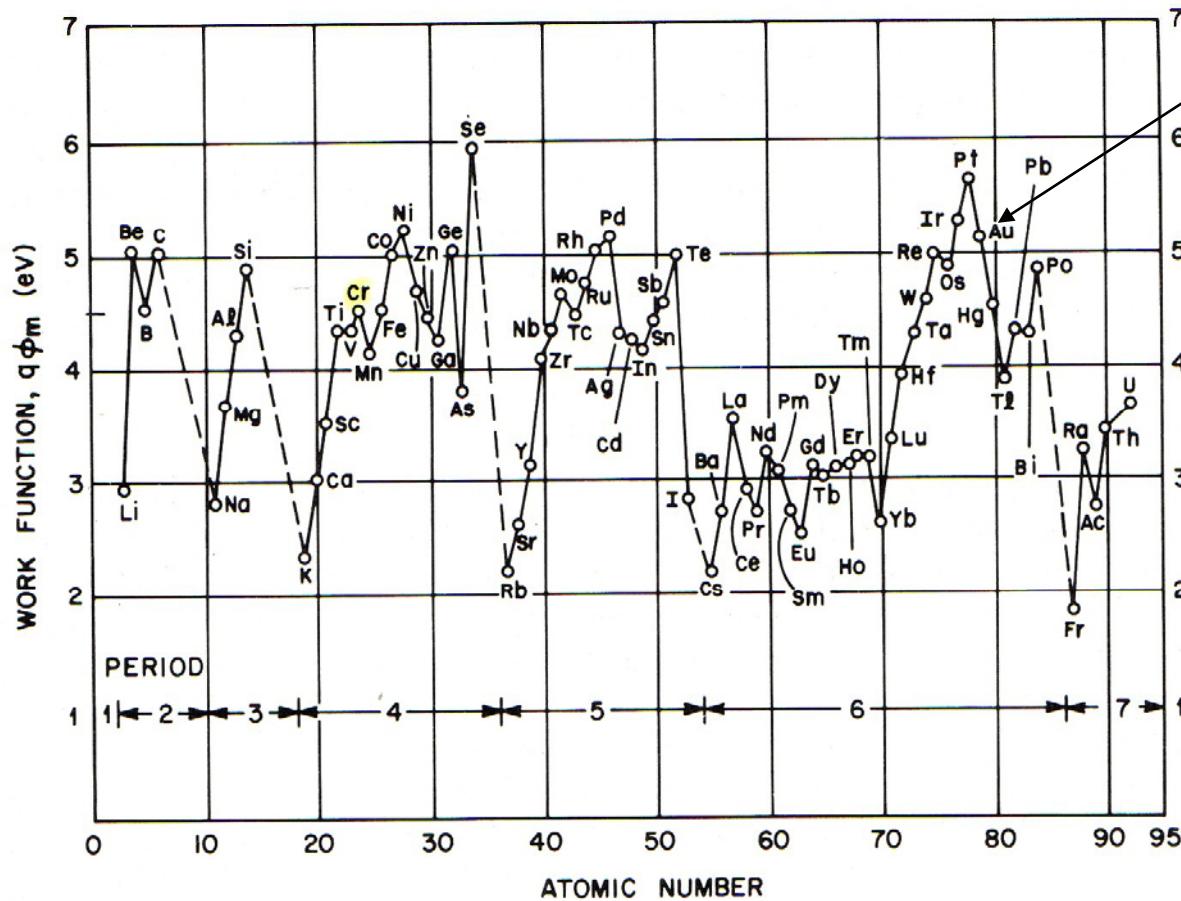


# 7. Contact Properties



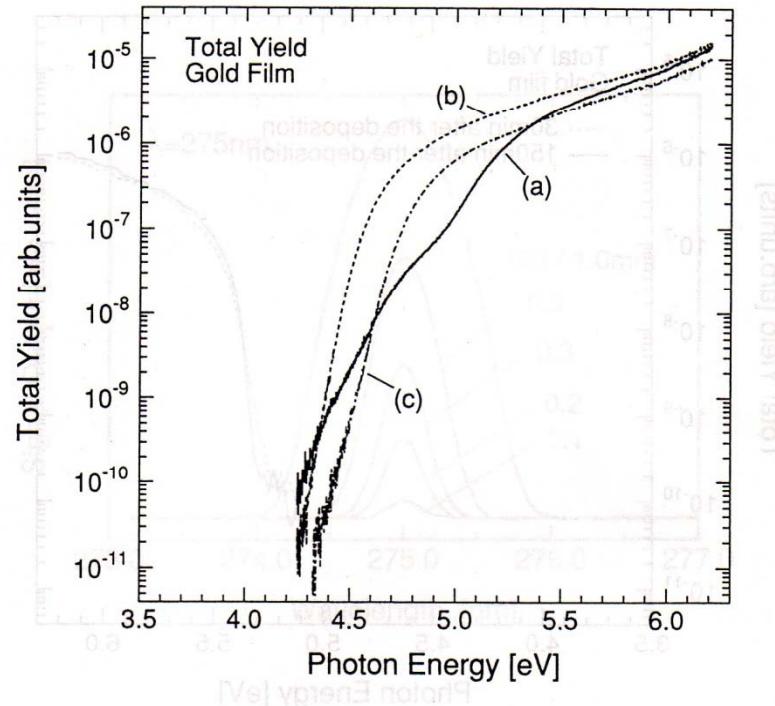
# Metal Workfunction (Sze ) $\Phi_m$

Au



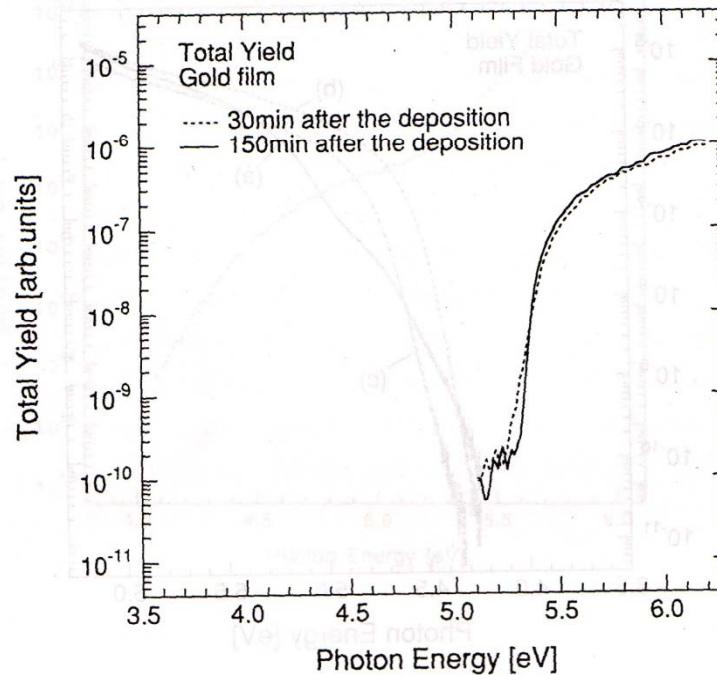
**Fig. 4** Metal work function for a clean metal surface in a vacuum versus atomic number. Note the periodic nature of the increase and decrease of the work functions within each group. (After Michaelson, Ref. 9.)

