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

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Diamond is ULTRA COLD

Assumptions: $T = 300$ K, $\nu_o = 10^{13}$ 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 involved:

- one longitudinal acoustic phonon
- Two transversal acoustic phonons
Temperature dependent absorption

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):

\[ E_{act} = 1.7 \, \text{eV} \]
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 cm$^2$/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

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Why different phonon scattering?
CVD Hole Mobility Limitations:
Scattering due to residual impurities like Fe and Mo

Scattering at ionized impurities:

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

Nava: Time-of-flight on natural undoped diamond
Konorova: Hall effect
Redfield: Hall effect

Koizumi et al.: Hall effect on Phosphorus doped diamond
The saturation velocity limitation:

Energy relaxation
\[ \frac{d\Delta E}{dt} = eFv_s - \frac{E_{phonon}}{\tau_e} \]

Impulse 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 one scattering process (one phonon)
\[ \tau_e = \tau_m \]

Saturation velocity:
\[ v_s = \left( \frac{E_{phonon}}{m^*} \right)^{1/2} \]
\[ v_s = 3.8 \times 10^7 \text{ cm/s} \]
for 165 meV and \( m = 0.2 \text{ m}_o \)

Better:
\[ v_{sat} = \left[ \frac{8E_{opticalphonon}}{3\pi m^*} \right]^{1/2} \]
Drift Velocity in Diamond: Holes

Saturation hole velocity: $1.1 \times 10^7$ cm/s

Reggiani et al, PRB 23 (1981) p. 3050
Drift Velocity in Diamond: Electrons

Saturated drift velocity: $1.5 \times 10^7$ cm/s

Anisotropy: multivalley band structure

Drift velocity

Drift velocity: \( v_D = F\mu = F\frac{e}{m}\tau \)

Scattering time: \( \tau = \tau_0 \left( \frac{\varepsilon}{kT} \right)^r \)

- \( r = -0.5 \) acoustic deformation potential scattering
- \( r = +3/2 \) ionized imurity 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
Deep trapping of carriers

Hecht equation:

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

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:

\[ E(r) = \frac{1}{4\pi\varepsilon_0 \varepsilon_r} \frac{1}{r^2} \]

\( \varepsilon_r \) in diamond much smaller!

\( \varepsilon_r(\text{Diamond}) = 5.7 \)

\( \varepsilon_r(\text{Si}) = 11.9 \)
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 $\sigma$) 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

![Graph showing current (A) vs. time (s) under different electric fields (V/cm)].

- **A**: F = 1.2x10³ V/cm
- **B**: F = 0 V/cm
Model:

pos. applied el. field

Laser Excitation

E

E_c

E_v

Metal

Diamond

Metal

X

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

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

(a) neg. applied el. field

(b) short circuit illumination

(c) pos. applied el. field

(d) short circuit illumination