# Au Workfunction (S. Gonda, PhD Tokyo Institut of Technology 1995)



Workfunction: 4.5 eV

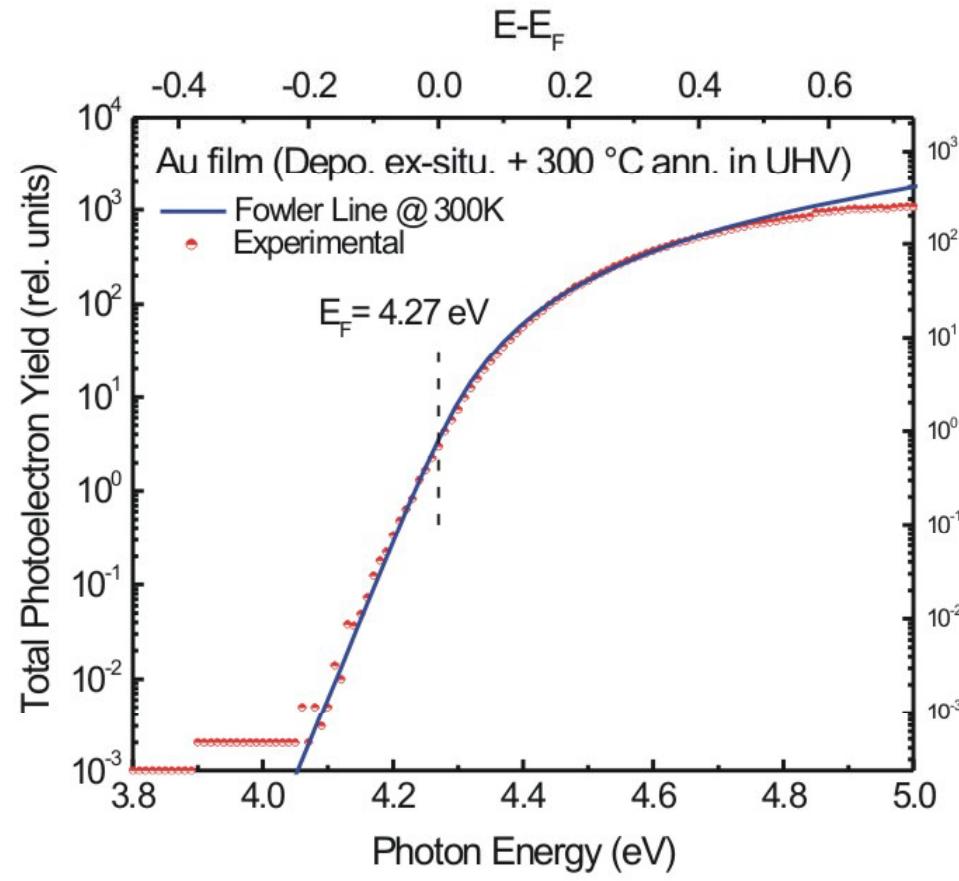
Au TPYS of AU: a) measured after 30 min,  
b) after 150 min in-situ evaporation in a vacuum of  $4 \times 10^{-8}$  Torr  
c) ex-situ evaporation



Workfunction: 5.2 eV

Au TPYS spectrum measured a) after 30 min  
and b) after 150 min. in-situ evaporation at  $5 \times 10^{-10}$  Torr

# TPYS on Au at DRC/AIST:

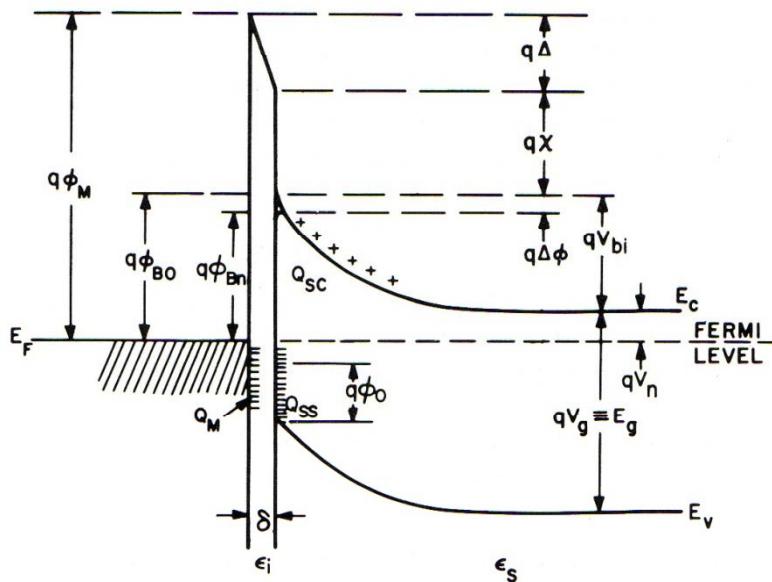


Workfunction 4.27 eV

# Real Schottky Contact

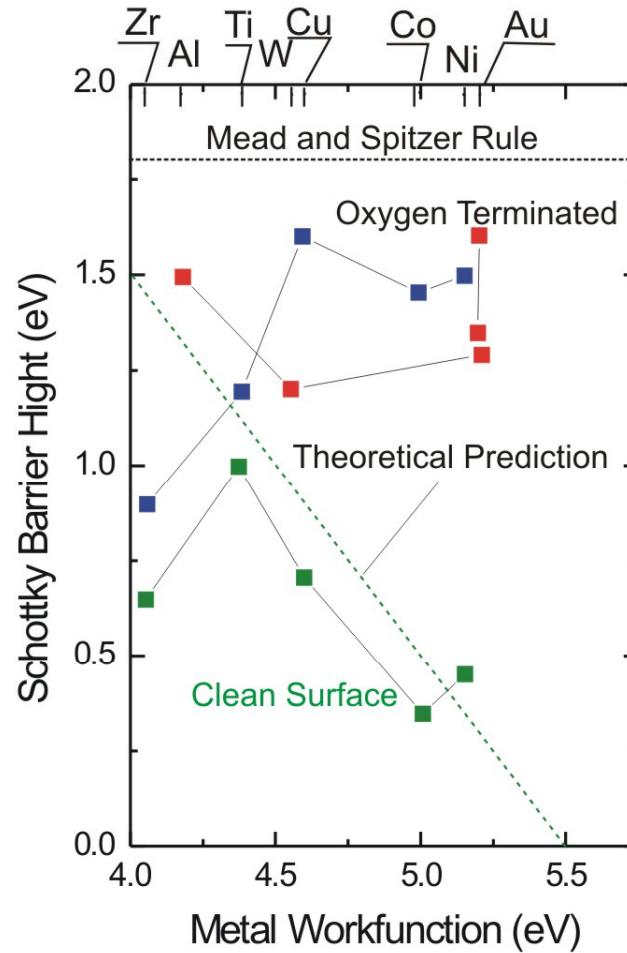
Surface Fermi-level pinning by surface defects

Schottky barrier is not dependent on metal.



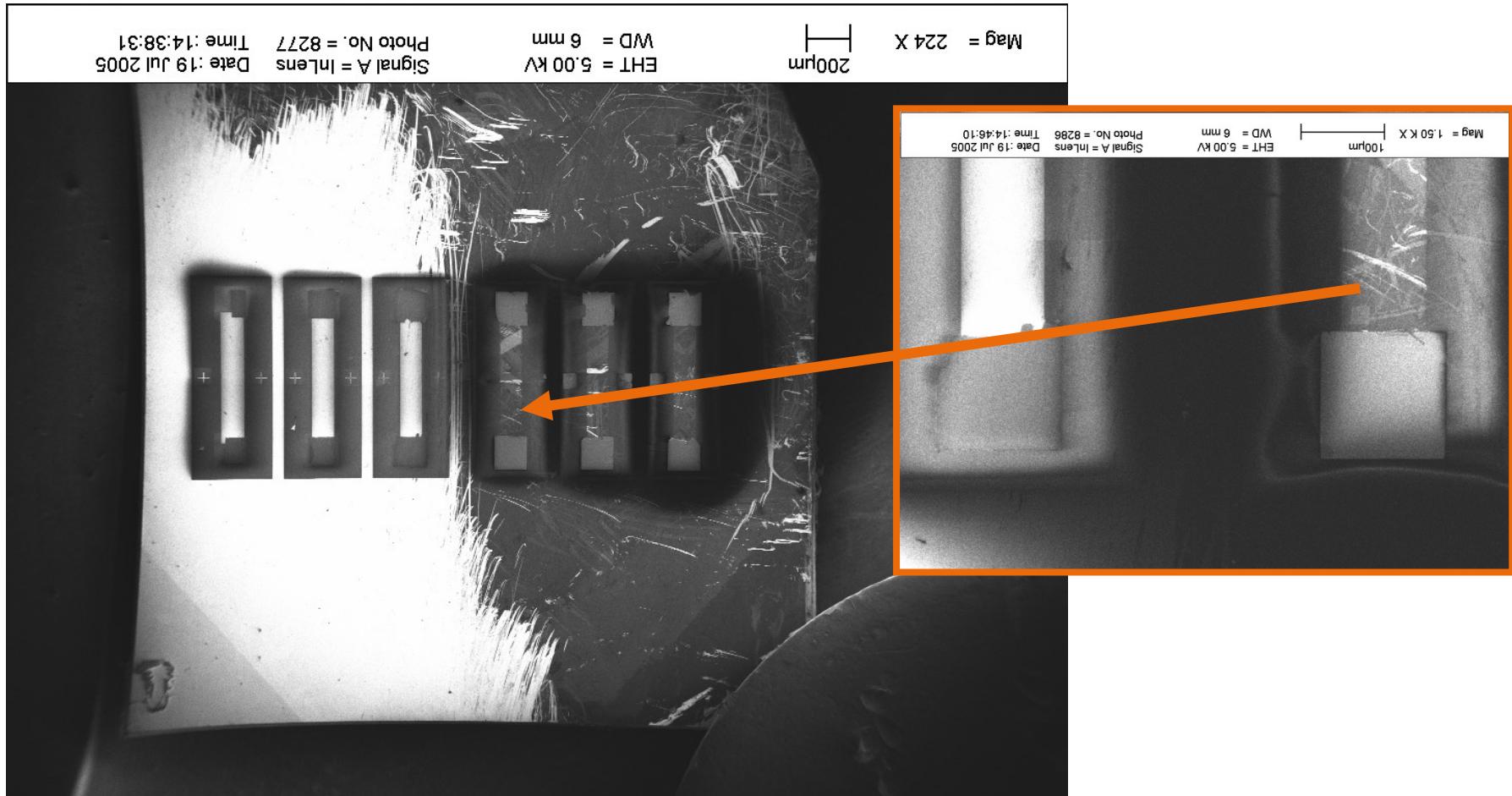
- $\phi_M$  = WORK FUNCTION OF METAL
- $\phi_{Bn}$  = BARRIER HEIGHT OF METAL-SEMICONDUCTOR BARRIER
- $\phi_{B0}$  = ASYMPTOTIC VALUE OF  $\phi_{Bn}$  AT ZERO ELECTRIC FIELD
- $\phi_0$  = ENERGY LEVEL AT SURFACE
- $\Delta\phi$  = IMAGE FORCE BARRIER LOWERING
- $\Delta$  = POTENTIAL ACROSS INTERFACIAL LAYER
- $X$  = ELECTRON AFFINITY OF SEMICONDUCTOR
- $V_{bi}$  = BUILT-IN POTENTIAL
- $\epsilon_s$  = PERMITTIVITY OF SEMICONDUCTOR
- $\epsilon_i$  = PERMITTIVITY OF INTERFACIAL LAYER
- $\delta$  = THICKNESS OF INTERFACIAL LAYER
- $Q_{sc}$  = SPACE-CHARGE DENSITY IN SEMICONDUCTOR
- $Q_{ss}$  = SURFACE-STATE DENSITY ON SEMICONDUCTOR
- $Q_m$  = SURFACE-CHARGE DENSITY ON METAL

# Schottky Properties: Clean and Oxygen Terminated Diamond



from:  
M. Werner, Semicond.  
Sci. Technol. 18 (2003) S41

# Cleanliness: SEM image of Bar-Contact structures



partially wiped  
in ethanol

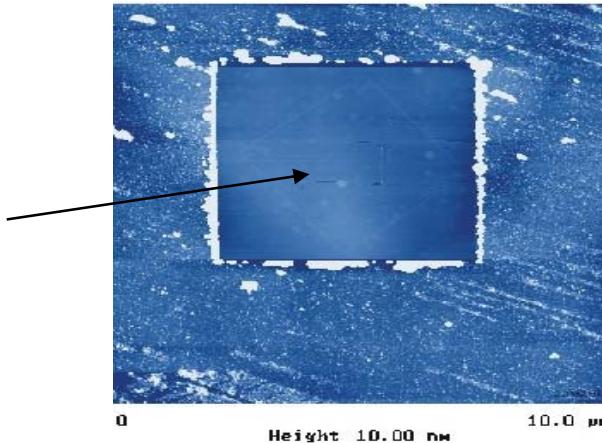
# Cleaning by contact mode AFM

Tapping Mode AFM  
Surface Morphology

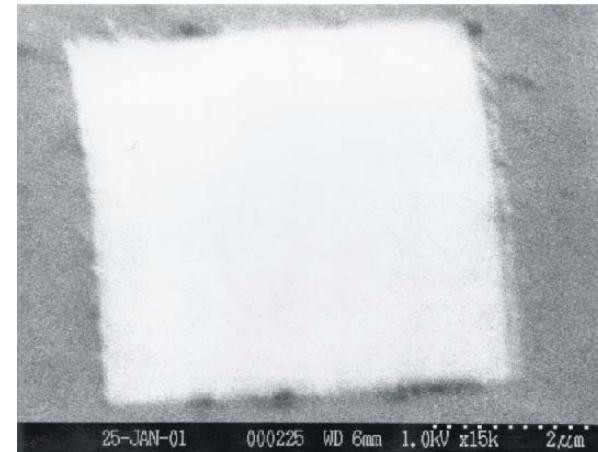
Contact Mode AFM  
Cleanning

Surface is covered with a thin  
(1 -10) nm thick adhesive layer.

AFM Image



SEM Image



B. Rezek, C.E. Nebel, M. Stutzmann  
Diam. and Rel. Mat. 13, 740-745 (2004)

## 8. Summary:

***Alles ist einfacher,  
als man denken kann,***

***zugleich verschränkter,  
als zu begreifen ist.***

Johann Wolfgang von Goethe